DYNAMICS OF MULTISTAGE SYSTEMS

BY

R. M. NEALE

A Thesis

Submitted for the degree of

Doctor of Philosophy

Loughborough University of Technology

Supervisor: H. W. KROPHOLLER

DEPARTMENT OF CHEMICAL ENGINEERING FEBRUARY 1971

To Beryl.

CONTENTS

CHAPTER 12 CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK.

ABSTRACT.

The project evolved from a discussion between academic staff at Loughborough University of Technology and staff from The British Petroleum Co. Ltd. A study was required of the dynamic characteristics of a particular 44-plate crude oil distillation unit at BP Refinery (Llandarcy) Ltd. A programme of experiments was conducted on the industrial unit. Step perturbations in the overhead reflux and sidestream offtakes were found to give oscillatory response curves decaying over a two hour period. A qualitative explanation for these results is given.

A theoretical model of the hydraulic and heat transfer contribution to the system dynamics is described. The applicability to the unsteady state of the published steady state correlations for the hydraulic parameters is verified using a laboratory sieve tray unit. The method and details of the computer solution are given. The results indicate that flow and heat transfer disturbances decay over 4-5 minutes in a 15-plate column. The model requires considerable computer core store and a computation time of sixty times real time on an ICL 1905 computer. Hence it is not considered suitable as a basis for controller design. The shape of the response curves obtained using the mathematical model matches the general experimental response curve indicating that the correct type of mechanism has been simulated.

Comments are made on the application of results to crude oil distillation and a simple control strategy is suggested. A test run on the industrial column using this strategy achieves the desired objective of minimisation of disturbance following a major flow change.

A comparison is given of the two main methods for modelling multicomponent distillation systems (applicable to similar multistage systems). The more widely used of these, that due to Mah et al, is shown to be inherently unsuitable and quite invalid for multicomponent systems. The other, due to Wood, is used to construct a state variable model describing the response to a feed composition disturbance of a ten plate column distilling a three component mixture.

Various methods of elucidating transfer functions from state variable models are described. The results of each are demonstrated by application to the distillation model described in the previous paragraph. The application is demonstrated of the method of continued fraction expansion (due to Chen and Shieh) to obtain equivalent simple forms from high order polynomial ratio transfer functions obtained from the state variable distillation model.

Finally the results of the analytical solution of the ten plate three component distillation model are compared with a numerical solution and the predictions of various simplified models. Very good agreement is obtained for some variables.

CHAPTER 1 INTRODUCTION.

Over the past ten years the understanding of the mechanisms of separation techniques and reaction kinetics have led to the confident design of increasingly large plants. It has been reported (65) that over this same period the over design of distillation equipment has been greatly reduced. Thus there is an increased need for the careful selection of the optimum operating point for these units.

However, although modern units are increasing in capacity they are not decreasing in complexity. Control of such systems is consequently achieving even more importance. The absolute value of fractional increases in efficiency, always important in the petroleum and heavy chemical industries, now more than ever merits detailed studies of processes at both steady and unsteady state.

Mathematical modelling, computer control and control engineering science all have a part to play in such studies, but the central discipline must be chemical engineering. Without a fundamental understanding of the mechanisms involved in the process that is to be controlled, elegant mathematics justifying elaborate computer systems are often a sophisticated way of wasting money and effort. Conversely, the use of mathematical analysis can be invaluable - for example, to simplify a complex control system whereby say 80% of the potential improvement is obtained for a fraction of the original cost.

This research project was formulated whilst the author was employed by BP Research Centre. Much of this thesis is concerned with crude oil distillation - a process which is typical of the comments in the first paragraph of this introduction. BP have carried out extensive studies of steady state operating conditions for crude units. This present work investigates some aspects of their operation at unsteady state.

In addition, the fundamental methods of the mathematical modelling of multicomponent multistage systems are considered. The way in which mathematics, control and chemical engineering can profitably be used together to produce simple but adequate models of such systems is demonstrated.

CHAPTER 2 OBJECTIVES.

2.1 Origin of the project.

This project was originally evolved as the study of the dynamic behaviour of a particular distillation unit. The following problem was produced from discussions between the staff in the Department of Chemical Engineering at Loughborough University of Technology and members of the staff of The British Petroleum Co. Ltd. at BP Research Centre, Sunbury-on-Thames and BP Refinery (Llandarcy), South Wales.

Crude oil distillation units were being operated in widely different ways depending on the source of the crude oil they were refining and also on current product requirements. At BP Llandarcy it was necessary to change the method of operation of Crude Distillation Unit No. 3 (CDU 3) perhaps fifty times per year. The main variables were column throughput, heat input and the relative amounts of each of the six products to be withdrawn. The method of changeover employed at the time of the above discussion was not standardised and depended on each operator's preference and experience.

A typical change was achieved by a series of small adjustments. After each one the column was allowed to settle and the product properties were checked against the required specification. This resulted in further small changes and checks until a suitable operating condition was achieved. This whole process took 8-12 hours on average.

The problem posed by BP was to study the column dynamics and reduce this changeover time. The immediate financial benefit from this was difficult to ascertain due to the complexity of downstream blending operations commonly found on a modern refinery. However, it was felt by British Petroleum that this area of operating knowledge required clarification.

2.2 Practical and theoretical studies connected with the BP crude distillation unit.

The two objectives described below, 2.2.1 and 2.2.2, were formulated at an early stage in the project.

2.2.1 Assessment of the effect of the hydraulic and heat transfer transients on the column response.

This objective was to be achieved by the construction of a detailed mathematical model. This was to be capable of describing the dynamics of a crude unit on the basis of the assumption that mass transfer played no part and each tray behaved only as a heat transfer stage. The hydraulic effects contributed the bulk of the column response under these conditions. This is developed in detail in Chapter 4.

2.2.2 Determination of the open loop response of the column.

Experiments were to be performed to determine the transient response of the column variables to flow changes. It was also required to know which variables responded greatly to small changes in operating conditions and to know how long was required for an upset to pass through the system. Loughborough University in particular wanted information on the feasibility of carrying out experiments on an industrial sized unit with only one or two men and no special equipment beyond the normal plant instrumentation. Also, an indication of operator liaison problems, and the reproducibility and accuracy of results was required. It was hoped to use the results to evolve a simple control strategy by which to achieve a major change in operating conditions with minimum disturbances. This work is described in Chapter 5.

2.2.3 Experimental work at Loughborough to assess the validity of static design correlations in a dynamic situation.

A paper by Bernard and Sargent (5) cast serious doubts on the validity of the existing design correlations for distillation hydraulics. These referred to sieve plates and related liquid and vapour rates and properties to froth height and density, pressure drop and plate hold-up. This work caused the present author to re-examine the assumptions made in the construction of the mathematical model described in section 2.2.1. It was thus decided some twelve months after the start of the project to carry out a short programme of experiments on a laboratory sieve tray unit. It was not feasible to employ a hydrocarbon mixture in these experiments so air and water had to be used. The object of these experiments was to determine the degree of error associated with the use in a dynamic model of some of the published static design correlations. The apparatus, method and results are described in Chapter 6.

2.2.4 Application of the results of this work to crude oil distillation.

An assessment was to be made of the use of this work in the operation of a crude oil distillation unit. This is given in Chapter 7.

2.3 Multicomponent mass transfer models.

The plan for this part of the work was formulated at the start of the last year of the project. Prior to this it had become apparent that models of the complexity of the one referred to in 2.2.1 were unsuitable for incorporation in any sort of control system. This particular model had the drawback of excessive computation time on an ICL 1905 computer and a large computer core store requirement. It will also be recalled that this model did not attempt to describe the mass transfer dynamics of the distillation process.

Hence a program of work was planned to investigate the application of some recently derived model simplification techniques to models of multicomponent multi-stage systems such as distillation. In general, the distillation of a three component mixture in a ten plate column was used as a vehicle to test ideas and demonstrate results. This distillation system is described in Chapter 8.

2.3.1 Selection of the unsimplified model to describe the distillation process.

Recent papers by Wood (25) and by Mah, Michaelson and Sargent (23) proposed fundamentally different ways of describing multicomponent distillation dynamics. These methods were to be investigated and the characteristics of each formulation compared. This comparison is given in Chapter 8.

2.3.2 Conversion of a model from state variable form to conventional transfer function representation.

The description of the distillation process normally employs the concentrations of one or more components at each stage as the state variables. The formulation of Wood (25), mentioned in 2.3.1, in particular leads to a large number of equations. In the design of the control system the response is required of a particular variable to a particular input (e.g. top product variation following a feed disturbance). This section of the work is aimed at the recommendation of a method for generating the necessary transfer function, and is described in Chapter 9.

2.3.3 Simplification of a complicated transfer function.

When the objective described in section 2.3.2 was decided it was recognised that this would generate a further problem. An nth order system will in general lead to a transfer function with an nth order denominator polynomial in the complex variables for any response to any input. The numerator of the transfer function may contain a polynomial of order up to n-1. The final stage of the work was to be the investigation of the reduction of this to a simpler equivalent form paying particular attention to a recent paper by Chen and Shieh (47). This is described in Chapter 10.

2.3.4 Analytical and numerical solutions to complete problems.

Features of the analytical and the various numerical solutions to a complete problem were to be described. This is done in Chapter 11.

Note.

The conclusions from the work given in the body of this thesis are given in Chapter 12. This has been structured so that each section corresponds with a section in this chapter.

CHAPTER 3 LITERATURE SURVEY.

3.1 Hydraulic performance of distillation trays.

The literature concerned with plate hydraulics has mainly dealt with the steady state behaviour of different designs. The object of much of the work reviewed in this section has been to develop the understanding of the way in which hydraulic factors influence plate efficiency and plate spacing and leads in general to improved design correlations and techniques. Little work has been done on the extension of steady state correlations to describe unsteady state systems.

Bolles (1) makes recommendations concerning bubble-cap tray design. These include the use of the Francis weir formula(2) for the flow of froth over the outlet weir:-

$$(\text{liquid rate}) = \text{constant} \times (\text{head over weir})^{3/2} \qquad \ldots(3\text{-}1)$$

and the expression to calculate the head of liquid in the downcomer:-

head in downcomer	=	head of foam on plate	+	force to drive liquid under downcomer weir	+	force to drive vapour through tray above	+	force to cause vapour to overcome head on tray above	+	liquid gradient

...(3-2)

An A.I.Ch.E. report(3) gives an indication of the form of relationship between mass transfer coefficients, gas and liquid rates, hold-up and weir height. In this report liquid hold-up appears to have been calculated from the clear liquid height - i.e. the manometric pressure at the tray floor - with no correction for capillarity or vapour momentum. These workers noted that the liquid properties of density, viscosity and surface tension had no significant effect on the hydraulic parameters. No correlations

GLOSSARY OF NOMENCLATURE USED IN CHAPTER 3.

A, B	square matrices.
d	the differential operator.
E	overall liquid Murphree plate efficiency.
F_s	F - factor for vapour based on superficial vapour velocity. $F_s = u_s \sqrt{\rho_v}$ (ft/sec $\sqrt{(\text{lb/ft}^3)}$).
g_c	acceleration due to gravity. (ft/sec^2.)
g	function of the liquid composition.
H	liquid hold-up on plate. (moles).
I	the unit matrix.
k	the equilibrium constant.
L	liquid rate. (moles/second).
L_A	liquid rate. (US.gpm/foot of weir length).
L_R	liquid rate. (Imp.gpm/foot of average plate width).
M	momentum head (feet).
r	total number of components.
R	reflux ratio.
s	the Laplace variable.
t	time (seconds).
u_H	vapour hole velocity. (ft/sec).
u_s	superficial vapour velocity. (ft/sec).
V	vapour rate. (moles/second).
W	weir height. (inches).
x	mole fraction in liquid.
y	mole fraction in vapour.
Z_c	clear liquid height (inches).
Z_F	froth height (inches).

Z_D dynamic head (the clear liquid height uncorrected for manometric capillarity or vapour momentum). (inches).

Subscripts

E enriching section.

n plate n (unless used to subscript a determinant, in which case it has the meaning assigned to it in section 3.5.)

i component i.

Superscript

* refers to the vapour which would be in equilibrium with the tray liquid at its bubble point.

Greek

ρ_V vapour density. (lb/ft^3)

ρ_L liquid density. (lb/ft^3)

μ (i) liquid viscosity (in distillation equations).

(ii) a variable parameter (in numerical integration).

α slope of equilibrium line in binary system, relative volatility in multicomponent system.

σ liquid surface tension (N/m).

ε absorption factor.

Δ deviation from steady state flow, or increment of time.

δ deviation from steady state composition.

∂ partial differential operator.

Note: (i) A bar below a variable thus: $\underline{u}$ denotes that u is a column vector.

(ii) A bar above a variable thus: $\overline{L}$ denotes that it is the steady state value that is referred to.

concerning liquid hold-up were presented, it being recognised that this was a function of weir height, liquid rate and (via the hydraulic gradient) the length of the liquid flow path. The single unifying factor was found to be the relative froth density $Z_F/(Z_F-Z_c)$ which appeared to be a function only of the F-factor for the vapour.

Gerster(4) in another A.I.Ch.E. report recommends a correlation for the uncorrected clear liquid height of bubble cap trays:-

$$Z_D = 0.19W - 0.65F_s + 0.02L_A + 1.65 \qquad \text{....(3-3)}$$

This same report gives a froth height correlation for bubble cap trays:-

$$Z_F = 0.73W + 3.24F_s - 0.084L_A \qquad \text{....(3-4)}$$

Bernard and Sargent(5) studied the hydrodynamic performance of a four inch diameter sieve plate distillation column. They report the three clearly discernible zones on a normally operating sieve plate - a region that is substantially liquid near the plate floor through which vapour bubbles rise, a foaming region, and finally a spray regime. It is noteworthy that although a four inch column might seem small for this type of work, by the careful use of foam baffles to support the foam the workers sought to simulate conditions at the centre of an industrial sized plate. Gamma radiation was used to measure foam density and it was found that this remained substantially constant over a major part of the liquid depth. However, this constant density region did not correspond exactly to the foaming region mentioned above. The authors found a linear relationship between the froth height and the F-factor for the vapour (based on a superficial vapour velocity)

$$Z_F = 3.7F_s \qquad \text{....(3-5)}$$

and note that this predicts values of Z_F for their sieve plate system within a few tenths of an inch of those given by equation (3-4) for bubble cap plates. Liquid hold-up was found to have significant dependence on four factors, increasing with increases in superficial vapour rate, weir height and hole diameter, but decreasing with increasing free area. The authors could not find a satisfactory way of expressing the variation in a single equation.

Bernard and Sargent(6) present a more recent paper describing work on a 16" diameter column. In this three formulas for correlating froth height were investigated:-

(i) the simple formula applicable to their 4" column - equation (3-5).

(ii) that given by the Delaware University Report for bubble cap plates - equation (3-4).

(iii) the recommendation of the Bubble Tray Design Manual(7) for bubble cap plates:-

$$Z_F = 2.53 F_s^2 + 1.89W - 1.6 \qquad \text{....(3-6)}$$

It was found that only (iii) gave results of the right order of magnitude for the 16" column without foam baffles and that no correlation was adequate with the foam baffles fitted. The workers also considered the following liquid hold-up correlations:-

(i) $Z_c = W + 0.092 L_A^{2/3}$ (Bolles (1))

(ii) $Z_D = 0.19W - 0.65F_S + 0.02L_A + 1.65$ (Gerster (4))

(iii) $Z_c = Z_D + M$

$$\text{where } M = \rho_v u_s (u_H - u_s)/(\rho_L g_c) \qquad \text{...(3-7)}$$

None of these was found to be reliable.

Rodionov(8) investigated the dependence of the volume fraction of gas in the foaming region on various parameters. This was found to be a weak function of liquid viscosity:-

$$(1 - Z_c/Z_F) \propto \mu^{-0.045} \qquad \text{....(3-8)}$$

and surface tension:-

$$(1 - Z_c/Z_F) \quad \propto \quad \sigma^{-0.16} \qquad \text{....(3.9)}$$

Thomas and Campbell(9) describe hydraulic studies in a sieve plate downcomer system. A froth height correlation of the following form is proposed:-

$$Z_F = 2.45F_s + 0.053L_R + 1.24W \qquad \text{....(3-10)}$$

They find the dynamic head (the uncorrected clear liquid height) to be given by:-

$$Z_D = 0.19W - 0.040F_s + 0.013L_R + 1.56 \qquad \text{....(3.11)}$$

which they found gave similar results to those of the Delaware University Report(4) when momentum head was taken into account:-

$$Z_c = Z_D + M$$

Gardner and Maclean (10) found that the conclusion of the A.I.Ch.E. Report(4), that froth characteristics were essentially independent of physical properties, was not valid for the systems they studied. These were the adiabatic evaporation of water to air, the non-adiabatic evaporation of carbon tetrachloride to air and the absorption of carbon tetrachloride from air by decalin.

Thus there seems to be considerable scope for more work in this basic field. The rather empirical approach of making measurements on an experimental unit and producing a correlation to fit the results does not seem capable of yielding reliable general predictions. Perhaps the approach of Ho, Muller and Prince(66), although more complex, will result in better design data. These workers consider the basic physical properties for the fluids to arrive at polyhedron models for cellular foam. At this level much work in the field of transport phenomena becomes relevant.

3.2 Mathematical models of distillation systems.

Wilkinson and Armstrong(11), (18) describe a model for a binary system based on many simplifying assumptions. For plate n in the enriching section:-

$$(L_E\, x_{n+1} + V_E\, y_{n-1}) - (L_E\, x_n + V_E y_n) - H_n dx_n/_{dt} = 0 \qquad \text{....(3-12)}$$

From which

$$(H_n/L_E)\ (dx_n/dt) = x_{n+1} - x_n\ (1 + \mathcal{E}) - \mathcal{E}\, x_{n-1} \qquad \text{....(3-13)}$$

where

$$\mathcal{E} = V_E \alpha_E/L_E = (1 + R)\alpha_E/R$$

The assumptions are (i) equimolal overflow (ii) constant tray liquid holdup (iii) a linear equilibrium line (iv) plate efficiency independent of composition (v) adiabatic operation (vi) the time to reach fluid dynamic equilibrium is small compared with that to reach mass transfer equilibrium. The authors go on to reduce their equations to partial differentials and effect a solution.

Rosenbrock(15) extends the above model to include non-linear equilibrium line and a Murphree vapour efficiency. He describes a numerical integration technique after Crank and Nicolson (16) and notes that doubling the time step every four steps is acceptable since the major non-linear part of the response curve occurs at the start - an important point for computational efficiency.

Rijnsdorp(17) considers two special cases of a distillation model. The first is a model resembling those of Wilkinson and Armstrong(11) and Rosenbrock(15) already mentioned, in which it is the slow dynamic effects (due to the mass transfer) which are considered. The second case considers the fast effects produced by pressure and liquid flow changes. Rijnsdorp found that it was possible to produce a model which gave results close to experimental results. This incorporated a relation:

$$L_n = K_1 H_n + K_2 V_{n+1} \qquad \text{....(3-14)}$$

K_1 determines the time delay for the propagation of a liquid flow disturbance through the column. K_2 measures the influence of vapour flow variations on the liquid overflow. The paper also goes on to show analytically how large values of K_2 can give rise to non-minimum phase responses.

A paper by Armstrong and Wood(19) describes the response of a 21-plate column to changes in the reflux and vapour flow-rates. It was noticed that with the initial mathematical model, which did not include a hold-up variation with reflux-rate, the composition response of trays below the top tray was slower than that obtained experimentally. Modification of the theory to include the assumption that over the small range the plate hold-up is a linear function of the reflux-rate produced a correction of the right order of magnitude. (cf. Rijnsdorp's K_1 factor(17)). The authors extended the theory with quite good success to changes in reflux and vapour rates with varying feed plate composition. It was noted that the response of the 21-plate column was so slow that the time to reach fluid equilibrium had little effect on the slope of the transient.

In a second paper Armstrong and Wood(20) demonstrate the application of frequency response analysis to the same problem. They show that there is very little interaction between the lag due to the delay in the reflux rate and that for mass transfer assuming no delay in reflux rate. Townend makes a pertinent suggestion in the reported discussion on the above paper. The basic mass balance equation assuming constant liquid hold-up is:-

$$(L_E + \Delta L_E)\,\delta x_n + V(\delta y_{n+2} - \delta y_{n+1}) - (L_E + \Delta L_E)\,\delta x_{n+1}$$

$$= H\,\frac{\partial\,\delta x_{n+1}}{\partial t} - \Delta L_E\,(x_n - x_{n+1}) \qquad \ldots.(3\text{-}15)$$

On elimination of all reflux rate delays from the column the effect of a step change in reflux at the top, ΔL_E, would be an equal and immediate change in the reflux flow at all plates in the column. Immediately after this change δx_n, δy_{n+2}, δy_{n+1}, δx_{n+1} will be zero since there will be no time for them to have changed. Hence:

$$\frac{\partial}{\partial t}(\delta x_{n+1}) = \Delta L_E \left(\frac{x_n - x_{n+1}}{H}\right) \qquad \ldots.(3\text{-}16)$$

Townend suggests that to the delay obtained from this equation be added the non-interacting delays obtained from the reflux rate change.

Baber and Gerster(21) calculate the predictions of the perturbation equations of Lamb, Pigford and Rippin(22) in modelling the response of a distillation column to reflux and vapour flow changes. They correct for variation of liquid flow with the relation:-

$$\frac{dLn}{d\Theta} = \left(\frac{1}{\beta_n}\right) \quad (L_{n-1} - L_n) \qquad \ldots.(3\text{-}17)$$

where

$$\beta_n = (\bar{L}_n/\bar{H}_n) \;/\; (d\bar{H}_n \;/\; d\bar{L}_n) \qquad \ldots.(3\text{-}18)$$

but do not appear to include any allowance for the effects due to vapour flow changes.

Mah, Michaelson and Sargent (23) present a mathematical formulation for the dynamic response of a multicomponent multistage system but neglect hydraulic effects. This paper also contains an excellent review of numerical methods for the solution of this type of problem. The model is set out in matrix form and includes a rigorous proof purporting to show that the mass transfer responses of a multicomponent distillation system must always be non-oscillatory. The poles are shown to be real, negative and distinct for continuous systems and form a Sturm sequence, the zeroes interlacing with the poles along the real axis. It is thus implied that right half plane zeroes cannot exist. These results are not correct and are discussed in greater detail in Chapter 8 of this thesis. In a later paper Sargent (24) extends the classical solution to avoid the problem:-

$$\sum_{i=1}^{r} x_i \neq 1.0$$

at each time step, but retains the relationship:-

$$y_{n,i} = k_{n,i} \; x_{n,i}$$

However, the new formulation does not require the assumption of constant coefficients over each time step.

Peiser and Grover(26) describe a mathematical model that is much more comprehensive. Mass and energy balances for each tray are constructed assuming unit plate efficiency and negligible heat losses. The tray hydraulics are modelled using the Francis formula for flow over a weir and a pressure balance to give the downcomer head. They report the successful application of the model to an industrial column to pinpoint flooding and aid in the redesign of certain trays. After modification the column then functioned correctly.

Robbins(28) describes work using a ternary mixture in an industrial column. A perturbation equation is used to describe the mass transfer:-

$$\bar{H}_n \frac{d\vec{x}_n}{dt} = \Delta L_{n-1} (\bar{x}_{n-1} - \bar{x}_n) - \Delta V (\bar{y}_n - \bar{y}_{n+1})$$
$$+ \bar{L}_{n-1} \delta x_{n-1} - \bar{L}_n \delta x_n + \bar{V}_{n+1} \delta y_{n+1} - \bar{V}_n \delta y_n \quad \ldots.(3\text{-}19)$$

Treating n as a continuous variable this is expanded by a Taylor series:-

$$\frac{\partial}{\partial t} (H_n \delta x_n) = \frac{\partial}{\partial n} \left[(\Delta L. \delta x - \Delta V. \delta y) + \tfrac{1}{2} \frac{\partial}{\partial n} (\Delta L. \delta x + \Delta V. \delta y) \right] \quad \ldots.(3.20)$$

Applying the Laplace transform method:-

$$\left[E^2 - E(1 + \mathcal{E} + s) - \mathcal{E}\right] \delta x_n(s) = 0 \quad \ldots.(3\text{-}21)$$

where $\mathcal{E} = Vk/L$

and E = overall liquid Murphree plate efficiency.

Tray hydraulics are expressed after Rijnsdorp(17) mentioned earlier in this section. Robbins solves the model using matrix complex arithmetic to get attenuation and phase shift for the variation of any tray composition relative to any perturbation. Using the ternary mixture MEK/benzol/toluene Robbins measured the response of the experimental column to step changes, sine waves and stochastic signals. Response measurements were at the fifth tray from the top and the sixth tray from the bottom. Reflux flowrate, feed pre-heat, reboiler steam, feed flowrate and feed composition were perturbed. Estimates of the Rijnsdorp K_1 and K_2 effects were made by achieving steady state under various flowrates and then bypassing the flows and allowing the column to drain into the base.

Wood(25) uses the perturbation equation of previous workers(22),(28). The formulation is demonstrated whereby the deviations in the mole fraction of a component on a tray depend on the deviation in all the other component mole fractions. Previous workers had mainly considered binary mixtures for which this point is inherent anyway. Wood used:-

$$\delta y_i = f_i(\delta x_1, \delta x_2, \dots \delta x_r) \qquad \dots.(3\text{-}22)$$

so that $$\delta y_{n,i} = g_{n,i}\, \delta x_{n,i} \qquad \dots.(3\text{-}23)$$

where $$g_{n,i} = \frac{d\,\bar{y}^*_{n,i}}{d\,\bar{x}_{n,i}} = \sum_{m=1}^{r} \left(\frac{\partial\, i}{\partial \bar{x}_{n,m}} \cdot \frac{\delta x_{n,m}}{\delta x_{n,i}} \right) \qquad \dots.(3\text{-}24)$$

If the equilibrium data may be represented by constant relative volatilities:

$$\bar{y}^*_i = \alpha_i \bar{x}_i / \sum_{m=1}^{r} \alpha_m \bar{x}_m \qquad \dots.(3\text{-}25)$$

then $$\frac{\partial f_i}{\partial \bar{x}_i} = \alpha_i \sum_{m \neq i}^{r} \alpha_m \bar{x}_m / \left(\sum_{m=1}^{r} \alpha_m \bar{x}_m\right)^2 \quad ....(3\text{-}26)$$

$$\frac{\partial f_i}{\partial \bar{x}_j} = -\alpha_i \cdot \alpha_j \cdot \bar{x}_i / \left(\sum_{m=1}^{r} \alpha_m \bar{x}_m\right)^2 \quad j \neq i \quad ....(3\text{-}27)$$

Wood uses equations (3-22) to (3-27) to eliminate δy terms from equation (3-19) and solves the resulting equation in the frequency domain in the same way as Robbins(28). It is demonstrated that this form allows plate compositions to give inverse response in multicomponent systems. (See Fig. 3-1).

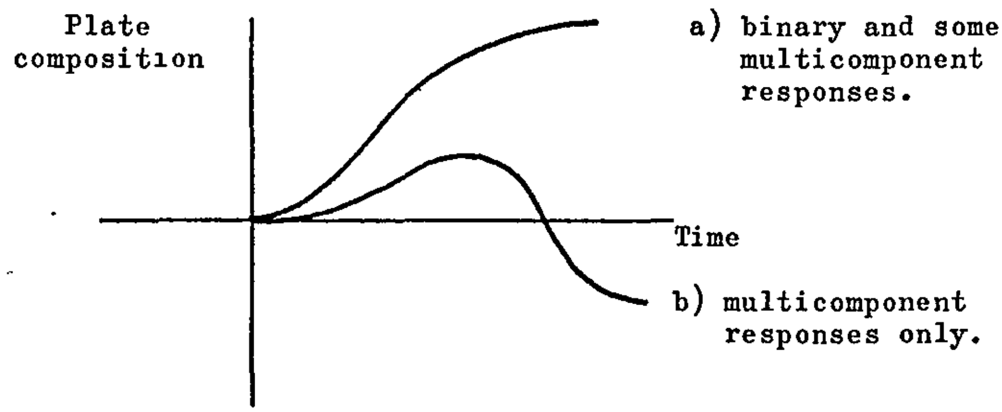


Fig. 3-1

3.3 Studies involving crude oil systems.

The main feature of the distillation of petroleum fractions is that in most cases consideration of individual components is not practicable because of the large number of these present and because of the difficulty of analysing the fraction on a component basis. For this reason dynamic models of distillation systems have not yet been extended to crude oil distillation. The papers reviewed here are concerned with steady state representation. The standard design procedure to avoid this problem is to break the fraction down into pseudo-components or narrow boiling range fractions. See for example Cecchetti et al(29) and Gilbert et al(30). Even with this simplification the number of components is still large - of the order of thirty for a crude oil. To reduce the number of pseudo components for a crude below this number would result in inadequate characterisation of each sidestream since a sidestream will typically contain only a few pseudo components in appreciable quantity.

Edmister(31) suggests a way of arriving at component distributions between offtake points in a distillation tower using absorption and stripping factors. The effective absorption factor concept is demonstrated whereby it is possible to define a single absorption factor for each component such that use of this factor for each plate produces the same separation for a particular component as use of the set of correct factors. An approximate method is given for obtaining the effective absorption factor from the absorption factor for the top and bottom plates of the column section under consideration.

Cechetti et al(29) demonstrate the application of a design method to a crude pipestill. The computer program based on the Thiele-Geddes method of calculation speeded by the Holland theta method of convergence is used. (The basis for this program is given by Holland(32) and a program listing is given by Clark(34)). This program assumes unit plate efficiency. The initial run uses the number of actual plates in the unit. Successive runs with the program then employ fewer plates in each section until a product match for a set of test data is obtained. The program is then used to predict product characterisation for other yield structures. Good agreement between predicted and observed results is demonstrated.

Hoffman(35) tackles the problem of a large number of components in a petroleum fraction from a different standpoint. This paper does not concern distillation as such but indicates a possible basis for petroleum distillation calculations. The petroleum fraction is represented by a continuous function - the true boiling point distribution curve. Use is made of the fact that TBP curves for petroleum fractions often follow a Gaussian distribution. Hoffman develops expressions for flash calculations via the bubble and dew points calculations, the liquid and vapour products again being characterised by their TBP distribution curves.

Gilbert et al(36) present an application of Edmister's(31) effective absorption factor method to yield a simple short-cut method for fractionator rating and preliminary design. They note the success of nominating as 'reference component' the TBP cut point. The results of the example they give are not particularly impressive from a steady state design viewpoint - even preliminary design would require better estimates than those quoted. However, this type of simplification might have potential control applications and for this reason is listed here.

<u>3.4 Obtaining information from distillation systems.</u>

Endtz, Janssen and Vermeulen(14) describe original equipment used to produce a sinusoidal perturbing signal. This was used to obtain the frequency characteristics of a refinery pipestill furnace. They found that the outlet temperature response to fuel-rate perturbations could be correlated with a time constant of 15 minutes, a time constant of 25 seconds and a dead time of 20 seconds. They also considered a pilot distillation column. Perturbations were injected into the steam flow to the reboiler, the water flow to the condenser, and the reflux flow. Response curves for the column conditions (including pressure) were plotted for each type of perturbation. It was noted that the temperature responses to changes in cooling water appeared somewhat unusual for some trays, especially those in the middle of the column. These temperature responses could not be represented by a number of exponential time lags in cascade. It was possible, however, to represent them by two transfer functions of a normal type in parallel. This indicated that the temperature response was brought about in two different ways - pressure and composition. Thus at some frequencies temperature effects may counteract each other whereas at others the effects may be additive.

Voetter(12) perturbs the feed stream to a distillation column to obtain concentration responses. He is keen to obtain simple correlations. The most striking feature of this paper is the care taken to investigate the magnitude of the simplifying assumptions. e.g. constant pressure, no vapour hold-up, unit tray efficiency, complete mixing and linearity. The main conclusions are:- (i) Concentration responses of distillation columns can be approximated by relatively simple formulae containing residence times and number of trays as main parameters (ii) The top concentration response to feed concentration disturbances is not very dependent on the properties of the bottom half of the column and vice versa. Only for low frequencies does a large second half give some correction to the responses. (iii) Within the precision desired flow rates and reflux ratios are only important insofar as they influence residence times.

Westcott(13) gives the groundwork on the practical approach to random disturbances. The idea is postulated of applying spectral analysis to the normal plant noise, defining and explaining auto- and cross-correlation functions. It is noted that more accurate measurements would be required than are found from the average plant recording equipment. Also the time scale is vital and must be precise.

Kuehn and Davidson (37) give the application of Lagrange multipliers to the problem of constraining on-line enthalpy and flow data to balance. These authors consider the inclusion of redundant information to improve estimates but do not include the weighting of instruments according to their reliability, a scheme now used in practice (38).

Clementson (39) tackles the same problem in a similar manner but uses regression analysis. This has the added attraction of giving error-bound estimates within defined confidence limits.

Robbins (28) describes the pseudo-random chain code method. Results for a random telegraph signal perturbation on various flows are given in the form of Bode plots, the composition response being measured on plage 5 from the top of the column and on plate 6 from the bottom. The ability to gain information over a wide range of frequencies with a single test is demonstrated.

Shelton and Hutchinson (40) discuss the use of two pseudo-random chain codes. The theoretical superiority of the pseudo random binary chain code as compared with the random telegraph signal is described. This is demonstrated with industrial experiments on a refinery depropaniser. It is shown that adequate information can be obtained by this method for the construction of a mathematical model based on a transfer function representation.

Rees (41) also describes the successful application of pseudo random binary chain code techniques to a pilot scale distillation column.

Stainthorp and Warren (42) describe another means of overcoming the long experimental effort required to obtain frequency response data over the wide range of frequencies normally of interest. It is proposed that pulse testing techniques could be of value in some circumstances. However, in quoted examples it was reported that averaging over five or six runs was necessary to eliminate the effects of noise.

3.5 Elucidation of transfer functions from state variable models

Consider the state variable equation for the general system :-

$$\frac{d}{dt}\underline{x} = A\underline{x} + B\underline{u} \qquad \text{....(3-28)}$$

The transfer function relating the response of any one variable in the state vector to a particular perturbation is given by :-

$$G_n(s) = \left|Is-A\right|_n \Big/ \left|Is-A\right| \qquad \text{....(3-29)}$$

where $\left|Is-A\right|_n$ refers to the matrix $\left[Is-A\right]$ but with column n replaced by $B\underline{u}$. The theory behind this is given in Chapter 9.

The problem of determining the transfer function is thus reduced to the one of evaluating the numerator and the denominator on the right hand side of equation (3-29).

The denominator presents no problem since it is well known that the roots of

$$\left| Is-A \right| = o \qquad \text{....(3-30)}$$

are the eigenvalues of the matrix A. Hence $\left|Is-A\right|$ may be obtained directly in factored form. Alternatively the method of Danislevsky as given for example in Pipes and Hovanessian (43) may be applied to reduce matrix A to Bush's form:-

$$A \equiv \begin{bmatrix} o & 1 & o & o & \cdots & o \\ o & o & 1 & o & \cdots & o \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & \cdot \\ \cdot & \cdot & & & & o \\ \cdot & \cdot & & & & 1 \\ -a_o & -a_1 & -a_2 & \cdots & & -a_{n-1} \end{bmatrix} \qquad \text{....(3-31)}$$

from which $\left|Is-A\right| = S^n + a_{n-1}s^{n-1} + a_{n-2}s^{n-2} + \ldots\ldots a_1 s + a_o$ ....(3-32)

as demonstrated for example by Chen and Haas P.298 (44).

The numerator presents more problems. Hennion (45) presents an algorithm for expanding a determinant, each element of which is a polynomial in s, to its factored form. The matrix is triangularised so that elements below the main diagonal are nulled and the required polynomial is the product of the diagonal elements.

Davison (46), (47), (48) presents a method for the evaluation of the numerator based upon the construction of the approximately equivalent eigenvalue problem. The eigenvalues obtained contain the roots of the numerator (the zeroes of the transfer function) together with some extraneous roots. This method is described and discussed in detail in Chapter 9.

Bosley et al (49) describe a method for determining the numerator polynomial coefficients by a simple recursion formula based on the Cayley-Hamilton theory. This is also described and discussed in detail in Chapter 9.

3.6 Simplification of transfer function models using continued fractions.

The algebraic manipulation of a ratio of two polynomials to give a continued fraction is given in classical mathematics (e.g. Hall and Knight (50) p.273). It is recognised that good approximations to C(s)/R(s) where

$$\frac{C(s)}{R(s)} = \cfrac{1}{H_1 + \cfrac{1}{\frac{H_2}{s} + \cfrac{1}{H_3 + \cfrac{1}{\frac{H_4}{s} + \cdots\cdots}}}} \qquad \ldots.(3\text{-}33)$$

are given by simple truncation of the fraction to say :-

$$\frac{C(s)}{R(s)} \doteqdot \cfrac{1}{H_1 + \cfrac{1}{\frac{H_2}{s}}} \qquad \ldots.(3\text{-}34)$$

Chen and Shieh (51), (52) use this method to obtain simplified transfer functions from complicated high-order polynomial ratios.

It is demonstrated (51) that an excellent fit can be obtained to transfer functions with seventh order polynomial denominators using second order models. The method is described fully and discussed in Chapter 10.

Maehly (53) gives a method for obtaining the best fit approximation to running fractions using Chebyshev polynomials, rather than simple truncation.

3.7 <u>Analytical and numerical methods for solving complete problems.</u>

Consider the equation :-

$$\frac{d}{dt}\underline{x} = A\underline{x} + B\underline{u} \qquad \text{....(3-28)}$$

The analytical solution to this has been given by Ogata (54) with additions by Lees (55) and Kropholler (56). It is developed in terms of the eigenvalues and eigenvectors of the A matrix and is described in detail in Chapter 11. It is of use to note that equation (3-28) may be converted to the equivalent initial value problem by writing :-

$$\underline{y} = \underline{x} + A^{-1}B\underline{u} \qquad \text{....(3-35)}$$

whence $\frac{d}{dt}\underline{y} = A\underline{y}$ ....(3-36)

the solution to which is :

$$y(t) = e^{At}\,y(o) \qquad \text{....(3-37)}$$

Of the numerical methods available for solving equation (3-28) the simplest is probably that of Euler :

$$d/dt \; \underline{x} = f(\underline{x})$$

$$\underline{x}_{n+1} = (t_{n+1} - t_n) \; f(\underline{x}_n) \qquad \text{....(3-38)}$$

Since equation (3-37) may be expanded by series summation to give :-

$$y(t) = (I + At + \frac{A^2t^2}{2!} + \frac{A^3t^3}{3!} + \ldots) \; y(o) \qquad \text{....(3-39)}$$

it is evident that Euler's method is equivalent to the truncation of the series solution after the second term. This leads to large truncation errors with the method unless small time steps are employed.

Runge, Heun and Kutta make use of a weighted sum of results of several applications of Euler's method to give a better fit to the series in equation (3-39). This gives rise to the widely used Runge-Kutta method and auxiliary methods.

Predictor corrector methods are generally more efficient then either Euler or Runge-Kutta methods. They consist of finite difference formulae giving a rough approximation for the interval (the predictor) followed by an improvement according to some consistency criterion (the corrector). This generally permits the use of larger time steps without the equivalent loss of accuracy.

Of more recent interest are the implicit methods, so called because the end-point appears on both sides of the finite difference approximation. A typical implicit form is :

$$\underline{x}_{t+\Delta t} = \left[(1-\mu) f(\underline{x}_t) + \mu f(\underline{x}_{t+\Delta t}) \right] \Delta t \qquad \text{....(3-40)}$$

For $\mu = \frac{1}{2}$ this reduces to the method of Crank and Nicolson (16). Holland (33) demonstrates the use of the method for solving unsteady state distillation problems, and notes that a minimum value of $\mu = 0.6$ is essential for stability with larger time steps. A graphical interpretation of the meaning of a particular choice of μ is given in section 4.4.1 of this thesis.

Gibilaro, Kropholler and Spikins (57), (58) present a numerical integration procedure based on a probabilistic mechanism. This méthod was originally written to solve flow mixing problems for systems of interconnected vessels but can equally be applied to any equation of the form of equation (3-36). The solution to equation (3-36) is given by equation (3-37) and is approximated by :

$$y\ (t) \quad = \quad P^n y(o)$$

where the matrix P is termed the transition matrix. The computational efficiency of the method lies in the fact that it allows the benefits of a small integration step length to be obtained, the matrix P being powered the requisite number of times to match the time intervals at which the response is required.

CHAPTER 4 A MATHEMATICAL MODEL OF A CRUDE OIL DISTILLATION UNIT.

4.1 Introduction.

This chapter describes the construction and solution of a mathematical model of a crude distillation unit. This model describes the unsteady state hydraulics and heat transfer but takes no account of the mass transfer processes.

4.2 Selection of the model.

The prime variables in a distillation column are the flow rates of liquid and vapour, the temperature and the composition. To completely specify the state of a unit at any point in time it is necessary to know the values of these variables at many points in the column.

A model is required which takes account of the liquid and vapour rates and the tray temperatures. For a crude oil fractionator a convenient simplification is possible. The enthalpy of an internal liquid or vapour stream is a simple function of the tray temperature alone. This is because crude oil fractions of similar bubble point have similar specific gravities. Hence since the tray temperature is assumed to be near the bubble point of the liquid on the tray specific gravity does not enter the correlation. Hence for a crude oil system it is possible to estimate stream enthalpies without knowing stream composition.

As mentioned in the literature survey, chapter 3, there proved to be a paucity of information on the hydraulic relations in a distillation column. Such correlations as did exist had several shortcomings :-

a) they had been formulated as an aid to the design or rating of equipment.

Glossary of nomenclature used in Chapter 4

Algebraic variable	Computer variable	Units	Meaning
A	A	-	Matrix in the final formulation of the model.
A_D	AD	ft^2	Cross-sectional area of downcomer.
A_T	AT	ft^2	Area of tray covered by bubbling liquid.
A_{UD}	AUD	ft^2	Area for liquid flow under downcomer (measured in vertical plane).
B	B	-	Matrix in the final formulation of the model.
C_L	CL	-	Discharge coefficient for flow of liquid under downcomer weir.
C_V	CV	-	Discharge coefficient for flow of vapour through holes in plate.
C	F	-	Matrix in the final formulation of the model.
d	-	-	Differential operator.
e_1, e_2 etc.	E1,E2 etc	-	Constants used in the empirical correlations.
E	D	-	Matrix used in the solution of the model by the implicit method.
f	-	-	e.g. $f(x)$ denotes the function of x.
F	E	-	Matrix used in the solution of the model by the implicit method.
g	G	$ft.sec^{-2}$	Acceleration due to gravity.
h	HL	$BTU.lb^{-1}.deg.F^{-1}$	Tray liquid enthalpy.
h_D	HLD	"	Downcomer liquid enthalpy.
H	HV	"	Vapour enthalpy.
l	AVL	ft	Average width of plate for liquid flow.
L	L	$lb.sec^{-1}$	Liquid flow rate from plate.
L_D	LD	"	Liquid flow rate from downcomer.

Algebraic variable	Computer variable	Units	Meaning
m	HTC	$BTU.sec.lb^{-1}deg.F^{-1}1^{1}$	Heat transfer coefficient for the plate.
p	C(3)	$BTU.lb^{-1}deg.F^{-1}$	Coefficients in the linear relationships by which liquid and vapour enthalpies are calculated from tray temperature.
q	C(4)	$BTU.lb^{-1}$	
r	C(11)	$BTU.lb^{-1}deg.F^{-1}$	
s	C(12)	$BTU.lb^{-1}$	
S_L	SL	$lb.sec^{-1}$	Rate of liquid withdrawal from plate.
S_R	SR	"	Rate of liquid return to plate.
S_V	SV	"	Rate of vapour return to plate.
t	CUMTIM	sec	Elapsed time.
V	V	$lb.sec^{-1}$	Vapour rate from plate.
W_D	WD	lb.	Hold-up of liquid in downcomer.
W_L	WL	lb.	Hold-up of liquid on plate.
X	DELTA1	$lb.sec^{-1}$ and deg.F	State vector used in the matrix formulation of the model.

Greek	Computer	Units	Meaning
ε	EPS	-	Liquid fraction in froth on plate.
ρ_L	RHOL	$lb.ft^{-3}$	Density of liquid on plate
ρ_{LD}	RHOLD	"	Density of liquid in downcomer.
ψ_W	PSIW	ft	Weir height.
ψ	PSI	ft	Head of froth over the weir.
ψ_D	PSID	ft	Head of liquid in the downcomer.
θ	T	deg.F	Liquid temperature on plate.
θ_D	TD	"	Liquid temperature in downcomer.
Δ	-	-	e.g. ΔL is the change in variable L in small time Δt measured from a reference state.
μ	XMU	-	Parameter used in the implicit method of numerical solution

Subscripts

	Refers to :-
D	Downcomer.
L	Liquid from the plate.
LD	Liquid from the downcomer.
n	Plate number.
SL	Liquid withdrawn from the plate.
SR	Liquid returned to plate.
SV	Vapour returned to plate.
T	Tray.
UD	Gap under the downcomer weir.
W	Weir.

Superscripts

	Refers to :-
$\overline{}$	Reference state.
p	Previous plate value.

b) they were not strictly applicable in the dynamic situation.

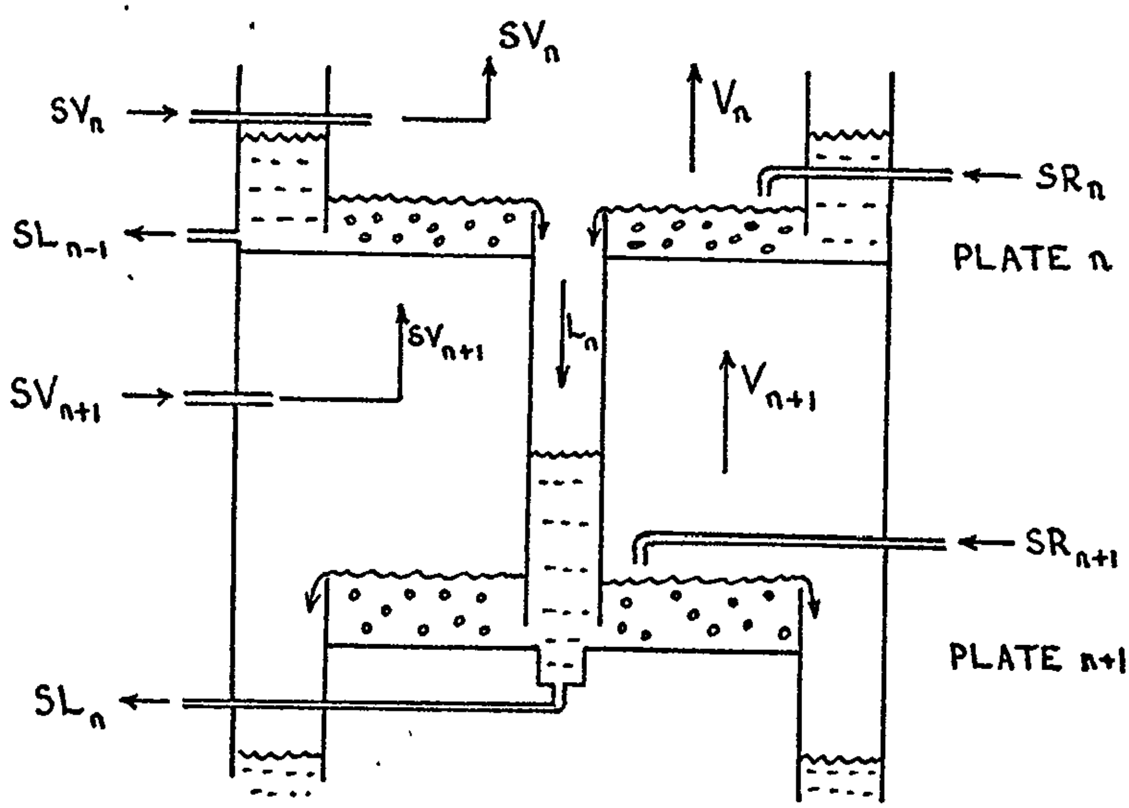
c) according to the work of Bernard and Sargent (6), the assumption that they were generally valid was incorrect.

In the absence of better correlations it was decided to proceed although such equations as it was essential to use would be viewed with circumspection. (These proved to be the Francis weir formula (2) and the correlations of froth height versus liquid and vapour rates given by Gerster (4) and Thomas and Campbell (9)). Facilities were not available for detailed checking although the limited experimental facility at Loughborough was used to its fullest extent. These experimental results gave an insight into the validity of some of the correlations and are described in chapter 6.

4.2.1 The system modelled.

The system modelled is a series of general distillation column bubble or sieve plates. The general plate (also valid as the feed plate) is shown in Fig. 4-1. The top plate differs from the general plate in that there is no downcomer before it, no liquid may be withdrawn from it and no vapour may be returned above it.

Note : The symbols used in the Fig. 4-1 and subsequently in this chapter have the meaning assigned to them in the Glossary of nomenclature at the beginning of the chapter.



THE SYSTEM MODELLED.

FIG. 4-1.

4.2.2 The assumptions made in formulating the model.

a) There is negligible vapour hold-up on a plate.

A typical ratio of liquid density to vapour density in a crude unit operating at one atmosphere pressure (gauge) is 100:1. The result of this assumption is to remove terms in dW_V/dt where W_V is the vapour hold-up. Vapour rate changes are thus instantaneous.

b) The liquid in the downcomer and the froth on the tray are each perfectly mixed.

This assumption is felt to be fully justified as regards the downcomer. This followed observation of the operation of the laboratory sieve tray unit in the Department of Chemical Engineering at Loughborough University. Considerable turbulence throughout the downcomer was visible in all cases except those of very low liquid rates. Inspection of the interior of the industrial unit during shutdown led the author to expect similar conditions to prevail in the full scale column.

However, the assumption of perfect mixing for the tray itself could be a source of error. This mean residence time for a tray as indicated by the model itself is of the order of fifteen seconds. The true situation may in fact be plug flow. Now other research workers have demonstrated cases of plug flow and also cases with considerable back mixing on a distillation tray (60). However, as will be seen at a later stage the model developed is sufficiently complex not to merit additional complication for what may well be only a limited improvement.

c) The liquid fraction in the froth is everywhere uniform for each particular tray.

This assumption is known to be untrue. Other workers (6) have described the foam on a distillation tray as being composed of three distinct layers: clear liquid, bubbles but mostly liquid, froth but mostly vapour.

It is difficult to say what errors this will introduce. Because the upper region of the froth is in fact of lower density than the mean then to achieve a given liquid flow the real situation will demand a greater froth height than predicted by the model. This could mean that the model will tend to err on the wrong side in the prediction of flooding.

d) <u>The Francis weir formula is a valid description of the flow of froth over the outlet weir.</u>

This correlation has the form :

$$L = ch^{3/2}$$

where L = liquid flow rate

h = head of liquid over the weir

c = a constant, the value of which depends on the units of L and h.

Bolles (1) recommends that this equation be used in tray design as if pure liquid not froth is flowing over the outlet weir. Inspection of the laboratory sieve tray in operation revealed as might be expected and as reported by other workers (6) that it is in fact froth flowing over the weir. Also this froth may persist into the downcomer depending on the characteristics of the liquid. Hence in this model the 'liquid' is assumed to have a density $\varepsilon\rho$ where ρ is the clear liquid density and ε is the liquid fraction of the froth.

e) <u>The froth height is an instantaneous function of the liquid and vapour rates.</u>

Qualitative considerations and also observation of the laboratory sieve plate support the validity of this assumption for the vapour rate dependence. However, it it not really true for a liquid rate variation. In the absence of a better model for the froth height correlation in a dynamic situation it was decided that this assumption would be the most adequate. Any imbalance in the mass balance thereby produced will be taken up by the froth density.

f) <u>The enthalpies of the liquid and vapour streams leaving each plate are linear functions of the tray liquid temperature.</u>

This is based on data supplied by BP. The relation for the liquid enthalpy is a true straight line. That for the vapour enthalpy curves slightly but is well approximated by a straight line.

g) <u>Representation of each plate as an effective heat transfer device with a heat transfer coefficient is an adequate description.</u>

In a distillation column tray design calculation liquid temperatures are generally obtained by a bubble-point calculation. i.e. the basis of the calculation is the liquid composition. This model proposes to neglect mass transfer considerations. Hence a different means of arriving at variations in the tray temperature is required. It is suggested that transfer of heat from the vapour entering the plate to the tray liquid is given by :-

Rate of heat transferred = (Constant) x (Vapour Rate) x (Temperature difference)

The initial data for the unit is used to provide a value for the constant. The vapour rate is included on the right hand side to replace the area term in the normal heat transfer equation. It is equivalent to the assumption that the interfacial area of the froth is a function only of the vapour rate, to which it is directly proportional.

h) <u>Vapour leaving a tray is at the same temperature as the liquid on the tray.</u>

This is a common design assumption. In this case it is the best estimate available.

i) <u>The presence of the steam in the unit as an inert may be ignored.</u>

With no inert gas present in a system the neglect of mass transfer effects is quite reasonable. Consideration of the process of distillation as being simply a heat transfer operation may be adequate. However, in the presence of inerts mass transfer might play a more dominant role. This is because condensation of vapour occurs by diffusion through the inert. In the present case this will occur in the bubbles in the liquid on the distillation trays. This effect is also a major one in a cooler-condenser and correct design of this apparatus must take account of the diffusion of the condensing vapour through the non-condensables.

The justification in the present case lies in the small amount of steam present - only a few pounds of steam per hundred pounds of crude feed.

4.2.3 The basic equations.

The dynamic mass balance for the tray gives :-

$$d/dt(W_{Ln}) = L_{Dn} + V_{n+1} + SV_{n+1} + SR_n - L_n - V_n \qquad \ldots.(4\text{-}1)$$

The dynamic mass balance for the downcomer gives :-

$$d/dt(W_{Dn}) = L_{n-1} - L_{Dn} - SL_{n-1} \qquad \ldots.(4\text{-}2)$$

The tray hold-up is (area) x (height) x (average density) :-

$$W_{Ln} = \varepsilon_n \rho_{Ln} A_{Tn} (\psi_{Wn} + \psi_n) \qquad \ldots. (4\text{-}3)$$

And similarly for the downcomer :-

$$W_{Dn} = \rho_{LDn} A_{Dn} \psi_{Dn} \qquad \ldots.(4\text{-}4)$$

The pressure head of liquid in the downcomer must balance four pressures on the tray :-   (ref. Peiser and Grover (26)).

$$\psi_{Dn} = \mathcal{E}_n(\psi_{Wn} + \psi_n) + C_{Ln}L_{Dn}^2 + C_{Vn-1}(V_n + SV_n)^2 + \mathcal{E}_{n-1}(\psi_{Wn-1} + \psi_{n-1}) \qquad \text{....(4-5)}$$

Head in downcomer.	Head on the tray.	Head to drive liquid under downcomer weir.	Head to drive vapour through holes in tray above.	Head to be overcome by vapour on tray above.

where

$$C_{Ln} = 1.5 \quad (0.36 \times 2.0 \times 32.2 \times [\rho_{Ln-1} \times A_{UDn}]^2) \qquad \text{....(4-5a)}$$

$$C_{Vn-1} = 2.0 \quad (32.2 \times \mathcal{E}_{n-1} \times \rho_{Ln-1} \times \rho_{Vn} \times (0.6 \times AP_{n-1})^2) \qquad \text{....(4-5b)}$$

The Francis weir formula gives the liquid flow over the outlet weir :-

$$L_n = e_9 l_n \mathcal{E}_n \rho_{Ln} \psi_n^{3/2} \qquad \text{....(4-6)}$$

The empirical correlation between the froth height and the liquid and vapour rates gives :-

$$\psi_n = e_1(V_{n+1} + SV_{n+1}) + e_2(L_{Dn} + SR_n) + e_3\psi_{Wn} + e_{10}(V_{n+1} + SV_{n+1})^2 + e_{11} \qquad \text{....(4-7)}$$

(From Gerster (4) for bubble cap plates and Thomas and Campbell (9) for sieve plates).

The enthalpy balance for the tray gives :

$$d/dt\ (h_n W_{Ln}) = h_{Dn}L_{Dn} + H_{n+1}V_{n+1} + H_{SVn+1}SV_{n+1} + h_{SRn}SR_n - h_nL_n - H_nV_n \qquad \text{....(4-8)}$$

The enthalpy balance for the downcomer gives :-

$$d/dt(h_{Dn}W_{Dn}) = h_{n-1}L_{n-1} - h_{Dn}L_{Dn} - h_{n-1}SL_{n-1} \qquad \text{....(4-9)}$$

The assumption that the heat transferred from the vapour entering a tray to the liquid on the tray = (constant) x (vapour rate) x (temperature difference) gives :-

$$H_{n+1}V_{n+1} + H_{SVn+1}SV_{n+1} - H_nV_n = m_nV_{n+1}(\Theta_{n+1} - \Theta_n) + m_nSV_{n+1}(\Theta_{SVn+1} - \Theta_n) \qquad \text{....(4-10)}$$

4.2.4 The linearised equations.

The equations set out in the previous section may be linearised about some suitable state. This need not be a steady state. The linearised equations are obtained by expressing each variable as the sum of two components - the value of the variable at the reference state plus the current deviation from that state, e.g. variable x is expressed as $\bar{x} + \Delta x$. The expressions are then multiplied out and terms of order Δ^2 and higher are neglected. Hence the linearisation is only true for small deviations from the reference state.

For example consider equation (4-6) :-

$$L_n = e_9 l_n \mathcal{E}_n \rho_{Ln} \psi_n^{3/2}$$

The variables are $L_n, \mathcal{E}_n, \psi_n$ the rest being assumed constant for the plate n. Expanding (4-6) by considering some state near to the reference state we obtain :-

$$\bar{L}_n + \Delta L_n = e_9 l_n(\bar{\mathcal{E}}_n + \Delta\mathcal{E}_n)\rho_{LN}(\bar{\psi}_n + \Delta\psi_n)^{3/2} \qquad \text{....(4-11)}$$

Now $\quad (\bar{\psi}_n + \Delta\psi_n)^{3/2} = \bar{\psi}_n^{\,3/2}\ (1 + \Delta\psi_n/\bar{\psi}_n)^{3/2}$

And by Taylor expansion $= \bar{\psi}_n^{\,3/2}\ (1 + \frac{3}{2}\frac{\Delta\psi_n}{\bar{\psi}_n} + 0\ (\Delta^2) + \dots)$

$$\doteqdot \bar{\psi}_n^{\,3/2} + \frac{3}{2}\,\bar{\psi}_n^{\,1/2}\Delta\psi_n$$

Substituting this in the expanded equation (4-11) gives :-

$$(L_n + \Delta L_n) = e_9 l_n (\bar{\varepsilon}_n + \Delta\varepsilon_n) \rho_{Ln} (\bar{\psi}_n^{3/2} + \frac{3}{2}\bar{\psi}_n^{1/2} \Delta\psi_n)$$

Multiplying out : -

$$(\bar{L}_n + \Delta L_n) = e_9 l_n \bar{\varepsilon}_n \rho_{Ln} \bar{\psi}_n^{3/2} + e_9 l_n \Delta\varepsilon_n \rho_{Ln} \bar{\psi}_n^{3/2}$$

$$+ \frac{3}{2} e_9 l_n \varepsilon_n \rho_{Ln} \psi_n^{1/2} \Delta\psi_n + \frac{3}{2} e_9 l_n \rho_{Ln} \bar{\psi}_n^{1/2} \Delta\varepsilon_n \Delta\psi_n$$

But applying (4-6) to the reference state gives :-

$$\bar{L}_n = e_9 l_n \bar{\varepsilon}_n \rho_{Ln} \bar{\psi}_n^{3/2}$$

Substracting this from the previous equation and neglecting the last term which is of order Δ^2 we finally obtain :-

$$\Delta L_n = e_9 l_n \rho_{Ln} \bar{\psi}_n^{3/2} \Delta\varepsilon_n + \frac{3}{2} e_9 l_n \bar{\varepsilon}_n \rho_{Ln} \bar{\psi}_n^{1/2} \Delta\psi_n \quad \ldots.(4\text{-}17)$$

A similar procedure is applied to each equation to give :-

(The bars above the reference state values are omitted for clarity.)

$$d/dt\ (\Delta W_{Ln}) = \Delta L_{Dn} + \Delta V_{n+1} + \Delta SV_{n+1} + \Delta SR_n - \Delta L_n - \Delta V_n + g_1 \quad \ldots.(4\text{-}12)$$

$$\text{where } g_1 = \left[L_{Dn} + V_{n+1} + SV_{n+1} + SR_n - L_n - V_n\right]\Big|\text{reference state.} \quad \ldots.(4\text{-}12a)$$

$$d/dt\ (\Delta W_{Dn}) = \Delta L_{n-1} - \Delta L_{Dn} - \Delta SL_{n-1} + g_2 \quad \ldots.(4\text{-}13)$$

$$\text{where } g_2 = \left[L_{n-1} - L_{Dn} - SL_{n-1}\right]\Big| \text{ reference state.} \quad \ldots.(4\text{-}13a)$$

$$\Delta W_{Ln} = \varepsilon_n \rho_{Ln} A_{Tn} \Delta\psi_n + \rho_{Ln} A_{Tn} (\psi_{Wn} + \psi_n) \Delta\varepsilon_n \quad \ldots.(4\text{-}14)$$

$$\Delta W_{Dn} = \rho_{LDn} A_{Dn} \Delta\psi_{Dn} \quad \ldots.(4\text{-}15)$$

$$\Delta\psi_{Dn} = \varepsilon_n \Delta\psi_n + (\psi_{Wn} + \psi_n)\Delta\varepsilon_n + 2C_{Ln} L_{Dn} \Delta L_{Dn}$$

$$+ 2C_{Vn-1}(V_n + SV_n)(\Delta V_n + \Delta SV_n) + \varepsilon_{n-1}\Delta\psi_{n-1} + (\psi_{Wn-1} + \psi_{n-1}).$$

$$\Delta\varepsilon_{n-1} \quad \ldots..(4\text{-}16)$$

$$\Delta L_n = e_9 l_n \int_{Ln} \psi_n^{3/2} \Delta \mathcal{E}_n + 3/2\, e_9 l_n \mathcal{E}_n \int_{Ln} \psi_n^{1/2} \Delta \psi_n \qquad \ldots.(4\text{-}17)$$

$$\Delta \psi_n = e_1 (\Delta V_{n+1} + \Delta SV_{n+1}) + e_2 (\Delta L_{Dn} + \Delta SR_n) + 2e_{10} (\Delta V_{n+1} + \Delta SV_{n+1}) (V_{n+1} + SV_{n+1}) \qquad \ldots(4\text{-}18)$$

In the manipulation of the heat balance equations the enthalpies are expressed as linear functions of the tray liquid temperature Θ or the downcomer liquid temperature Θ_D :-

Liquid enthalpy $h = r\Theta + s$

Vapour enthalpy $H = p\Theta + q$

The detailed manipulation of the heat balance equations is given in Appendix 1, section A1.2.

The resulting equations are :-

$$\begin{aligned} W_{Ln} r\, d/dt\, (\Delta\Theta_n) = {} & r (\Theta_{Dn} - \Theta_n) \Delta L_{Dn} + r L_{Dn} \Delta\Theta_{Dn} + (H_{n+1} - h_n) \Delta V_{n+1} \\ & + p V_{n+1} \Delta\Theta_{n+1} + (H_{svn+1} - h_n) \Delta SV_{n+1} \\ & + (h_{SRn} - h_n) \Delta SR_n - \left[r (L_n + g_1) + pV_n \right] \Delta\Theta_n \\ & - (H_n - h_n) \Delta V_n + (g_3 - h_n g_1) \qquad \ldots(4\text{-}19) \end{aligned}$$

$$\begin{aligned} W_{Dn} r\, d/dt\, (\Delta\Theta_{Dn}) = {} & (h_{n-1} - h_{Dn}) \Delta L_{n-1} + (rL_{n-1} - rSL_{n-1}) \Delta\Theta_{n-1} \\ & - rL_{Dn} \Delta\Theta_{Dn} + (h_{Dn} - h_{n-1}) \Delta SL_{n-1} \\ & - (h_{Dn} + r\Delta\Theta_{Dn})\, g_2 \qquad \ldots(4\text{-}20) \end{aligned}$$

$$\begin{aligned} & H_{n+1} - m_n (\Theta_{n+1} - \Theta_n) \Delta V_{n+1} - H_n \Delta V_n \\ & \quad = \left[pV_n - m_n V_{n+1} - m_n SV_{n+1} \right] \Delta\Theta_n + \left[m_n V_{n+1} - pV_{n+1} \right] \Delta\Theta_{n+1} \\ & \quad + \left[m_n (\Theta_{SVn+1} - \Theta_n) \Delta SV_{n+1} - H_{SVn+1} \Delta SV_{n+1} \right] \ldots. (4\text{-}21) \end{aligned}$$

4.3 Solution of the model.

We have obtained a set of ten equations per tray (4-12) to (4-21) in ten unknowns per tray :- ΔL, ΔV, ΔW_L, ΔW_D, ΔL_D, $\Delta \mathcal{E}$, $\Delta \psi$, $\Delta \psi_D$, $\Delta \Theta$, $\Delta \Theta_D$. Four equations are linear differential. The remainder are linear algebraic. The two variables $\Delta\Theta, \Delta\Theta_D$ occur only in equations (4-19), (4-20) and (4-21). i.e. the temperature effects on the liquid and vapour densities are not taken into account.

The initial manipulation of the equations into a form suitable for solution consists of the elimination of the three variables $\Delta \mathcal{E}$, $\Delta \psi$ and $\Delta \psi_D$ from equations (4-14) and (4-15) using (4-16), (4-17) and (4-18). Equations (4-14) and (4-15) then have the form :-

$$\Delta W_L = f_1 \ (\Delta L, \Delta V, \Delta L_D)$$

$$\Delta W_D = f_2 \ (\Delta L, \Delta V, \Delta L_D)$$

Differentiation of these yields expressions for $d/dt(\Delta W_L)$and $d/dt(\Delta W_D)$ which may be substituted into equations (4-12) and (4-13). Equations (4-12) and (4-13) thus remain linear differential equations, but are now in the unknowns ΔL, ΔL_D, and ΔV. The method of solution employed is then to assume a value for the vector ΔV and on this basis to solve the four linear differential equations (4-12) (4-13) (4-19) and (4-20) for the four unknowns ΔL, $\Delta L_D, \Delta\Theta, \Delta\Theta_D$. Equation (4-21) is then used to yield an improved estimate of ΔV. At some predetermined point in the computation of the transient the calculation is stopped and a new linear model is generated about the point reached. That is the elements of the system matrix are updated so that the non-linear problem is solved by a quasi-linear technique.

That then is the overall approach. Now consider the details of the method of solution. The manipulation by which equations (4-12) to (4-18) are reduced to two differential equations in three unknowns is given in Appendix 1. The two equations so obtained have the form :- ($\Delta\dot{L}$ denotes $d/dt(\Delta L)$).

$$b_1 \Delta\dot{L}_{Dn} + b_2 \Delta\dot{L}_n = \Delta L_{Dn} + \Delta V_{n+1} \Delta SV_{n+1} + \Delta SR_n - \Delta L_n - \Delta V_n + g_1 \qquad \ldots.(4\text{-}22)$$

$$b_3 \Delta\dot{L}_{Dn-1} + b_4 \Delta\dot{L}_{n-1} + b_5 \Delta\dot{L}_{Dn} + b_6 \Delta\dot{L}_n = \Delta L_{n-1} - \Delta L_{Dn} - \Delta SL_{n-1} + g_2 \qquad \ldots.(4\text{-}23)$$

where b_1 to b_6 are as follows :-

$$b_1 = \varepsilon_n \rho_{Ln} A_{Tn} e_2 \left\{1-3(\psi_{Wn} + \psi_n)\Big/(2\psi_n)\right\}$$

$$b_2 = \rho_{Ln} A_{Tn} \; (\psi_{Wn} + \psi_n)\Big/(e_9 l_n \rho_{Ln} \psi_n^{\;3/2})$$

$$b_3 = \rho_{LDn} A_{Dn} \varepsilon_{n-1} \; e_2^p \left\{1-3 \; (\psi_{Wn-1} + \psi_{n-1})\Big/(2\psi_{n-1}) \qquad n > 2\right.$$

$$b_3 = 0, \quad n = 2.$$

$$b_4 = \rho_{LDn} A_{Dn} (\psi_{Wn-1} + \psi_{n-1})\Big/(e_9^p \; l_{n-1} \rho_{Ln-1} \psi_{n-1}^{\;3/2})$$

$$b_5 = \rho_{LDn} \; A_{Dn} \left\{\varepsilon_n e_2 \left[1-3 \; (\psi_{Wn} + \psi_n)\Big/(2\psi_n) \right. + 2C_{Ln} L_{Dn}\right\}$$

$$b_6 = \rho_{LDn} A_{Dn} \left[(\psi_{Wn} + \psi_n)\Big/(e_9 l_n \rho_{Ln} \psi_n^{\;3/2})\right]$$

If we now select as our state vector $\underline{X}$ where :-

$$\underline{X}^T = \left[\Delta L_1, \Delta\theta_1, \Delta L_{D2}, \Delta\theta_{D2}, \Delta L_2, \Delta\theta_2, \Delta L_{D3}, \Delta\theta_{D3} \ldots \Delta L_{DnT}, \Delta\theta_{DnT}, \Delta L_{nT}, \Delta\theta_{nT}\right]$$

then we can write down the two equations for the top tray (equations

(4-12) and (4-19)) and the four equations for each remaining tray (equations (4-12), (4-13), (4-19) and (4-20) in matrix form :-

$$A\dot{\underline{X}} = B\underline{X} + C \qquad \ldots.(4\text{-}24)$$

where C, the vector of forcing functions, also contains the terms in V. The matrices A and B have the following form if the equations are written down in the order (4-13), (4-20), (4-12), (4-19) :-

(x denotes a non-zero element).

$$A:- \quad \left[\begin{array}{cccccccccccccc}
x & o & o & o & o & & & & & & & & & \\
o & x & o & o & o & o & & & & & & & & \\
x & o & x & o & x & o & o & & & & & & & \\
o & o & o & x & o & o & o & o & & & & & & \\
o & o & x & o & x & o & o & o & o & & & & & \\
 & o & o & o & o & x & o & o & o & o & & & & \\
 & & x & o & x & o & x & o & x & o & o & & & \\
 & & & o & o & o & o & x & o & o & o & o & & \\
 & & & & o & o & x & o & x & o & o & o & o & \\
 & & & & & o & o & o & o & x & o & o & o & o
\end{array}\right.$$

etc.

$$B:- \quad \left[\begin{array}{cccccccccccccc}
x & o & o & o & o & & & & & & & & & \\
o & x & o & o & o & x & & & & & & & & \\
x & o & x & o & o & o & o & & & & & & & \\
x & x & o & x & o & o & o & o & & & & & & \\
o & o & x & o & x & o & o & o & o & & & & & \\
 & o & x & x & o & x & o & o & o & x & & & & \\
 & & o & o & x & o & x & o & o & o & o & & & \\
 & & & o & x & x & o & x & o & o & o & o & & \\
 & & & & o & o & x & o & x & o & o & o & o & \\
 & & & & & o & x & d & o & x & o & o & o & x
\end{array}\right. \quad \text{etc.}$$

Equation (4-24) is solved numerically by the implicit method described by Holland (33), P.27. This is a generalisation of the approximation to $\int_t^{t+\Delta t} f(x)dt$ by the trapezoidal rule:-

$$\int_t^{t+\Delta t} f(x)dt \doteq \left[\mu f(x)\Big|_{t+\Delta t} + (1-\mu)f(x)\Big|_t\right]\Delta t \qquad \ldots.(4\text{-}25)$$

For $\mu=\frac{1}{2}$ the above approximation reduces to the trapezoidal rule. Application of equation (4-25) to equation (4-24) yiēlds:-

$$(A/\Delta t)(\underline{X}_{n+1} - \underline{X}_n) = \mu(B\underline{X}_{n+1} + C) + (1-\mu)(B\underline{X}_n + C) \qquad 0 \leq \mu \leq 1.$$

which on rearrangement gives:-

$$\underline{X}_{n+1} = \left[\frac{A}{\Delta t} - \mu B\right]^{-1}\left[\left\{(1-\mu)B + \frac{A}{\Delta t}\right\}\underline{X}_n + C\right] \qquad \ldots.(4\text{-}26)$$

Equation (4-26) may conveniently be written:-

$$\underline{X} = E^{-1}F$$

where E is a band matrix with nine elements in each row and F is a column vector. The shape of E is the same as A and B given above. The band elements of E are in general zero only if the corresponding elements of both A and B are zero.

This method of solution has been assembled as a computer program. This is described in the next section.

4.4. Computer program for the model solution.

The program is written in Fortran 4 for the ICL 1905 computer at Loughborough University. This third generation machine has 32,000 words of core store, a factor which affected the program considerably.

The program is described in detail in Appendix 2 and sample data and results are given. When the program was written no routine was available for the economical inversion of a large band matrix and a special routine (subroutine BMM3) was written. This employs Jordan's method (59) and incorporates partial (row) pivoting. ICL have since introduced a similar routine based on Gaussian elimination.

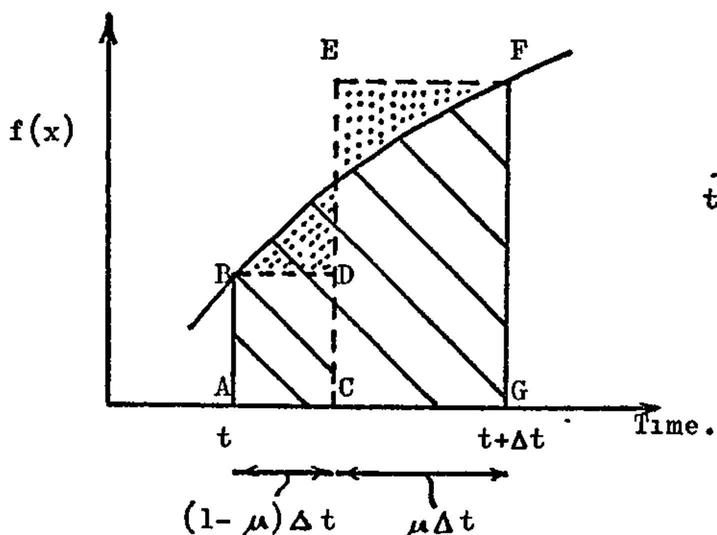
The method of solution requires the specification of a time increment for the numerical integration, the frequency with which the model is to be relinearised and a value for the implicit parameter μ. The author has found some interaction between these parameters. Indeed since the calculation iterates on the ΔV vector at each step it is possible for large integration steps to give such slow convergence of this iteration that small integration steps make more efficient use of computer time.

4.4.1 The effect of the implicit parameter μ.

The basic approximation made in the integration of the differential equation is:-

$$\int_t^{t+\Delta t} f(x)dt \doteqdot \left[\mu f(x)\Big|_{t+\Delta t} + (1-\mu)f(x)\Big|_t\right]\Delta t.$$

This is considered in geometric terms in Fig. 4-2.



$$\int_t^{t+\Delta t} f(x)dt = \text{shaded area}$$

Fig. 4-2

The approximation is equivalent to writing:-

$$\int_{t}^{t+\Delta t} f(x)dt = ABDC + CEFG$$

Clearly this approximation will become exact if a choice of μ is made which makes the stippled areas equal. If the curve between t and t+ Δt is a straight line then clearly the best value is $\mu = \frac{1}{2}$. If the curve is concave then $0.0 < \mu < 0.5$, if convex $0.5 < \mu < 1.0$.

Inspection of early results and intuition indicate that in the present problem transient response curves may follow either concave or convex paths depending on the variable and the elapsed time. At no one time is it reasonable to suppose that there will be a single choice of μ that will give the correct integral for all variables.

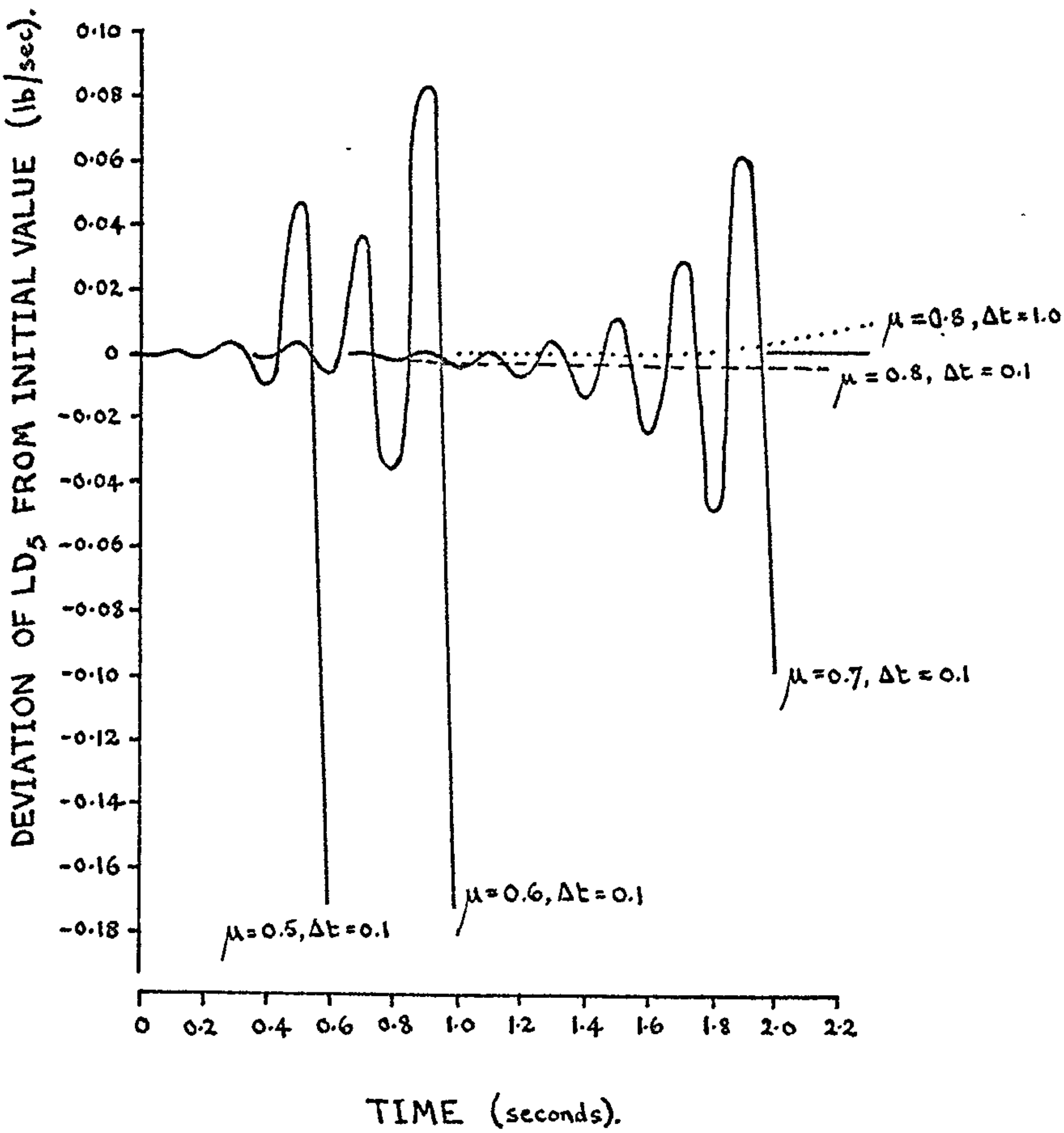
Experiments with different values of μ revealed that there is a minimum value of μ for which the response of the system is stable. The results of using different values of μ are demonstrated by plotting the transient for the liquid rate from downcomer 5 - see Fig. 4-3.

Because of the small time increment employed it is not felt that errors from a poor value of μ will accumulate rapidly. The variation in the transient for the liquid rate from plate 1 is given in Fig. 4-4. The response curves obtained using μ = 0.5,0.6 and 0.7 are almost coincident and that for μ = 0.8 is very close.

4.4.2 Effect of the time increment.

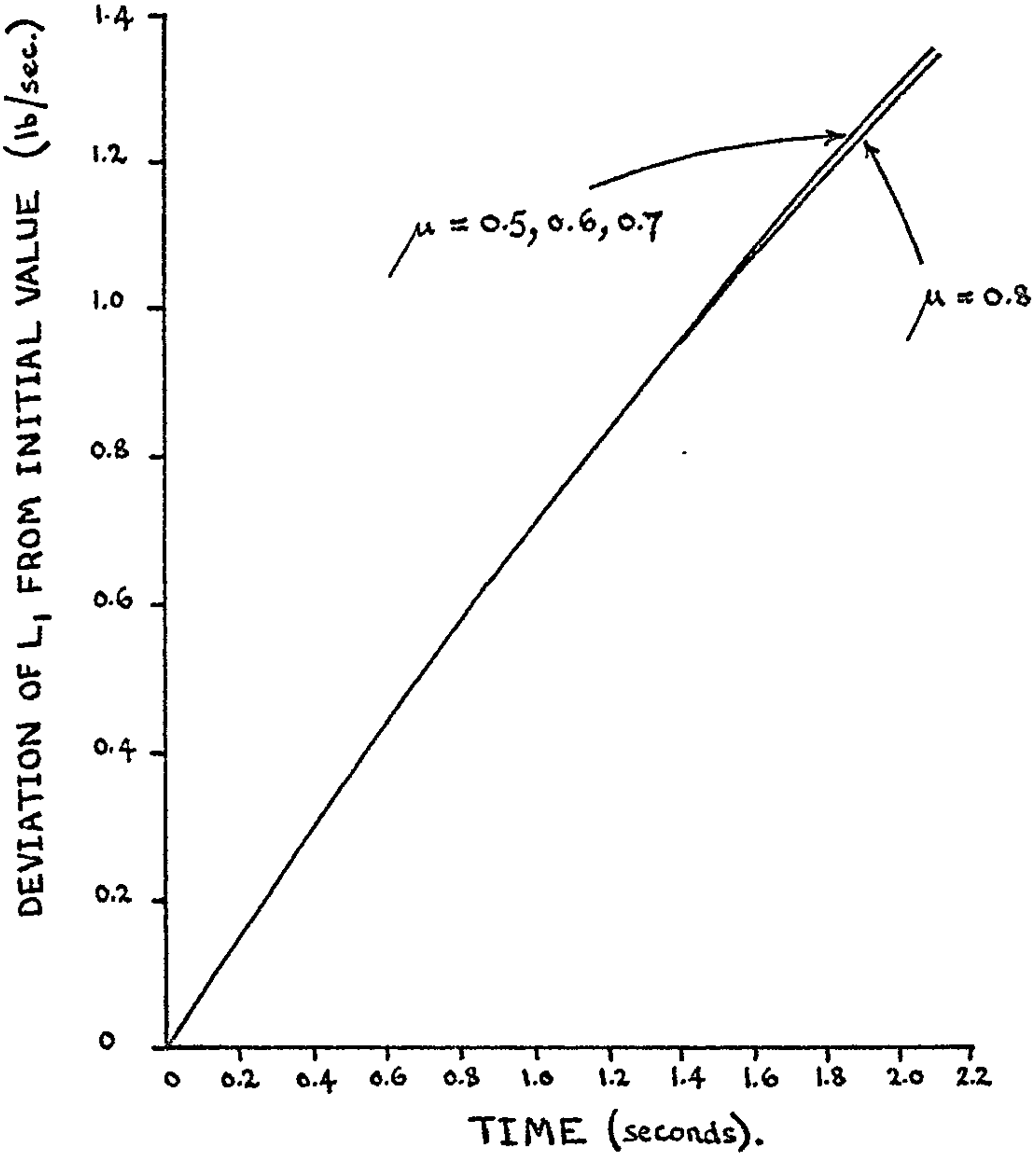
In selecting a time increment for a numerical integration three factors must be borne in mind. The first is that the time increment must clearly be less than or equal to the time over which the linearity of the mathematical model may be assumed valid. The second is that the approximation error for the calculation of

FIG. 4-3.



TRANSIENT RESPONSE OF LIQUID RATE FROM DOWNCOMER TO PLATE 5 FOR VARIOUS VALUES OF IMPLICIT PARAMETER.

FIG. 4-4.



TRANSIENT RESPONSE OF LIQUID RATE FROM PLATE 1 FOR VARIOUS VALUES OF IMPLICIT PARAMETER.

$\int_{t}^{t+\Delta t} f(x)dt$ will be zero if the correct value of μ is chosen for each variable. However, in general the correct value of μ cannot be chosen and so the error is proportional to the time increment. The third concerns accumulation of numerical error. Considerable computation is involved in calculating the response of all variables over one time step. If round-off errors result in an error say λ in one variable then after n steps the error may have accumulated to $n\lambda$. This could lead to serious error as well as being a waste of computer time. (The classic example of round-off error accumulation is given by Holland (32):-

'Using the formula $A_n = 10A_{n-1} - 10$ and given that $A_1 = 10/9$ calculate A_{10} using 7 figure arithmetic.

$A_1 = 1.111111$

$A_2 = 1.111110$

$A_3 = 1.111100$

..

..

..

$A_{10} = -110.0$ as compared with the obvious correct answer of 1.111111!)

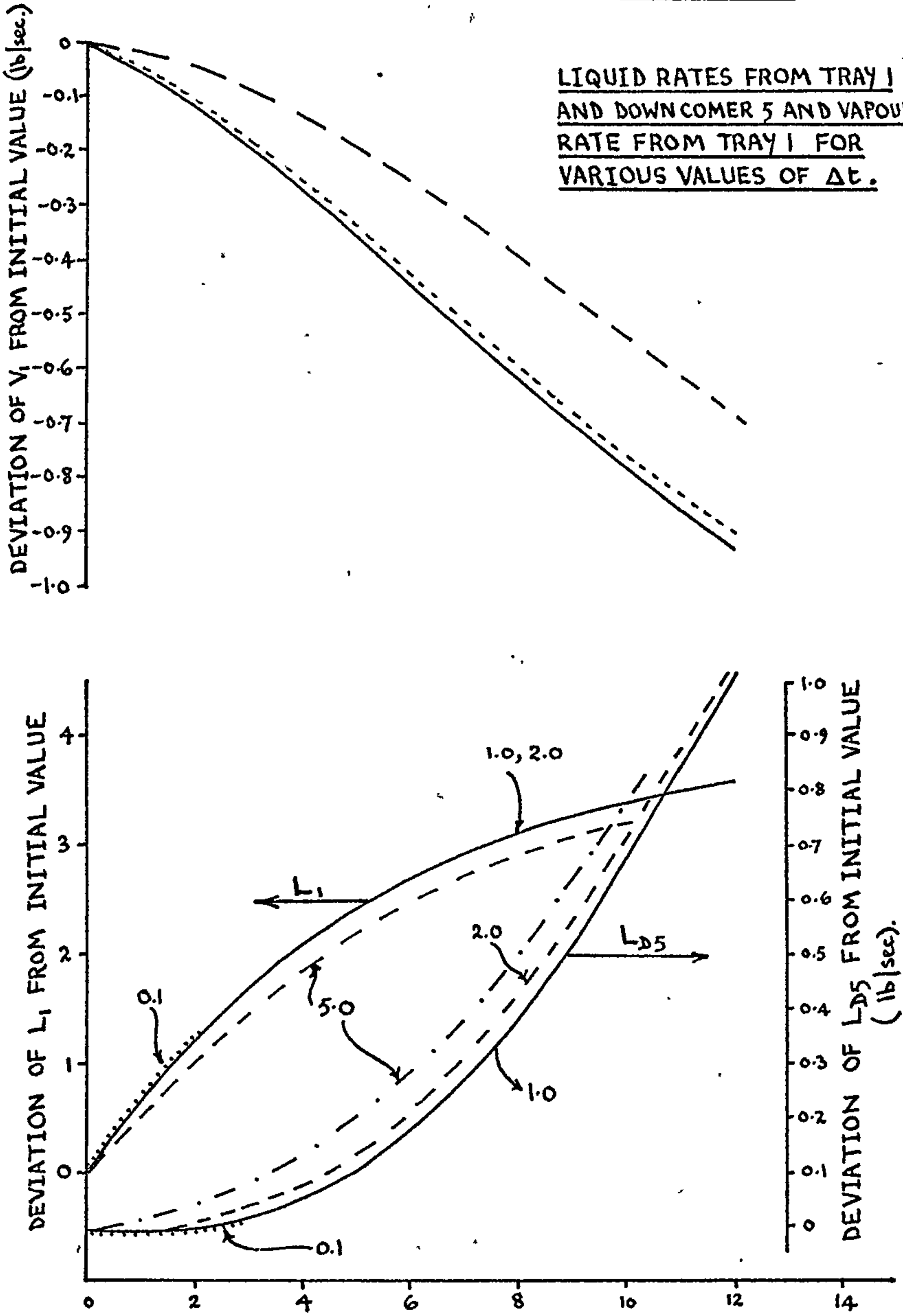
The results for a particular problem obtained using several values of the time increment are given in Fig. 4-5. It will be seen that the results using $\Delta t = 2.0$ seconds and $\Delta t = 1.0$ seconds are close. A time increment of 1.0 seconds was selected as giving a suitable compromise between accuracy and computation time in many of the computer runs.

4.4.3 Effect of relinearisation of the model.

Two long runs have been performed using a 15-plate column, a time increment of 1.0 second and a value of $\mu = 0.8$. The first

FIG. 4-5.

LIQUID RATES FROM TRAY 1 AND DOWNCOMER 5 AND VAPOUR RATE FROM TRAY 1 FOR VARIOUS VALUES OF Δt.



run incorporated re-evaluation of the system matrix at every time step. The second assumed linearity throughout. The results are given in Figs. 4-6 and 4-7.

It will be seen that the linear model did not give a stable response under the integration conditions used. Also it will be noticed that the linear and re-linearised runs were about coincident for the first few seconds. This suggests that a re-linearisation interval of greater than one second would be acceptable. However, the assumption of linearity throughout would not be valid.

4.5 The predictions of the mathematical model.

The computer program for the model solution was used to obtain the response for a reflux step increase on a hypothetical fifteen plate column, the details of which are contained in the sample data for the program in Appendix 2. For this size of problem the program required about one minute of computation time for each second of response time. Typical results from this run are given in Figs. 4-8 to 4-11. The first general point to note is that the major part of all the responses was completed within three to four minutes.

4.5.1 The liquid rate transient.

At the top of the column the liquid rate changes smoothly and is non-oscillatory. Fig. 4-8 shows that the liquid rate from tray 1 follows a smooth exponential decay lasting 30 seconds. Peaks on the response curves became evident lower in the column as a distinct surge passes down through the system. Fig. 4-9 shows that this surge reaches a peak after about 50 seconds for the liquid rate leaving the downcomer to the fifth tray and after about 110 seconds for the liquid rate leaving tray 12. It is

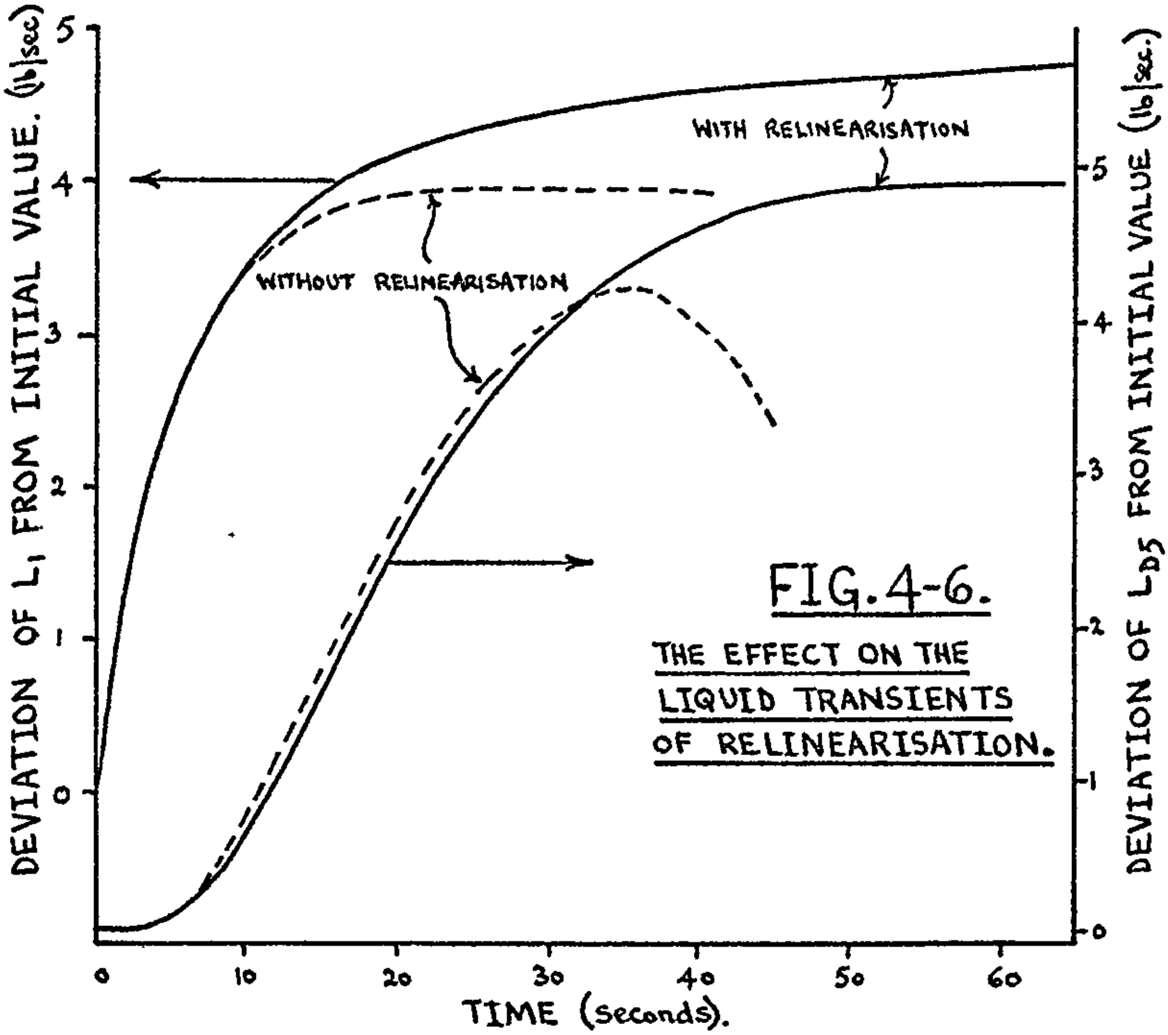


FIG. 4-6.

THE EFFECT ON THE LIQUID TRANSIENTS OF RELINEARISATION.

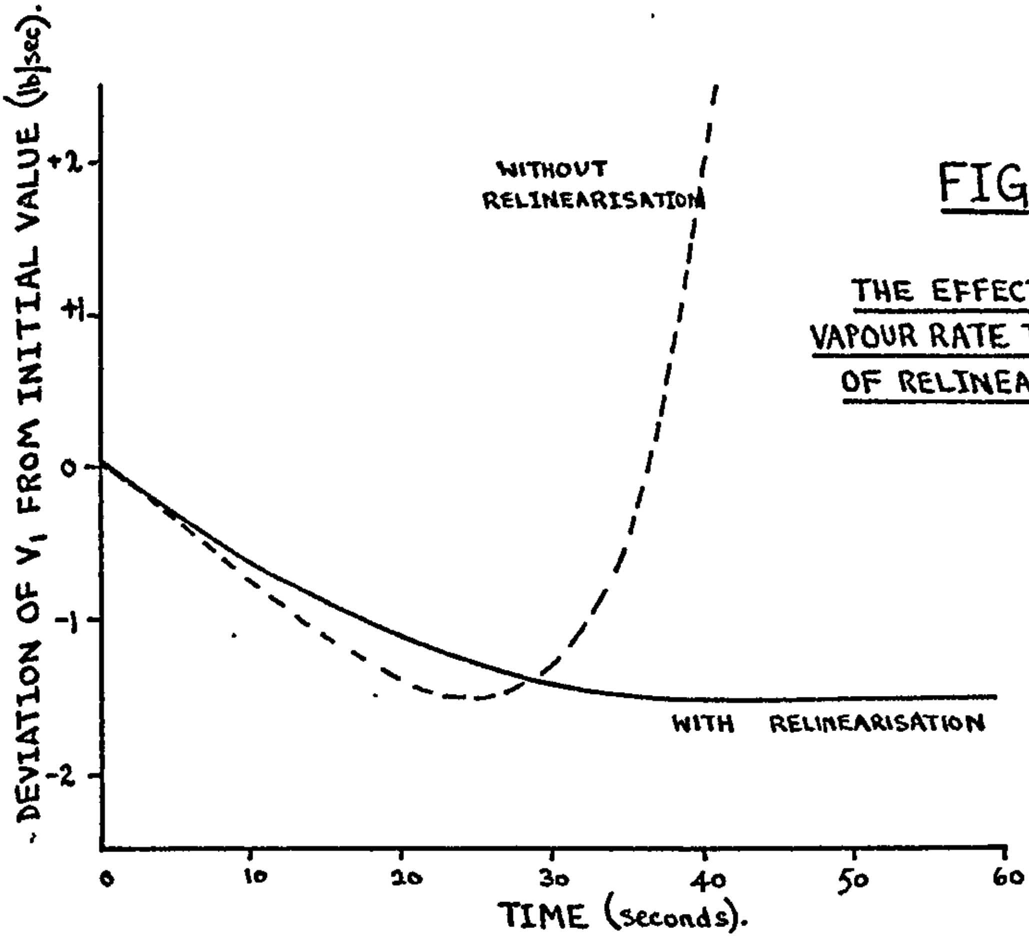


FIG. 4-7.

THE EFFECT ON THE VAPOUR RATE TRANSIENT OF RELINEARISATION.

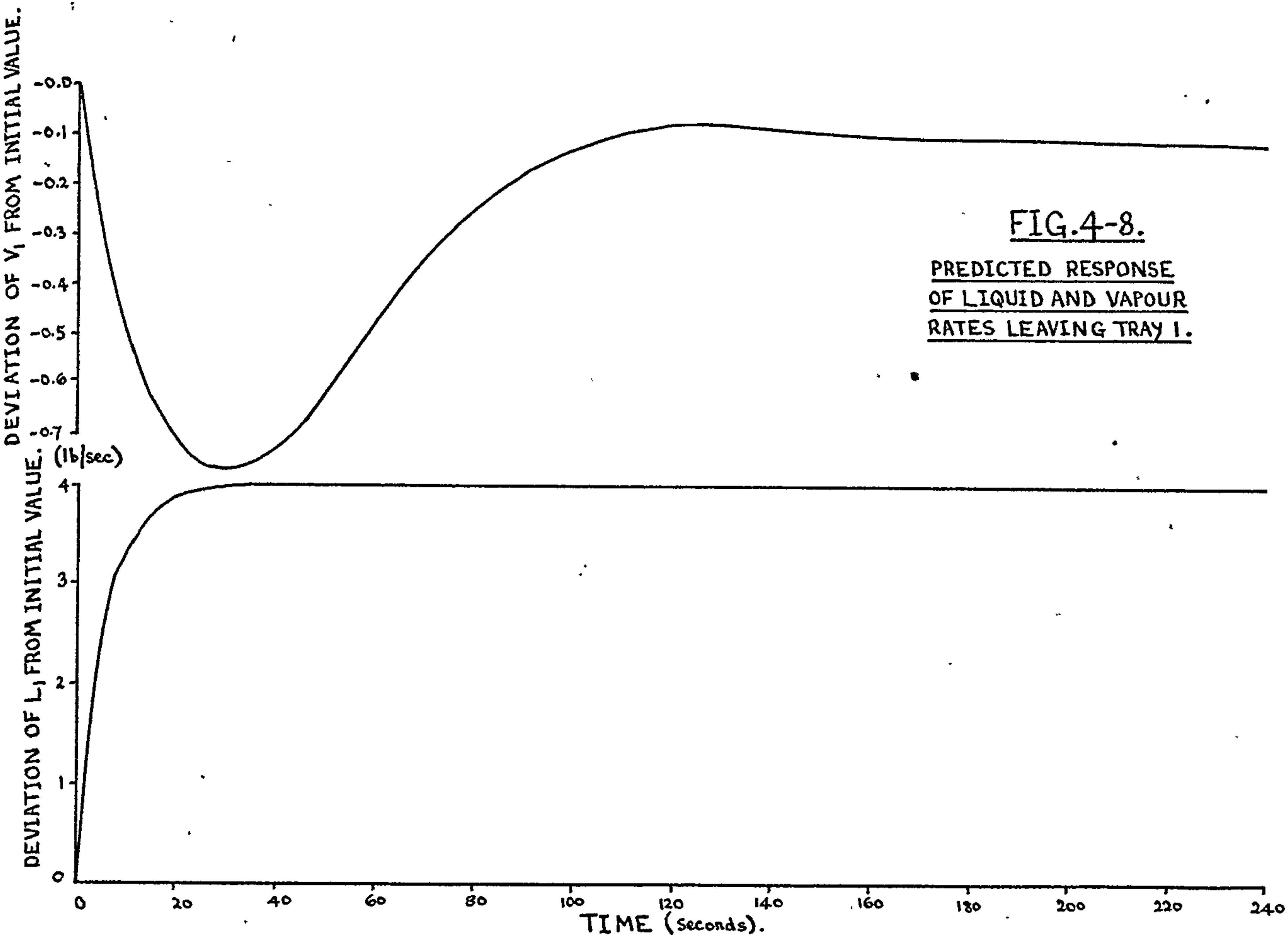


FIG.4-8.

PREDICTED RESPONSE OF LIQUID AND VAPOUR RATES LEAVING TRAY 1.

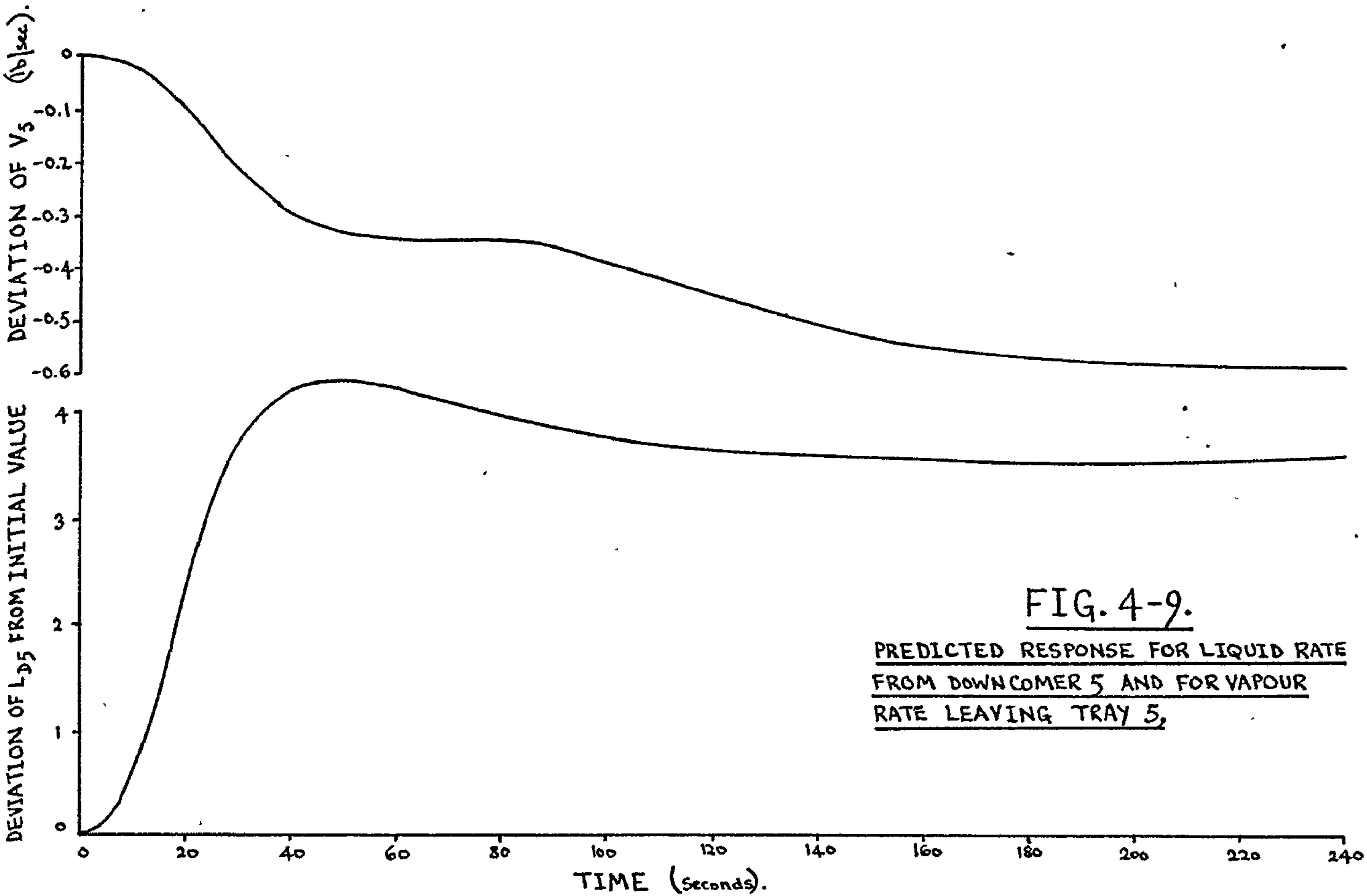


FIG. 4-9.

PREDICTED RESPONSE FOR LIQUID RATE FROM DOWNCOMER 5 AND FOR VAPOUR RATE LEAVING TRAY 5.

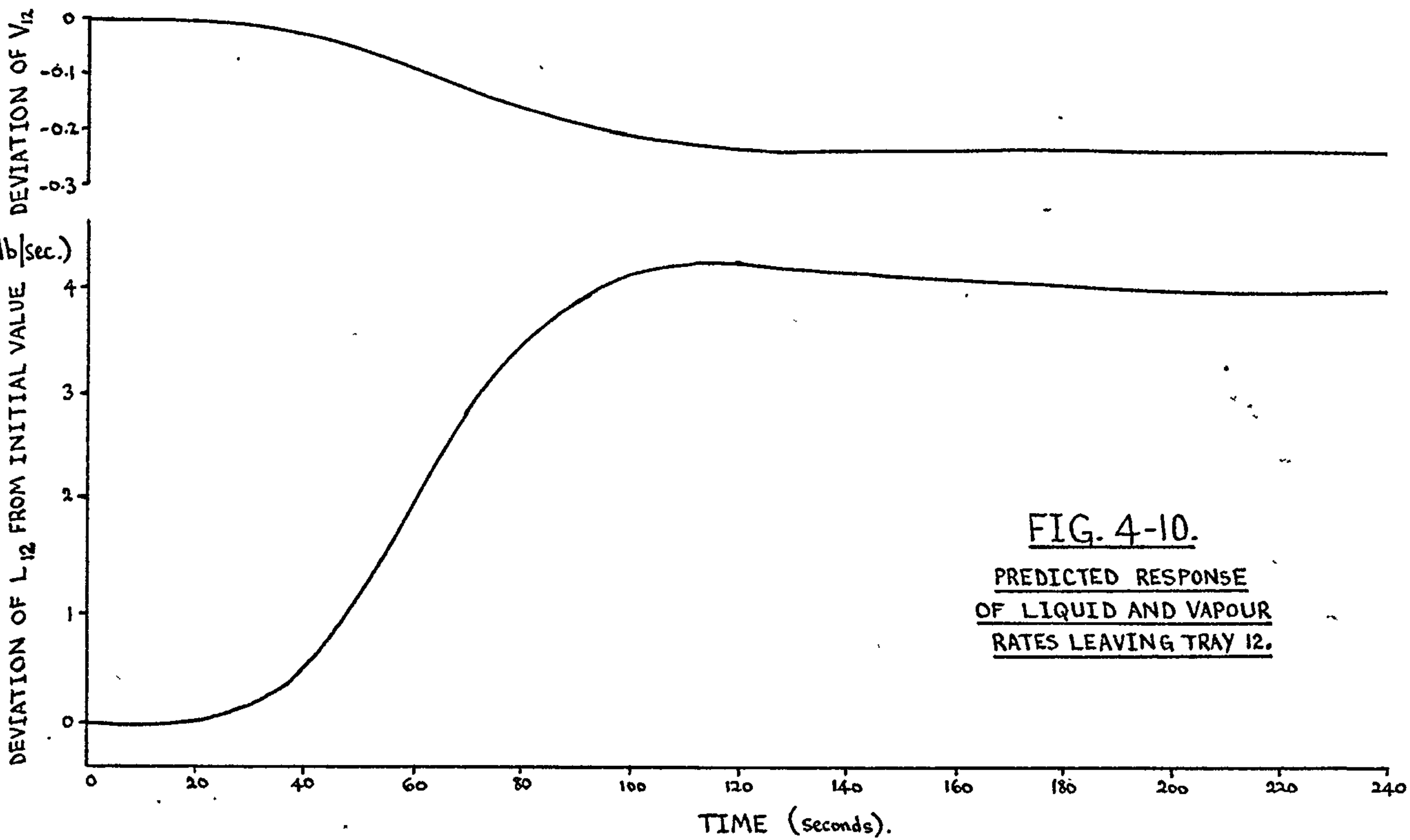


FIG. 4-10.

PREDICTED RESPONSE OF LIQUID AND VAPOUR RATES LEAVING TRAY 12.

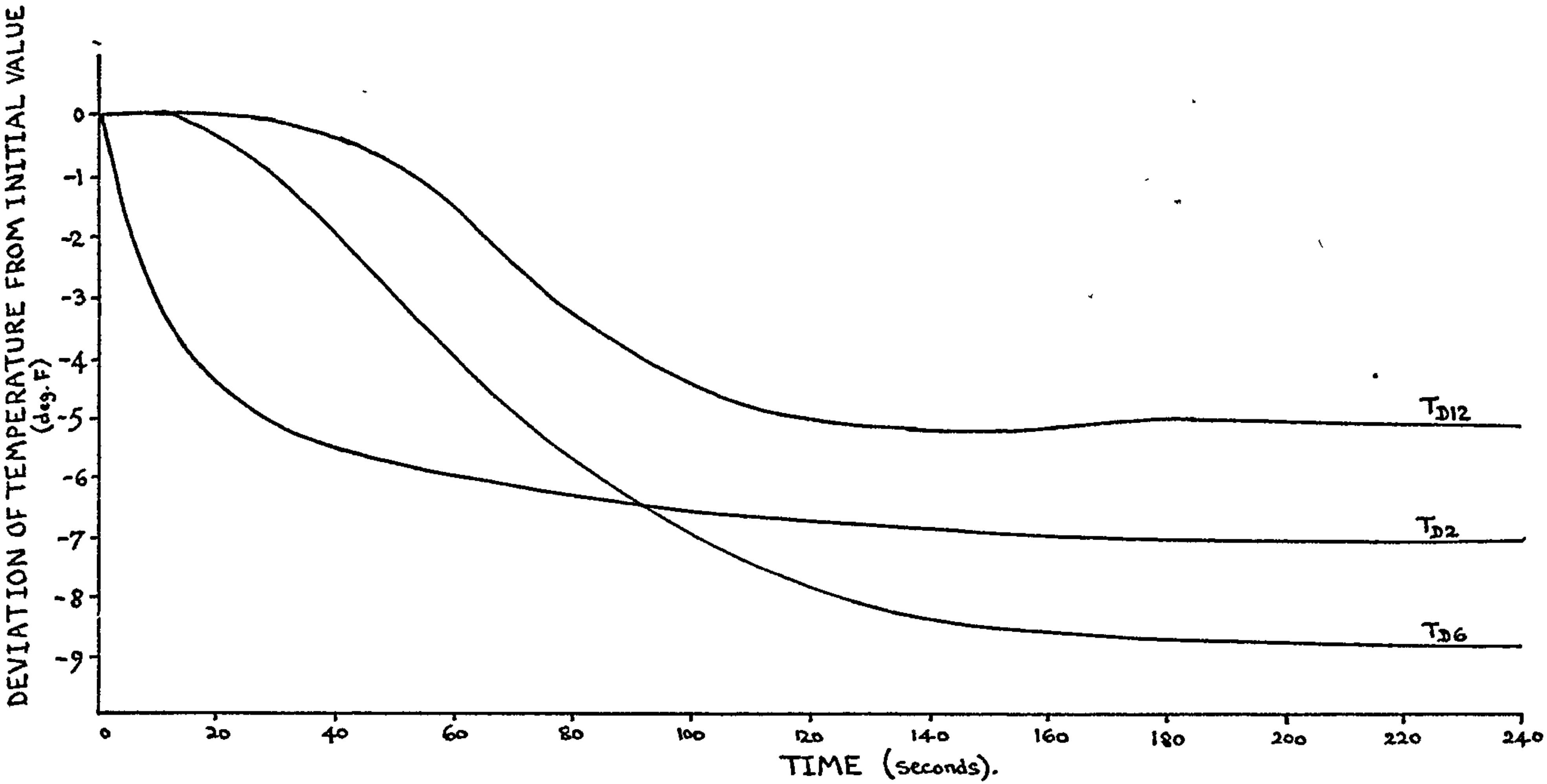


FIG. 4-11.

RESPONSE OF LIQUID TEMPERATURES IN DOWNCOMERS TO PLATES 2, 6 AND 12.

interesting to note the negligible effect on the liquid rate from the top tray of the varying vapour rate at the top of the column. (It should, however, be borne in mind that the scales on the liquid and vapour rate axes are in the ratio 5:1 in Figs. 4-8 to 4-10.)

4.5.2 The vapour rate transient.

The first point of note is the oscillatory response obtained at the top of the column, as shown for example by the vapour rate leaving tray 1 in Fig. 4-8. By tray 5 this is little more than a small irregularity - a plateau on an otherwise smooth response (Fig. 4-9). The vapour rate leaving tray 12 exhibits a smooth response that matches the liquid rate transient for tray 12 for the main part. The next point, not unexpected, is the wide discrepancy at the top of the column between the settling time for the liquid and vapour rates. Whereas the liquid rate equilibrates after 30 seconds, the vapour rate is barely steady after 200 seconds. At the bottom of the column the reverse is true, as Fig. 4-10 demonstrates, although the discrepancy is not so large. This is surprising since it would be expected that the changing liquid rate would cause the vapour rate to vary. However, the strong influence of the feed vapour just below this point is probably the reason for this steadiness. Support for this is given by the fact that liquid rate variations of similar magnitude have a decreasing effect on the vapour going down the column.

4.5.3 The tray temperature transient.

The main point of note with the transient response of the tray liquid temperatures is that at no point in the column has equilibrium been established in under 200 seconds. The temperatures at the top display the steepest rates of change but also appear to take the longest time to achieve final equilibrium. This indicates the strong feed-back effect due to the vapour. A pronounced oscillation is visible on the temperatures in the lower part of the column (see Fig. 4-11). This is probably due to the overcooling by bulk liquid dumping being reversed by the strong effect of the feed vapour only two trays below.

4.6 Conclusions.

The mathematical model of the hydraulics and heat transfer processes in a distillation column indicates settling periods of three to four minutes for flows and temperatures in a 15 plate industrial sized crude column following a step change in the flowrate of the overhead reflux return. The response curves appear consistent with each other and are not illogical from a practical point of view. The computer program required to solve the model is large and extremely time consuming. The mathematical method selected for numerical integration did not prove to be particularly robust or rapid, although this may have been partly due to the need for an iterative loop at each integration step. Thus, whereas this exercise is of use in assessing the contribution of two of the secondary effects in distillation dynamics, the model as such is not suitable for incorporation into any sort of control system.

CHAPTER 5 INFORMATION FROM THE INDUSTRIAL UNIT BY EXPERIMENT AND OBSERVATION.

5.1 Introduction.

The unit made available for experimental work was Crude Oil Distillation Unit No. 3 at BP Refinery (Llandarcy) Ltd. in South Wales. The operators on this unit were accustomed to assisting with BP test runs. These previous tests had been primarily concerned with achieving and maintaining steady state at specified operating conditions. Little dynamic investigation had been carried out on the main distillation column.

5.2 Objectives.

The objectives of the experiments were:-

(i) to obtain a 'feel' for the dynamics of the unit.

(ii) to establish a working method for performing dynamic experiments on this type of unit.

(iii) to familiarise the various operating crews with this type of test - in particular the importance of time as a variable and the danger of misguided 'trimming' of variables.

(iv) to provide a check on the predictions from a mathematical model of a crude distillation unit (described in Chapter 4.)

(v) to provide data from which to evolve a simple control strategy by which to achieve a major change in operating conditions with minimum disturbance.

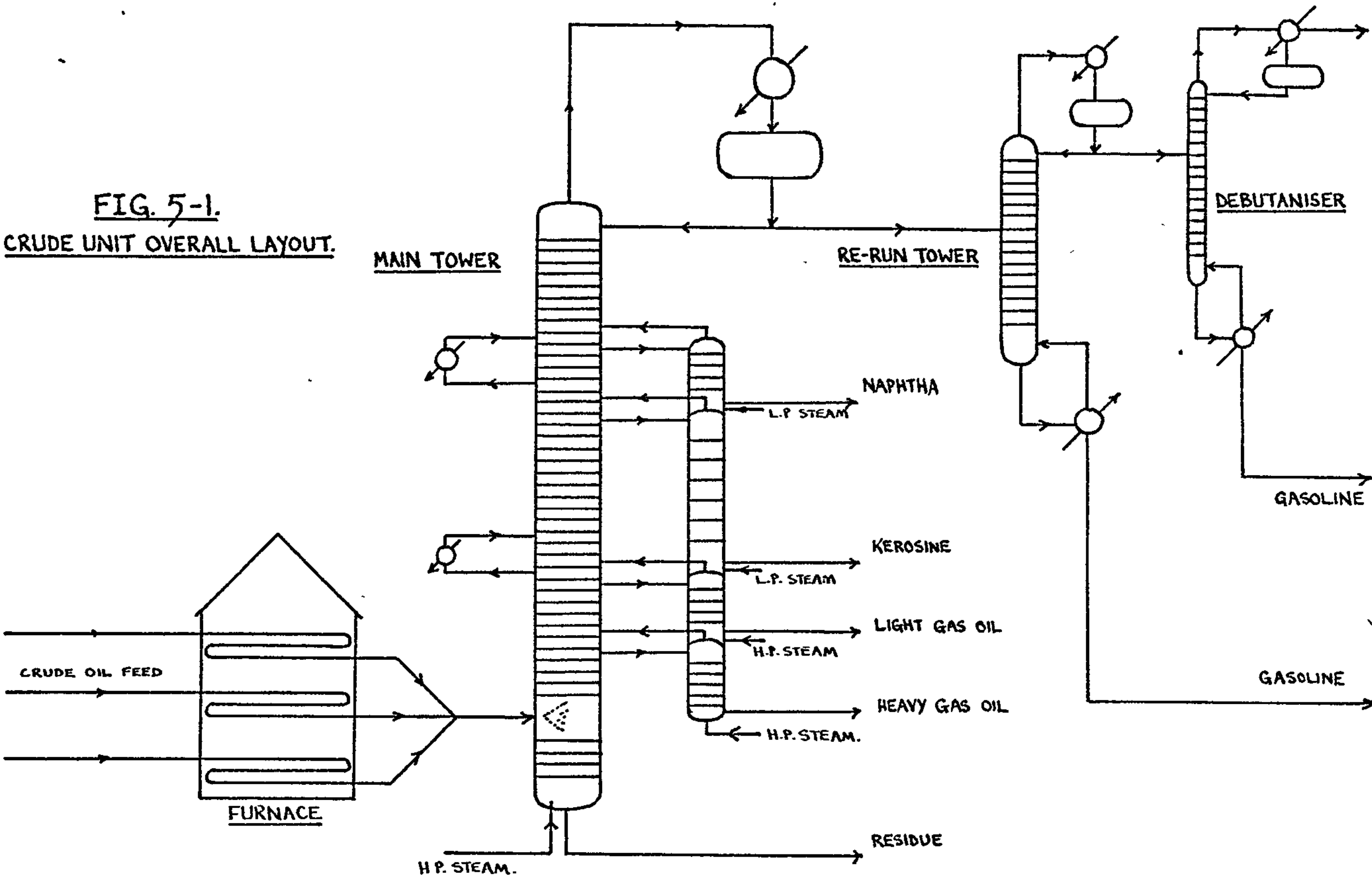
5.3 Description of the unit.

5.3.1 Overall layout.

A simplified flowsheet for the unit is given (Fig. 5-1). The crude enters the furnace in three passes, and is raised to a temperature of about 650°F. The three lines are then run together and the mixture of liquid and vapour is fed to the main column.

FIG. 5-1.

CRUDE UNIT OVERALL LAYOUT.



The overhead product from this is passed forward to the re-run tower. The sidestream products, which may include heavy naphtha, kerosine, light gas oil and heavy gas oil, are steam stripped before being passed to storage. The stripper vapours are returned to the main column. Reduced crude is pumped from the base of the main tower going forward to storage. The re-run tower makes a bottom product for straight-run gasoline blending and a top product for debutaniser feed. The debutaniser makes a fuel-gas overhead product and a bottoms for straight-run gasoline blending.

This project is solely concerned with the dynamics of the main tower, but it may be seen that any improvement in the main tower control during major changes in operating conditions should give a smoothly changing overhead product. The consequent improvement in the re-run and debutaniser tower feeds may be expected to improve the quality of control of these towers also.

5.3.2 The main tower and its operation.

The main tower has a straight length of 122 ft. and an internal diameter of 14 ft. 6 ins. It contains 44 plates, 40 in the rectification section and 4 in the bottoms' stripping section. Trays 1-4, and 37-40 are split flow bubble cap trays; trays 5-36 are split flow sieve plates; trays 41-44 are single pass bubble trays.

The feed enters the space below tray 40 - the flash zone - where some vaporisation occurs as the feed equilibrates at the column pressure. Vapour passes up through the rectification section and out of the column to the overhead condensers. Total condensation occurs and the liquid is passed to the overhead reflux drum. This has a capacity of 3560 gallons. A single pump is used to return part of this liquid to the main tower as overhead reflux and to pass part forward as re-run tower feed.

The sidestream products may be withdrawn as follows:-

heavy naphtha from tray 10

kerosine from tray 16

light gas oil from tray 30

heavy gas oil from tray 36

These products are steam stripped before being passed to storage. The heavy naphtha and kerosine are stripped with 50 psig saturated steam. The gas oils are stripped with superheated steam at a temperature of about 800°F. The strippers are mounted one above the other to form a single side tower.

It may be appreciated that if the system so far described were operated then very high liquid rates would occur in the top part of the tower, reducing at each offtake to low rates in the base of the rectification section. In order to produce a relatively uniform reflux ratio throughout heat is removed at two intermediate points. These 'pumparounds' remove liquid from one tray, pass it through a heat exchanger and return the cooled liquid a few trays higher up the column. In this way the reflux ratio above the pumparound is reduced, that below being unchanged. The unit used for this project had intermediate refluxes removing liquid from trays 13 and 29 and returning it to trays 10 and 27 respectively.

The liquid leaving the flash zone is joined by the liquid leaving the bottom of the rectification section (termed the 'true over-flash',) and passes across the four bubble plates in the base of the column. Light ends are stripped out with superheated steam, there being no reboiler on this type of unit.

The superheated steam serves two useful purposes. It strips out the light ends as mentioned above and also serves to reduce the partial pressure in and below the flash zone. This enables greater vaporisation to be achieved at a lower temperature, increasing the overflash. This permits lower pipestill outlet temperatures (PSO's) and increases the reflux ratio on the rectification section below the heavy gas oil take-off.

5.3.3 Main tower instrumentation.

The instrumentation on the experimental unit is more comprehensive than that normally associated with this type of unit insofar as temperature measurement is concerned. This was originally installed to facilitate experimental work. The main column was fitted with temperature indicators on the liquid and vapour streams listed in Fig.5-2. These were thermocouples wired into the main control room. The appropriate toggle switch is held to display the required temperature on the drum scale. It is possible to read this scale to 1^{o}F. Damping is rapid and reproducibility is better than $\frac{1}{2}^{o}$F. The absolute error on any reading was not known but was thought by BP instrument personnel to be small. These temperatures were regarded as adequate by BP for heat and mass balance purposes. These were carried out daily for this unit.

All main external flows and the tower top pressure are recorded in the control room on Swartout chart recorders. The PSO's are also recorded but the readings differed considerably from the thermocouple indications mentioned above. The latter were reputedly the more reliable and the plant operators only used the chart recorders for noting trends or keeping watch for sudden upsets.

There are no major feedback control loops on the unit. The side-stream product offtake rates from the strippers are controlled from the control room by set point adjustment of the two-term controllers. Some offset is normally evident. The products run from the main tower to the strippers under stripper base level control. The tower top temperature is used to control the tower top reflux rate. The overhead product flow is then adjusted by the operator to maintain a constant level in the overhead reflux drum. The intermediate reflux rates are controlled by manual setpoint adjustment. The PSO's provide furnace fuel rate control. The reduced crude runs from the base of the tower under tower-base level control. Tower top pressure is controlled by a bleed from the overhead vapour line to the reflux drum, bypassing the overhead condensers. On-line analysers are fitted but serve no servo-control function. These give naphtha and kerosine 10% and 90% ASTM distillation points and the residue viscosity.

Ref. No.	Variable
-	Raw data
T18	Temperature of liquid in crude tower bottom
T19	Heavy gas oil draw-off temperature ex-tower
T20	Light gas oil draw-off temperature ex-tower
T21	Kerosine draw-off temperature ex-tower
T23	Upper intermediate reflux draw-off temperature
T24	Lower intermediate reflux draw-o ff temperature
T25	Lower intermediate reflux return temperature
T26	Upper intermediate reflux return temperature
T27	Overhead reflux return temperature
T46	Crude oil feed to tower - stream A temperature
T47	Crude oil feed to tower - stream B temperature
T48	Crude oil feed to tower - stream C temperature
T49	Temperature of vapour below tray 40
T50	Temperature of overhead vapour to condensers
T71	Superheated steam exit temperature - stream A
T72	Superheated steam exit temperature - stream B
TA1	Tray 2 liquid temperature
TA2	Tray 9 liquid temperature
TA3	Tray 11 vapour temperature
TA4	Tray 11 liquid temperature
TA5	Tray 13 liquid temperature
TA6	Tray 17 liquid temperature

Ref. No.	Variable
TA7	Tray 19 liquid temperature
TA8	Tray 28 vapour temperature
TA9	Tray 28 liquid temperature
TA10	Tray 30 liquid temperature
TA11	Tray 31 liquid temperature
TA12	Tray 37 liquid temperature
TA13	Tray 41 liquid temperature
TA14	Tray 42 liquid temperature
TA17	Temperature vapour ex-kerosine stripper
TA18	Temperature liquid ex-kerosine stripper
TA19	Temperature vapour ex-light gas oil stripper
TA20	Temperature vapour ex-heavy gas oil stripper

Fig. 5-2

Temperature Indicators on CDU3

5.4 Experimental runs.

Five experimental runs were carried out on CDU3 involving one or more planned changes in liquid flowrates. In addition data was recorded for four 'observation runs'. These results gave data describing the common operations of crude oil feedstock changes and activity changes. The runs are listed in Figs.5-3 and 5-4.

EXPERIMENTAL RUNS

Run No.	Date	Crude	% Change	Type of change
TR1	18-6-68	Crude oil A	+8%	Reflux - step
TR2	17-9-68	Crude oil B	+12%	Reflux - step
TR3	21-5-69	Crude oil C	-14%	Reflux - step
TR4	2-7-69	Crude oil D	-10%	Light gas oil withdrawal - step
TR5	5-9-69	Crude oil B	-11%	Pre-planned change - reflux step followed by ramp.

Fig. 5-3

OBSERVATION RUNS

Run No.	Date	Crude	Operation
OB1	21-5-69	Crude oil C	Crude change to Crude oil A
OB2	3-9-69	Crude oil C	Crude change to Crude oil B
OB3	3-9-69	Crude oil B	Activity change.
OB4	4-9-69	Crude oil D	Crude change to Crude oil B

Fig. 5-4

5.4.1 Step change experiments on the overhead reflux - A comparison of runs TR1, TR2 and TR3.

Three experiments were performed to determine the response of the unit to a step change in the flowrate of the overhead reflux return. The first two runs permitted the development of experimental expertise. It was hoped that these would also provide a replication that would increase confidence in the reliability of the results.

The general pattern evolved for performing this type of experiment was first to set the unit on steady state operation for a period of four hours to note random variations and to check that the unit was truly steady. Then the step change would be injected and the column variables logged by hand for four to six hours. The step change in the overhead reflux rate was achieved by first disconnecting the tower top temperature controller so that the top reflux was on flow control only. The reflux controller set point was then stepped down. Frequent adjustment of this setpoint to maintain the indicated flow constant was essential.

All the temperature indicators for the distillation trays and the relevant external streams were monitored. All the external liquid flowrates were monitored. It was found that one person could read and note all the necessary temperatures and flows in three minutes. A higher frequency on the rapidly changing variables immediately following a change was achieved by recording only a representative selection of the available temperatures for short periods. Once the initial thirty minutes after a step change had elapsed, it proved adequate to monitor all variables every ten minutes.

Samples of the overhead and sidestream products were withdrawn during all three tests. Initially these were taken every ten minutes, the interval widening to twenty or thirty minutes as the test progressed.

Sample results from each test are presented in Figs. 5-5, 5-6 and 5-7. Fig. 5-5 gives the response of the temperature of the overhead vapour to the condensers for each test run. The vertical axes have been adjusted so that the initial 'steady state' values prior to each test coincide. The time scale has as zero the point at which the step change was injected.

The results from experimental runs TR1 and TR2 do not yield much useful information. As has been mentioned, these runs were primarily for the purpose of acquiring a suitable experimental technique rather than obtaining accurate results. The results from TR2 in particular are difficult to separate from normal process noise. However, the early runs do supply some support for the validity of the results of the third run, TR3.

The first point to emerge from TR1 and TR2 was that as large a change as possible was essential if the adequate separation of the response from process noise was to be achieved. The second feature of the results is the general pattern for most of the

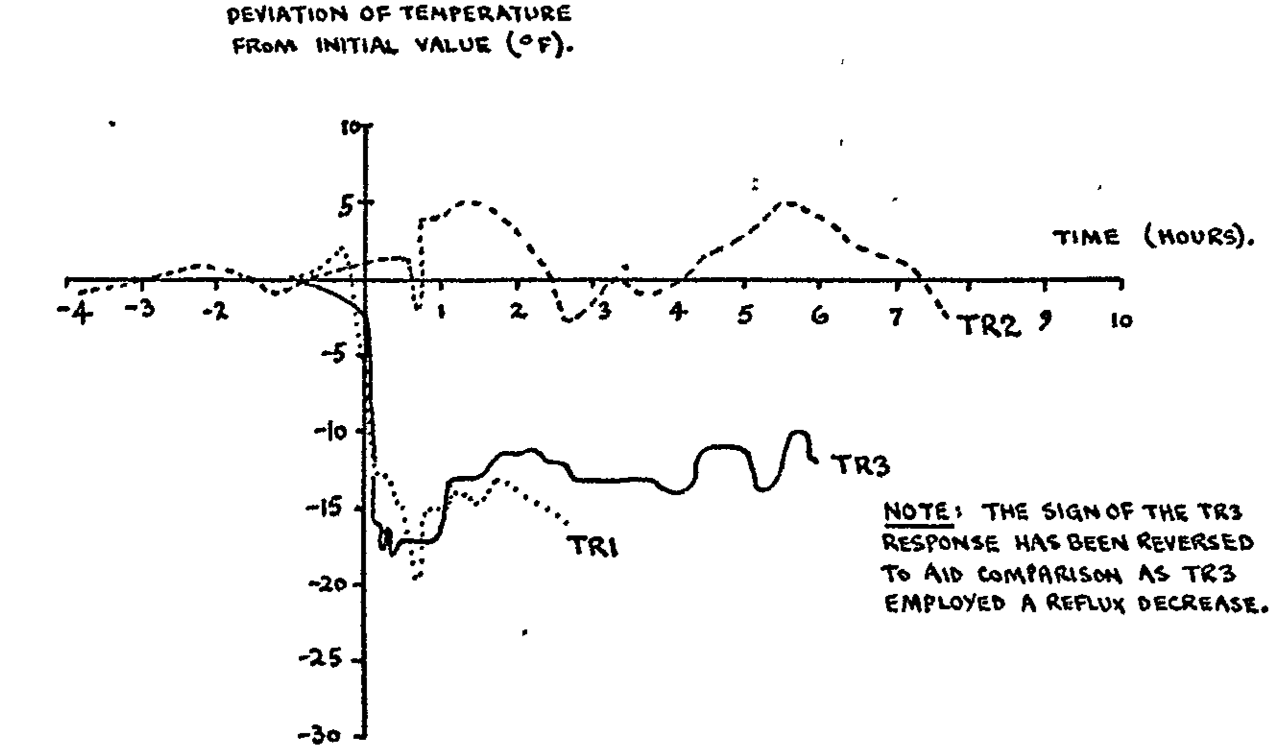


FIG. 5-5.

RESPONSE OF OVERHEAD VAPOUR TEMPERATURE FOR EXPERIMENTS TR1, TR2 AND TR3.

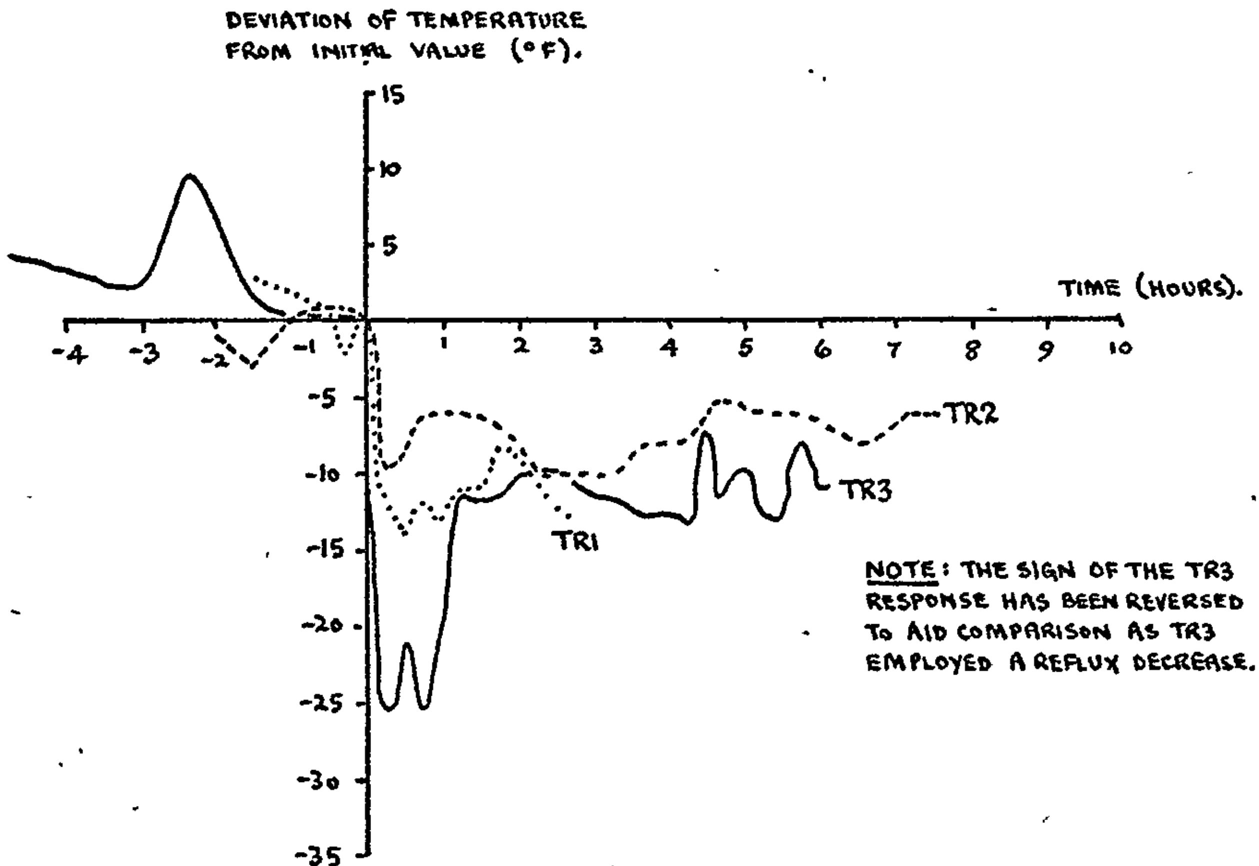


FIG. 5-6.

RESPONSE OF KEROSINE OFFTAKE TEMPERATURE FOR EXPERIMENTS TR1, TR2 AND TR3.

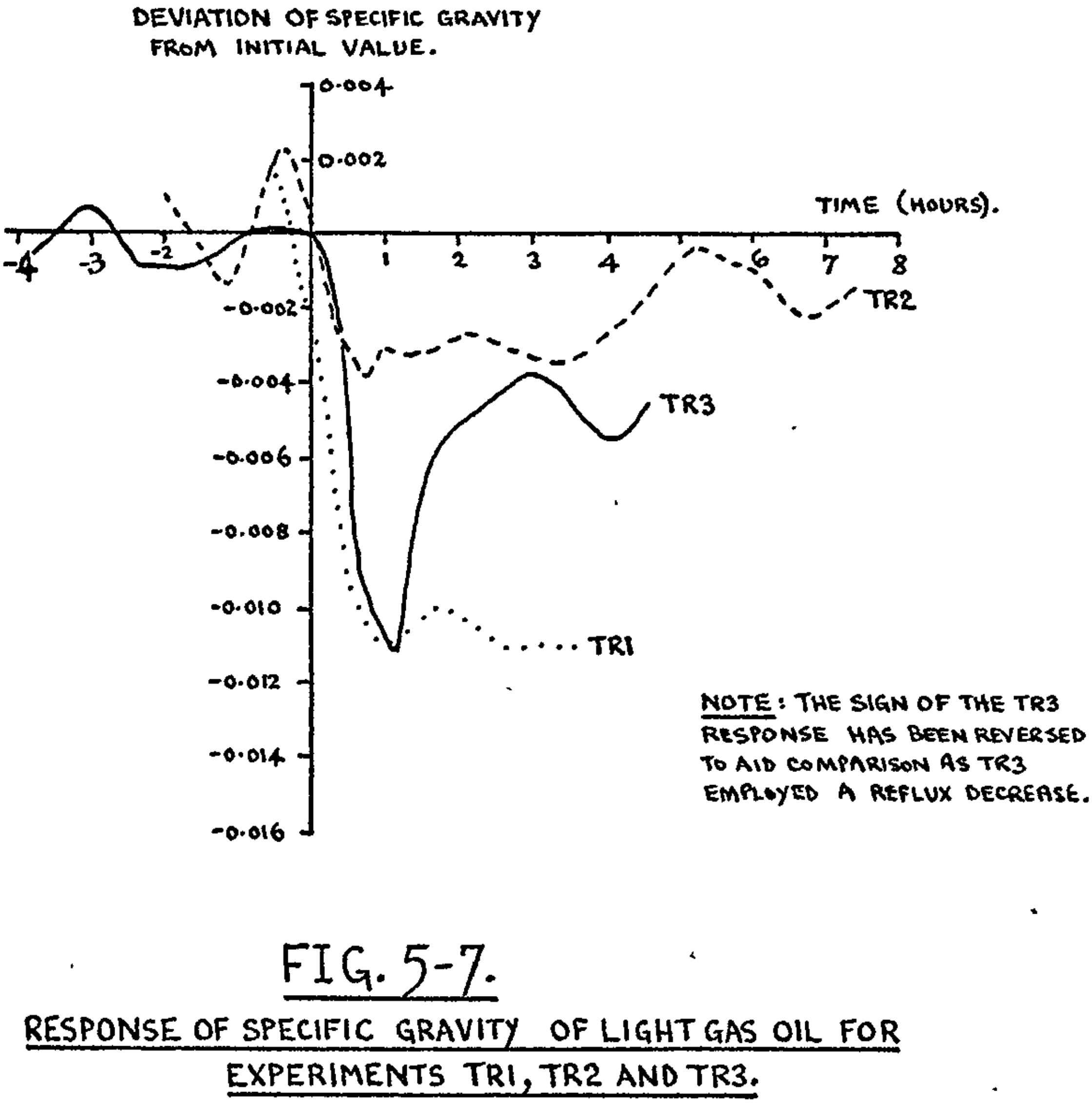


FIG. 5-7.

RESPONSE OF SPECIFIC GRAVITY OF LIGHT GAS OIL FOR EXPERIMENTS TR1, TR2 AND TR3.

response curves. Seven of the nine responses shown exhibit a rapid rise to a maximum. This is held for varying lengths of time before the variables settle out around steady state values intermediate between the initial steady state and the maximum. The two curves that are different are the response of the overhead vapour temperature in TR2 and the light gas oil gravity in TR1.

Examination of the 'peaks' on these response curves reveals no real correlation between those for the overhead vapour temperature. The kerosine offtake temperature responses exhibit peaks held for the following periods :-

TR1	0.25 - 1.05 hrs.
TR2	0.10 - 0.60 hrs.
TR3	0.10 - 1.00 hrs.

The light gas oil gravity curves, perhaps because of the lower sampling frequency, exhibit sharper peaks. Peaks occur at the following times :-

TR1	1.0 hrs.
TR2	0.7 hrs.
TR3	1.15 hrs.

Thus it may be concluded that broad agreement exists between the three experimental results for these last two responses. Together with the general characteristic shape of most of the curves mentioned earlier it was felt that the two initial runs provided general support for the validity of the interesting curves obtained in TR3. These are described in more detail in the next section.

<u>5.4.2 Step change experiment on the overhead reflux - Run TR3.</u>

a) <u>Method</u> The unit was operated in accordance with the normal procedure. The unit was running a feed of Crude oil C, making overheads, kerosine, light and heavy gas oil and residue. The column was under observation from 0900 hrs 21-5-69. Careful steady state operation was being maintained to comply with a BP test run. The metered feed and product flows, the thermocouple and pressure gauge readings were recorded at approximately forty minute intervals. Samples of the stripped sidestream products and the overheads and residue were also taken at forty minute intervals. The step decrease was made at 1400 hrs so that steady state had been observed for five hours. The decrease in reflux was -14% of the overhead reflux flow. Immediately after the step all charts and thermocouples were read and samples taken. Sampling was continued at ten minute intervals. The main thermocouples were read every three minutes and the chart readings and the auxiliary thermocouples were monitored every ten minutes. Readings were continued until 2015 hrs.

b) <u>Constancy of the primary and secondary forcing functions.</u>

The <u>crude oil feedrate</u> meters indicated mean value $\pm.2$ %. The mean crude feed temperature was 649 $\pm 2^{\circ}$F, from the thermocouples in each feed pass. (Figs. 5-8 and 5-9).

The <u>overhead reflux flow</u> prior to 1400 hrs was maintained at a constant flowrate. At 1400 hrs the flow was dropped steeply to 86% of its original value. Oscillations between 86% and 90% occurred over the next hour after which the step decrease of -14% was held steadily. . Pressure fluctuations at the top of the column during the early part of the response together with the extreme sensitivity of the flow to small set point adjustments made this vital flow one of the most difficult to control. (Fig. 5-10).

FIG. 5-8.

CRUDE OIL FEEDRATE - RUN TR3.

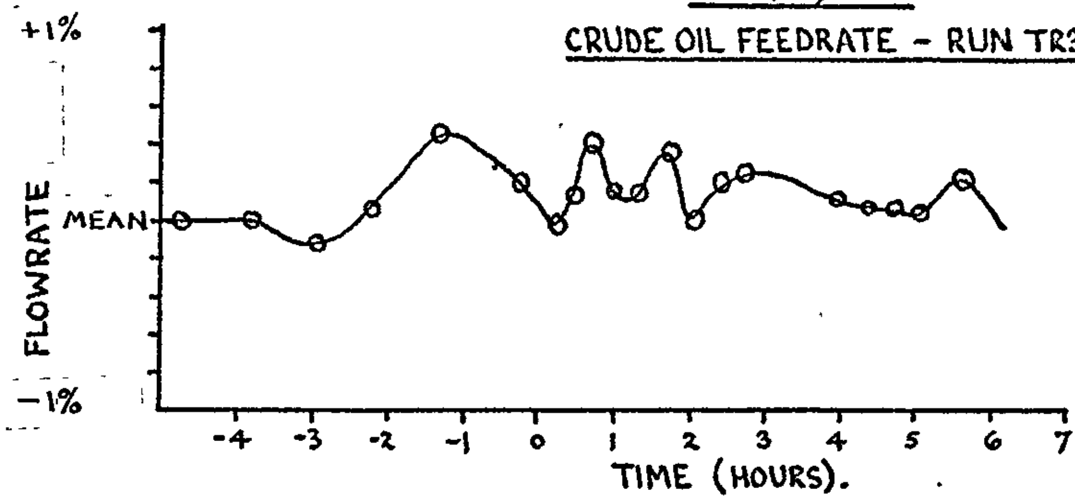


FIG. 5-9.

CRUDE OIL FEED TEMPERATURE - RUN TR3.

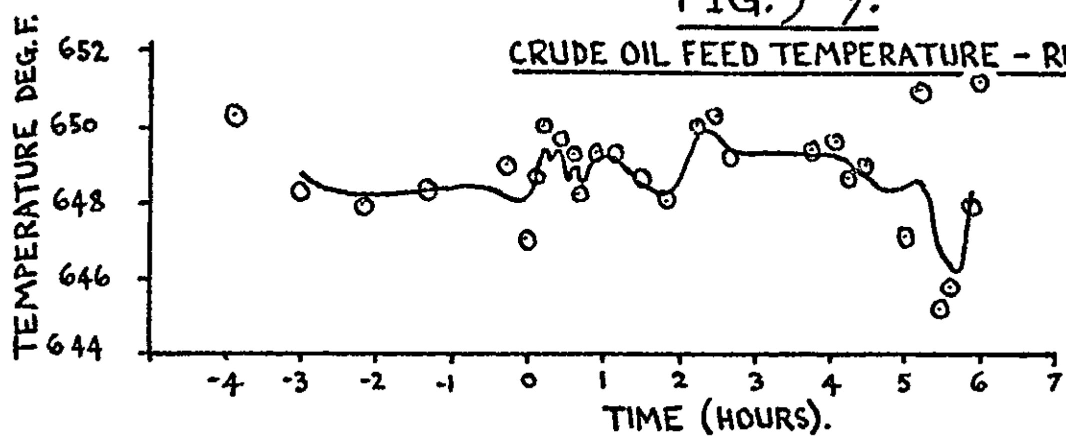
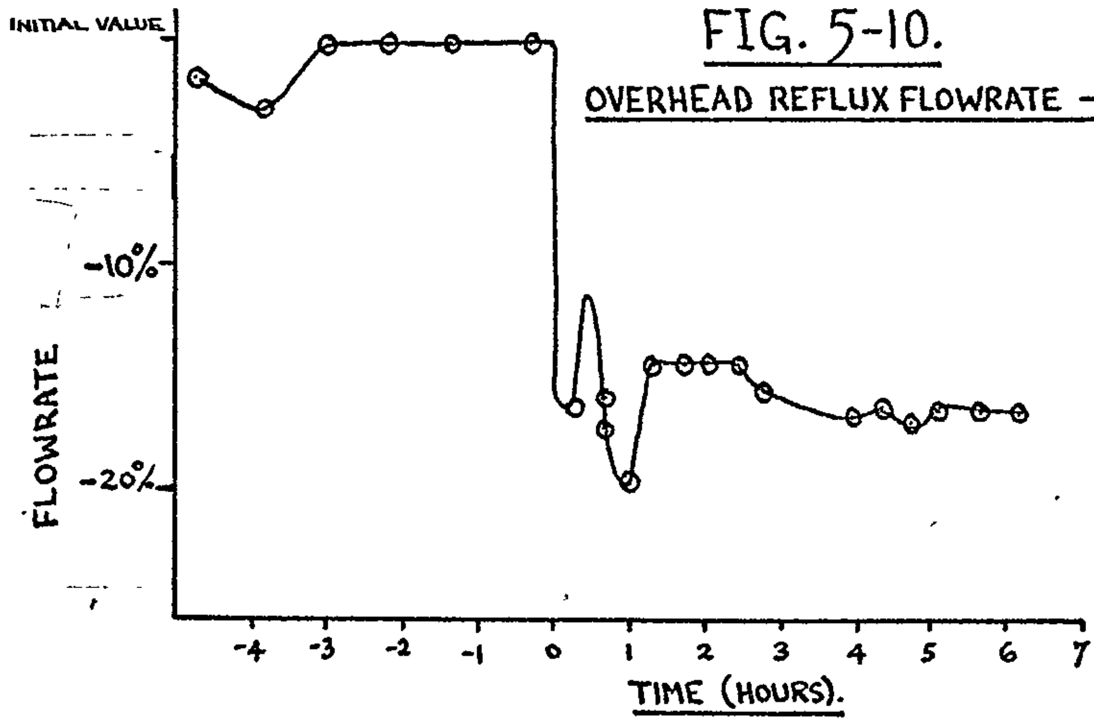


FIG. 5-10.

OVERHEAD REFLUX FLOWRATE - RUN TR3.



The overhead reflux return temperature was maintained steady at 106 $\pm1^{\circ}$F prior to the test. Over the first half hour after the step change the temperature rose to 109°F. This value was held for a half hour before falling again to 106°F over the next hour. (Fig. 5-11).

The upper intermediate reflux flow was maintained at 34250 gph prior to the step change but eased up to 34500 gph one hour after the step decrease. The return temperature rose rapidly by 3°F approximately six minutes after the step. This new value was held for 1¼ hours after which the temperature slowly moved down to 1°F above its initial value. (Figs. 5-12 and 5-13).

The lower intermediate reflux was maintained steady at 28150 gph throughout. The return temperature, initially 306°F rose to 316°F over the fifty minutes following the step. This value was held for 10 minutes and was followed by a fall over thirty minutes to 310°F. (Figs. 5-14 and 5-15).

The crude tower top pressure was better controlled in this test than in previous runs. It was mostly held at 26 psig but a drop to 25 psig immediately after the step was experienced, followed by an over correction to 26.5 psig. (Fig. 5-16).

The kerosine product withdrawal rate was generally held steady with the minor exception of short drops of 3% occurring one hour and three hours after the step. (Fig. 5-17).

The light gas oil product withdrawal rate was maintained within ±1% throughout. (Fig. 5-18).

The heavy gas oil product withdrawal rate was maintained within ± 1% throughout. (Fig. 5-19).

The returning vapour from the kerosine stripper rose to a peak fifteen minutes after the step and maintained this for about

FIG. 5-11.

OVERHEAD REFLUX TEMPERATURE - RUN TR3.

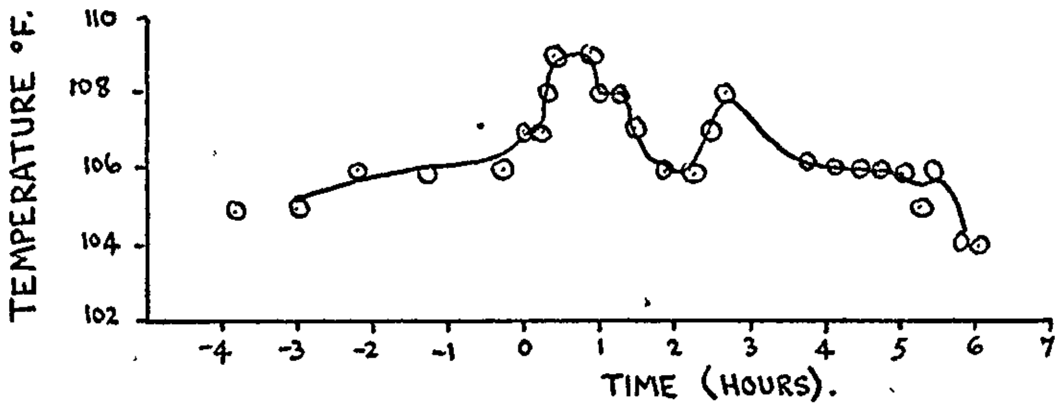


FIG. 5-12.

UPPER INTERMEDIATE REFLUX FLOWRATE - RUN TR3.

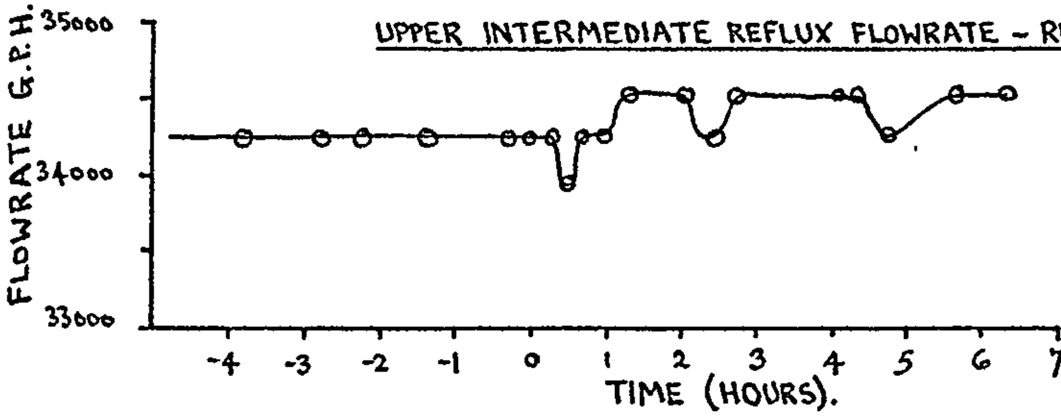


FIG. 5-13.

LOWER INTERMEDIATE REFLUX FLOWRATE - RUN TR3.

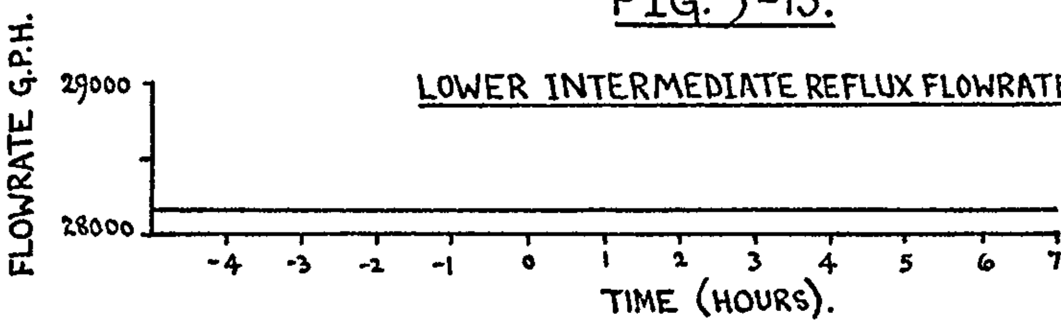


FIG. 5-14.

UPPER INTERMEDIATE REFLUX RETURN TEMPERATURE - RUN TR3.

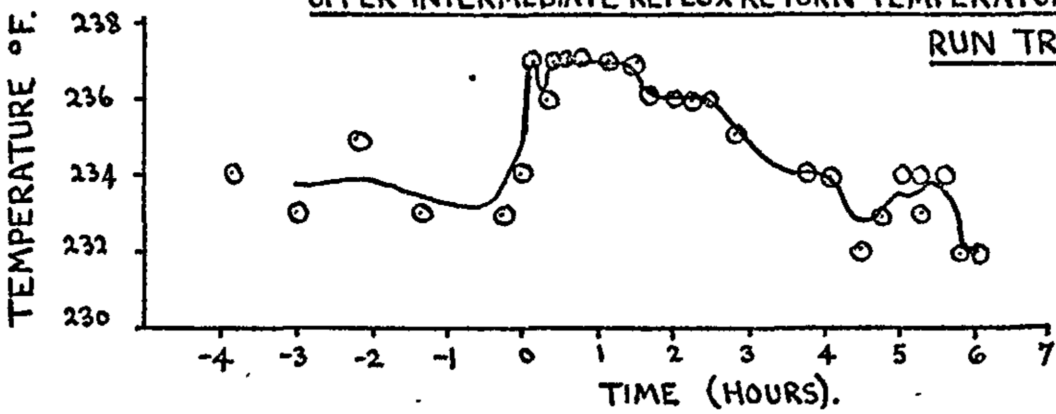


FIG. 5-15.

LOWER INTERMEDIATE REFLUX RETURN TEMPERATURE - RUN TR3.

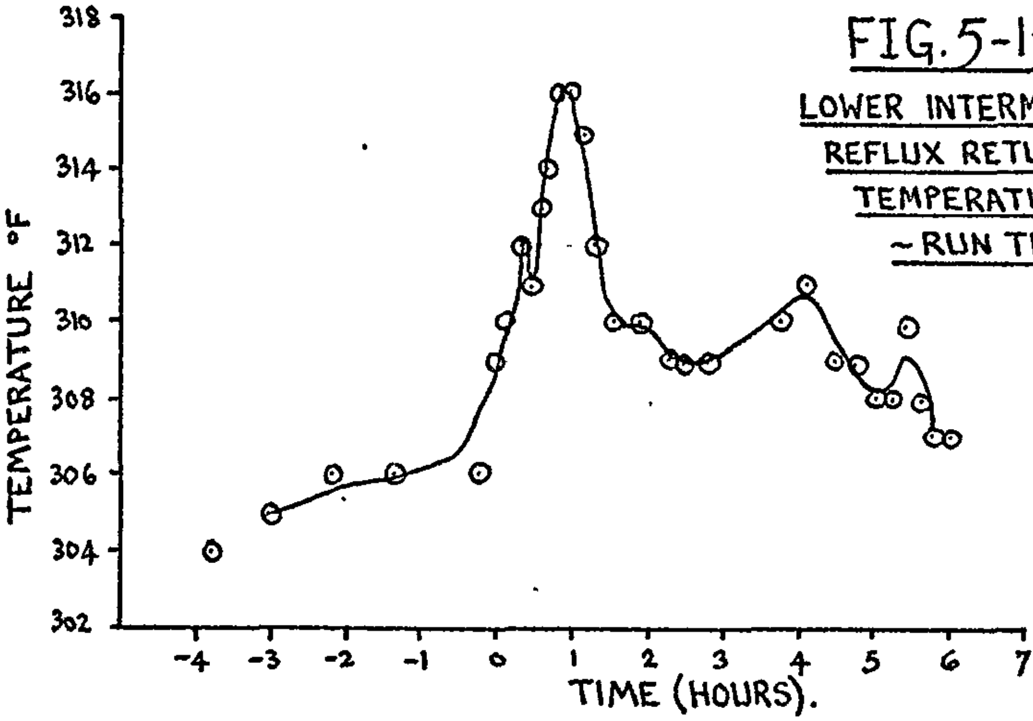


FIG. 5-16.

TOWER TOP PRESSURE - RUN TR3.

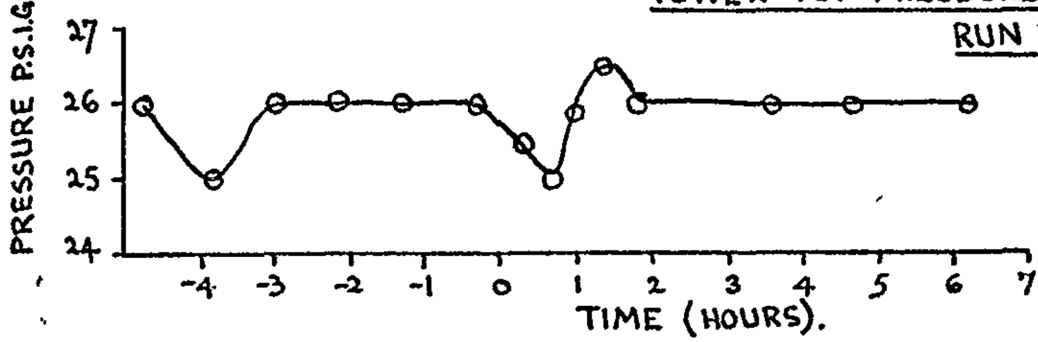


FIG. 5-17.

KEROSINE PRODUCT FLOWRATE - RUN TR3.

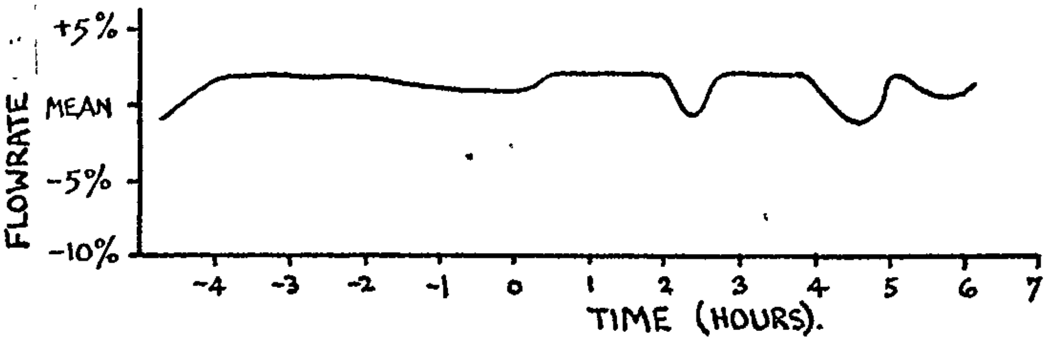


FIG. 5-18.

LIGHT GAS OIL PRODUCT FLOWRATE - RUN TR3.

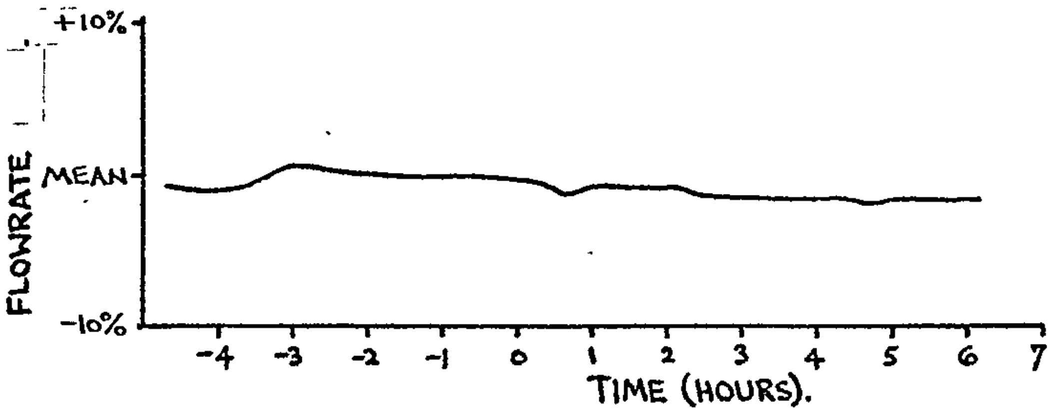
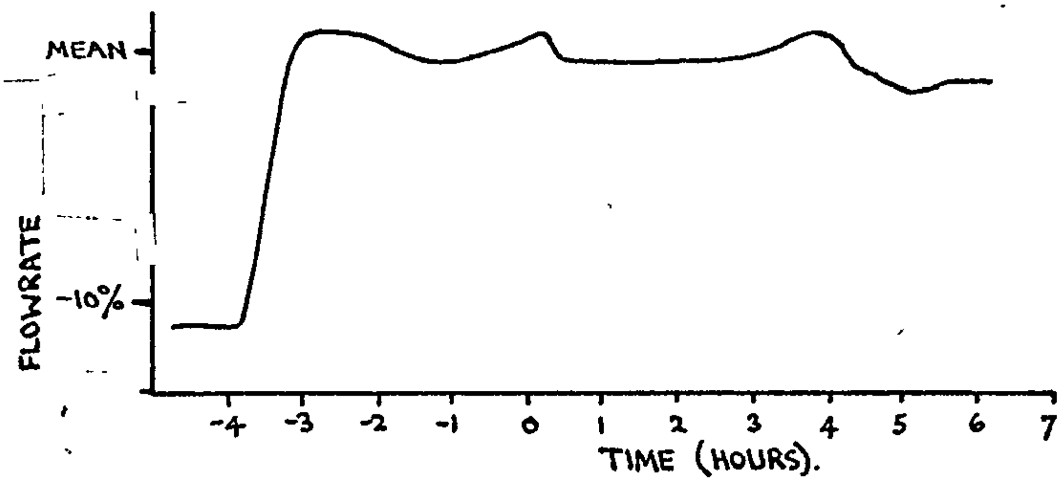


FIG. 5-19.

HEAVY GAS OIL PRODUCT FLOWRATE - RUN TR3.



thirty minutes before dropping 15°F back to a final equilibrium value. (Fig. 5-20).

The <u>returning vapour from the light gas oil stripper</u> achieved a peak forty minutes after the step but fell back 12°F over the next forty minutes to a final equilibrium value. (Fig. 5-21).

The <u>returning vapour from the heavy gas oil stripper</u> behaved in a similar manner to that from the light gas oil stripper. (Fig. 5-22).

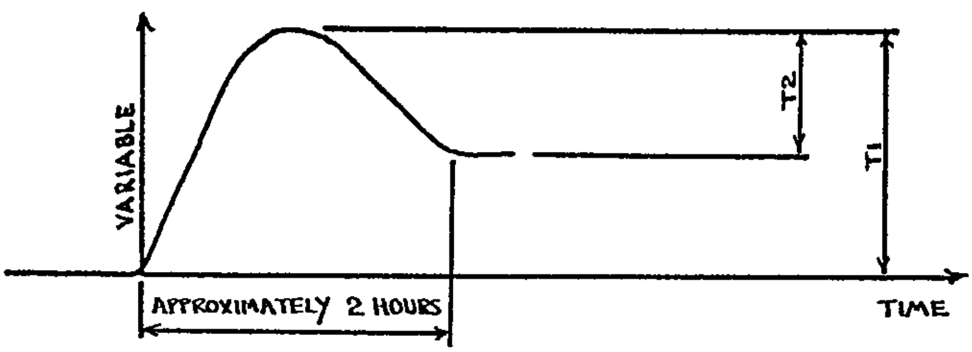
c) <u>The responses of the tray temperatures and the product properties.</u>

These are shown in Figs. 5-23 to 5-40. The results are smoothed to bring out the major response, the unsmoothed set of points X being related to the smoothed set of points Y by :-

$$Y_{N+1} = \tfrac{1}{4}X_N + \tfrac{1}{2}X_{N+1} + \tfrac{1}{4}X_{N+2}$$

The solid lines shown on the graphs are drawn through the points Y and the points X, the raw data, are shown thus o.

Examination of the tray temperature responses and product gravity curves reveals a similar shape as far as the rectification section is concerned as shown in Fig. 5-41.



<u>Fig. 5-41</u>

An analysis of the temperature responses may be carried out. In the table, Fig. 5-42, T1 is the temperature difference between

FIG. 5-20.

TEMPERATURE OF VAPOUR EX-KEROSINE STRIPPER - RUN TR3.

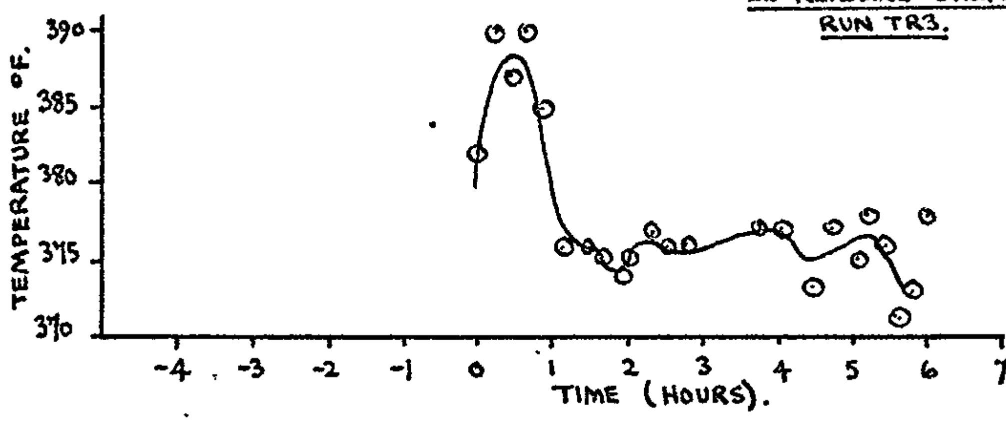


FIG. 5-21.

TEMPERATURE OF VAPOUR EX-LIGHT GAS OIL STRIPPER - RUN TR3.

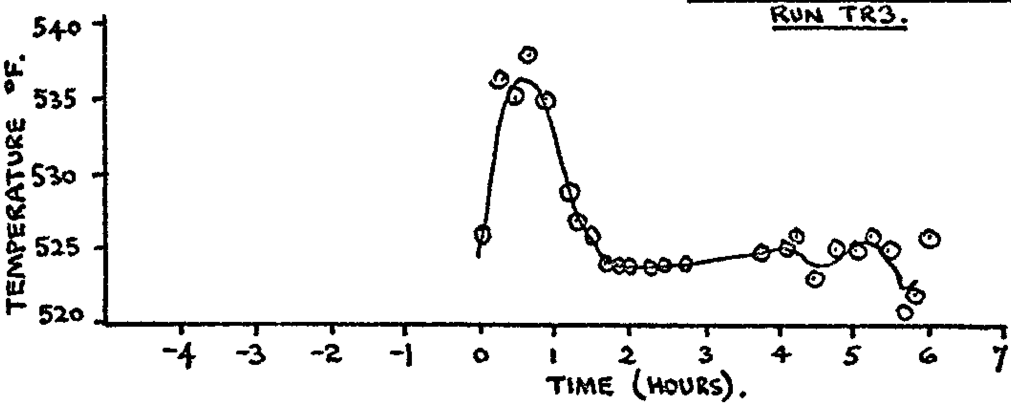


FIG. 5-22.

TEMPERATURE OF VAPOUR EX-HEAVY GAS OIL STRIPPER - RUN TR3.

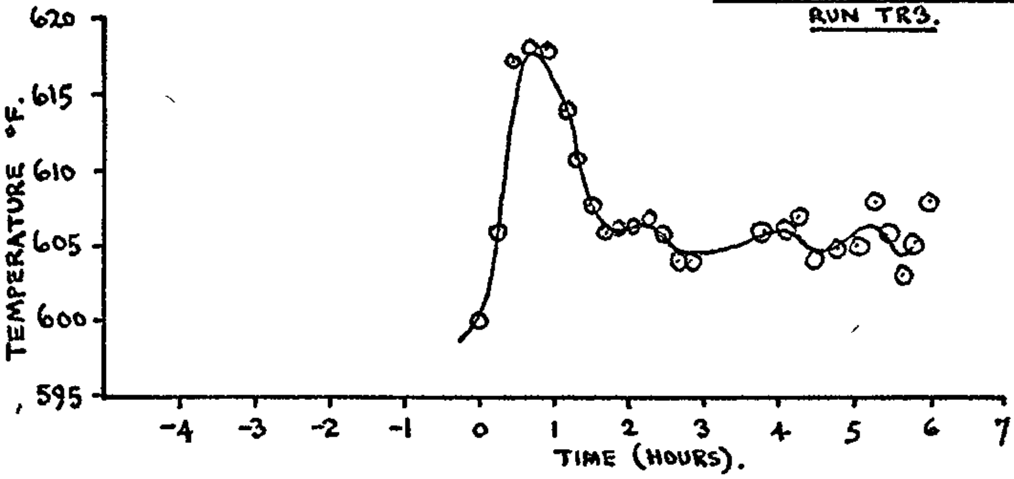


FIG. 5-23.

OVERHEAD VAPOUR TEMPERATURE - RUN TR3.

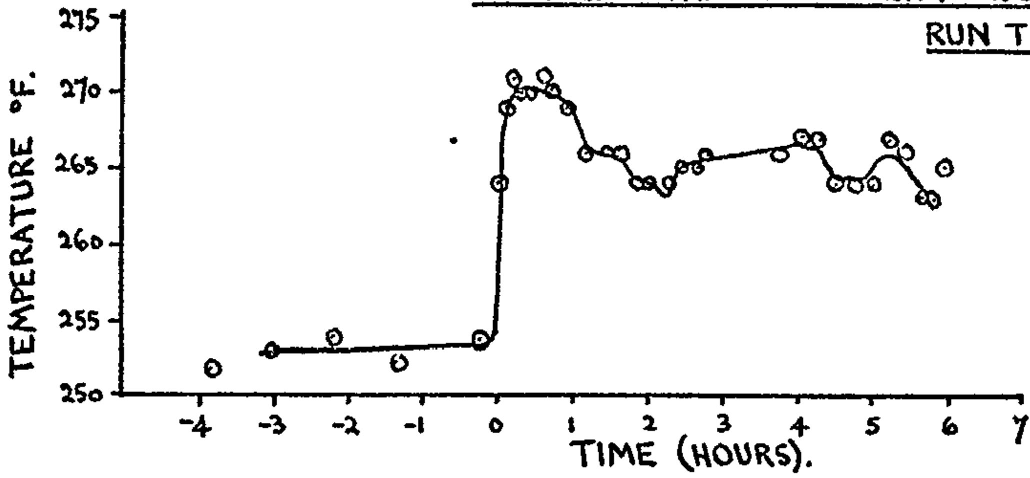


FIG. 5-24.

UPPER INTERMEDIATE REFLUX DRAW OFF TEMPERATURE (EX-TRAY 12) - RUN TR3.

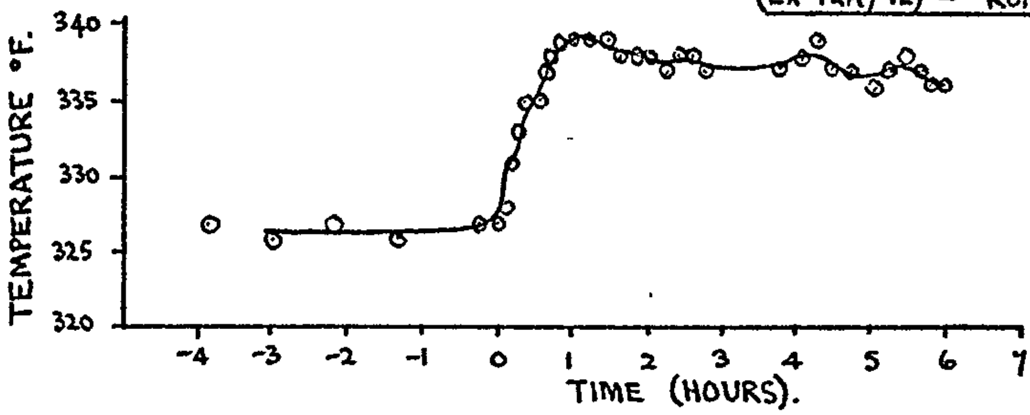


FIG. 5-25.

KEROSINE DRAW OFF TEMPERATURE (EX-TRAY 16) - RUN TR3.

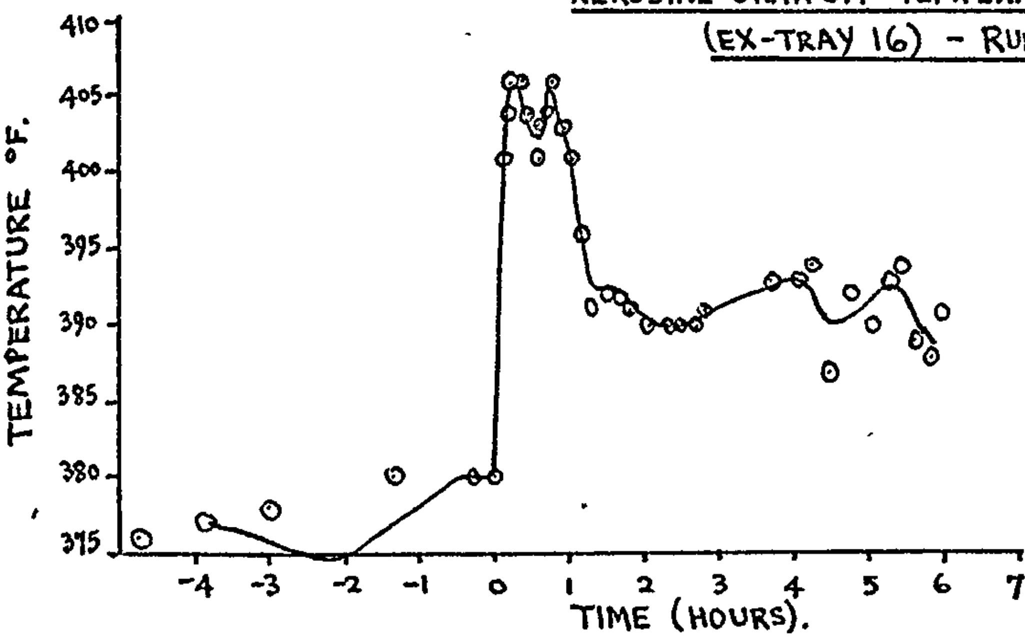


FIG. 5-26.

LOWER INTERMEDIATE REFLUX DRAW OFF TEMPERATURE (EX-TRAY 29) - RUN TR3.

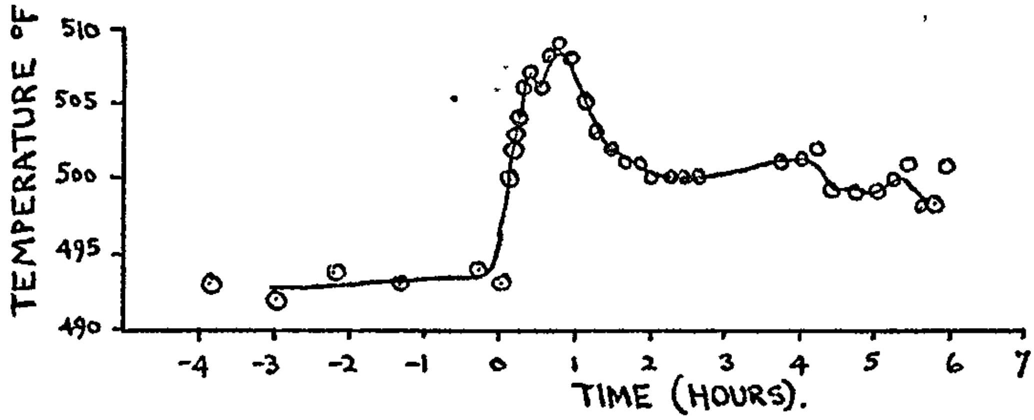


FIG. 5-27.

LIGHT GAS OIL DRAW OFF TEMPERATURE (EX-TRAY 30)-RUN TR3.

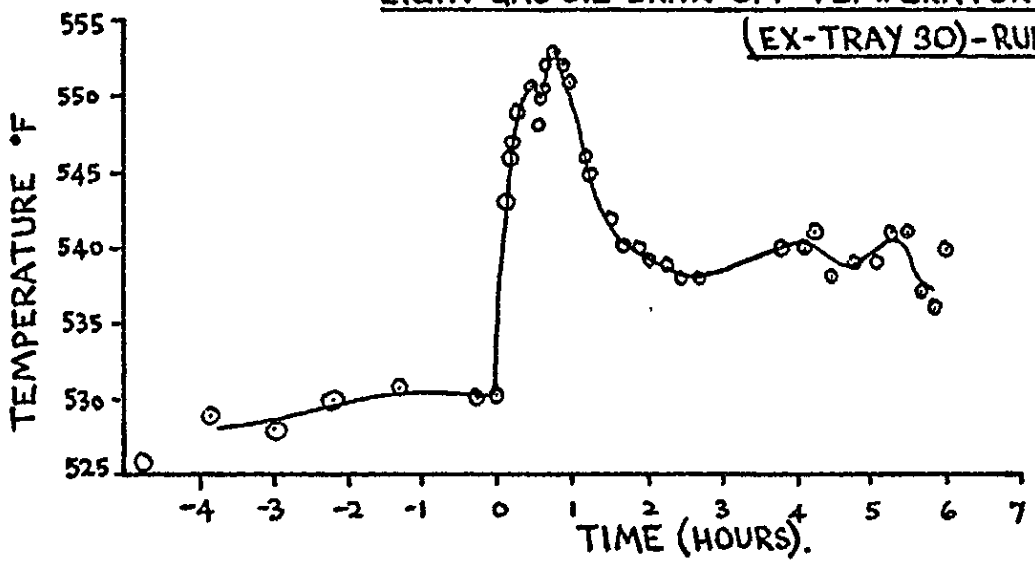


FIG. 5-28

HEAVY GAS OIL DRAW OFF TEMPERATURE (EX-TRAY 36)- RUN TR3.

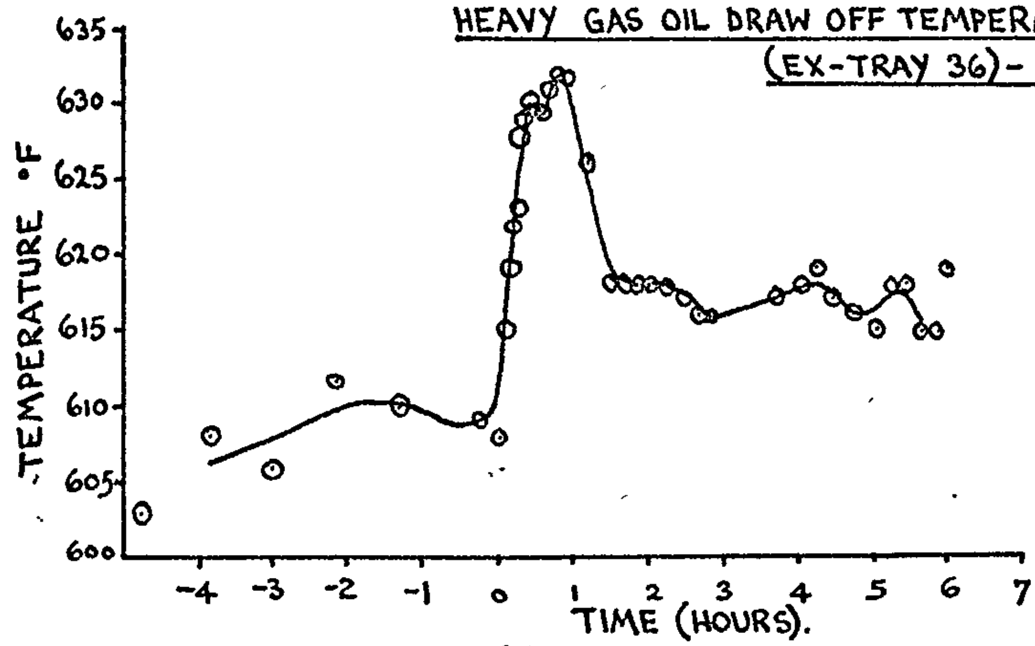


FIG. 5-29.

TEMPERATURE OF VAPOUR BELOW TRAY 40. RUN TR3.

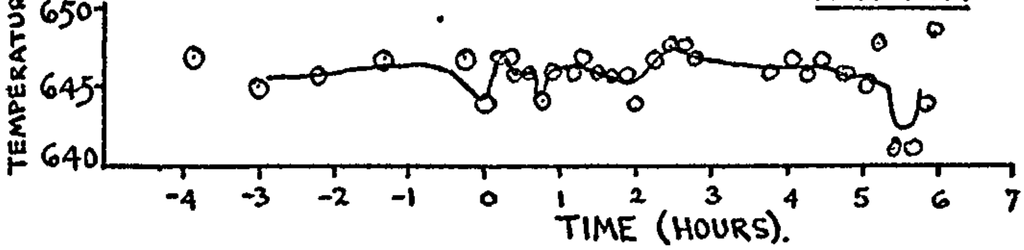


FIG. 5-30.

TEMPERATURE OF LIQUID IN TOWER BASE - RUN TR3.

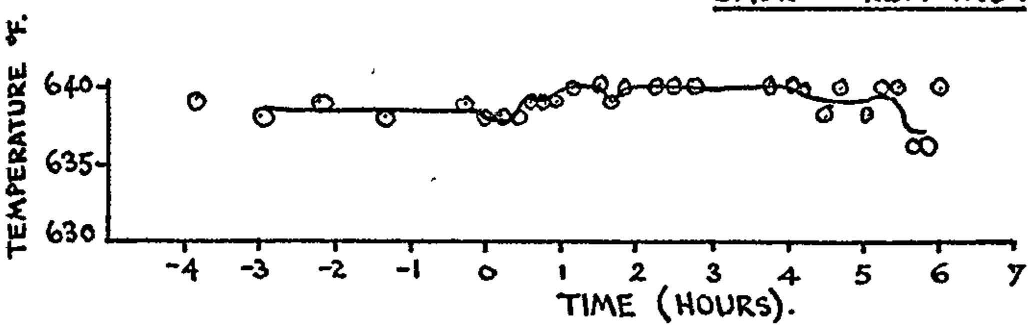


FIG. 5-31.

SPECIFIC GRAVITY OF OVERHEAD PRODUCT AT 60°F - RUN TR3.

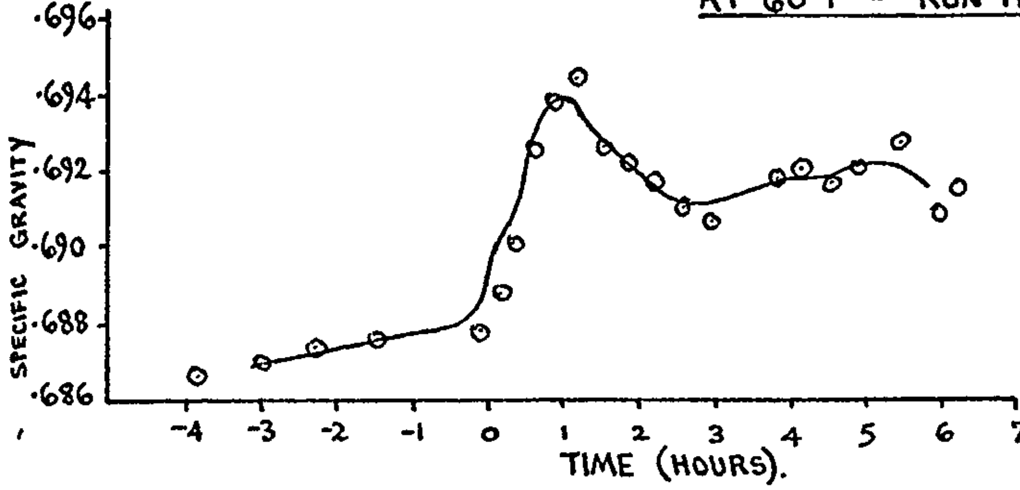


FIG. 5-32.

SPECIFIC GRAVITY OF KEROSINE PRODUCT - RUN TR3.

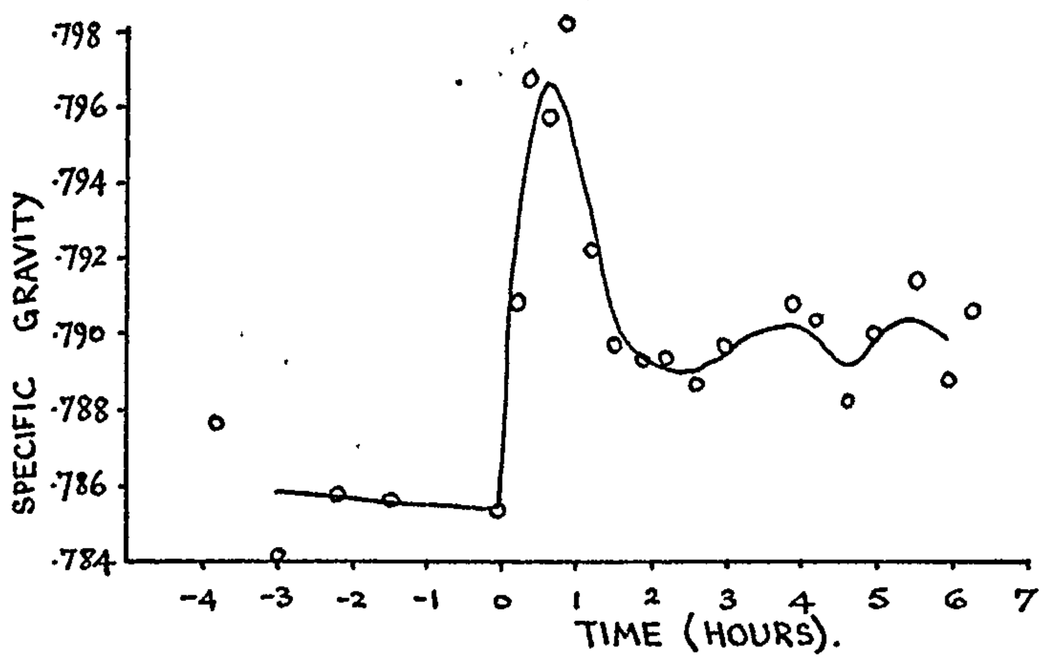


FIG. 5-33.

SPECIFIC GRAVITY OF LIGHT GAS OIL PRODUCT - RUN TR3.

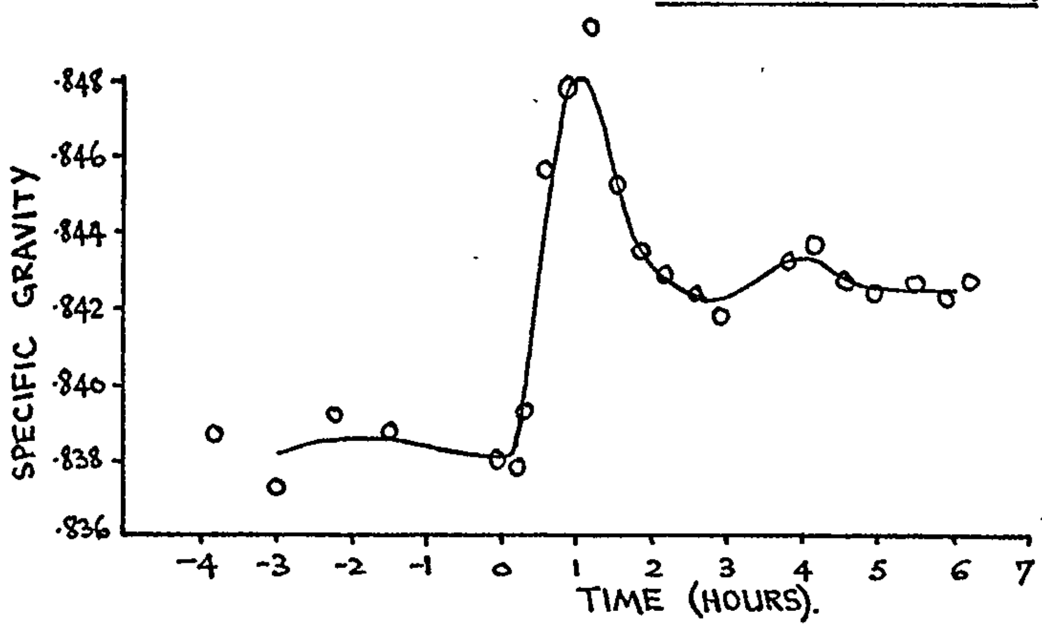


FIG. 5-34.

SPECIFIC GRAVITY OF HEAVY GAS OIL PRODUCT - RUN TR3.

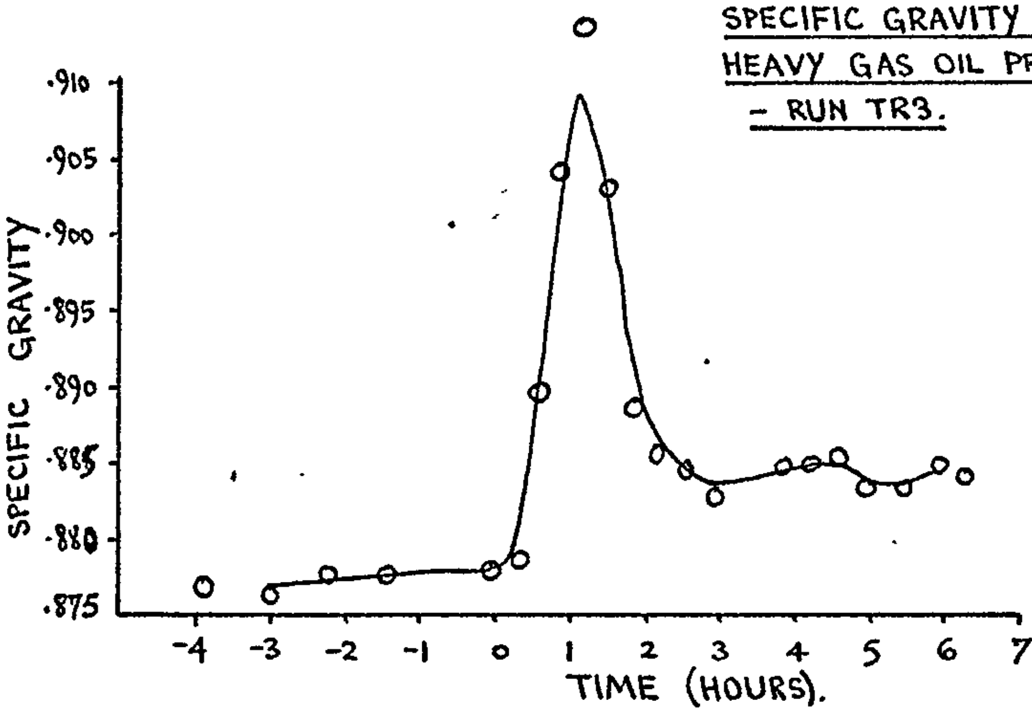


FIG. 5-35.

SPECIFIC GRAVITY OF RESIDUE (BOTTOM PRODUCT) - RUN TR3.

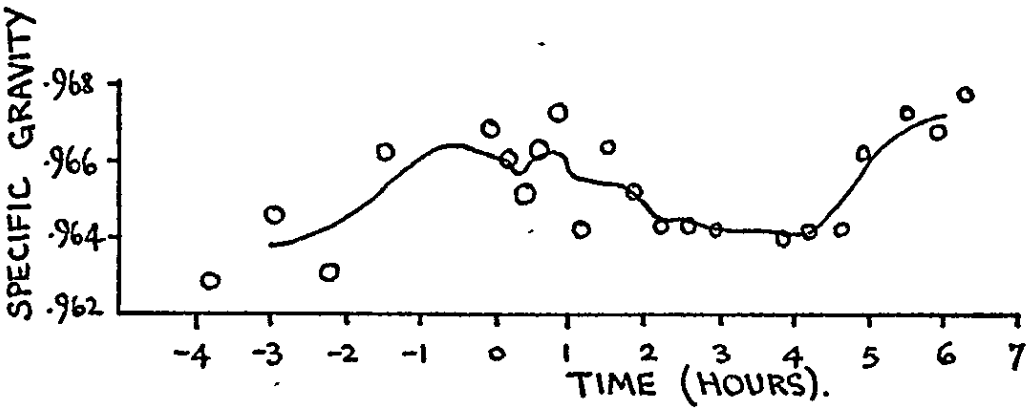


FIG. 5-36.

ASTM DISTILLATION 10% POINT FOR KEROSINE PRODUCT - RUN TR3.

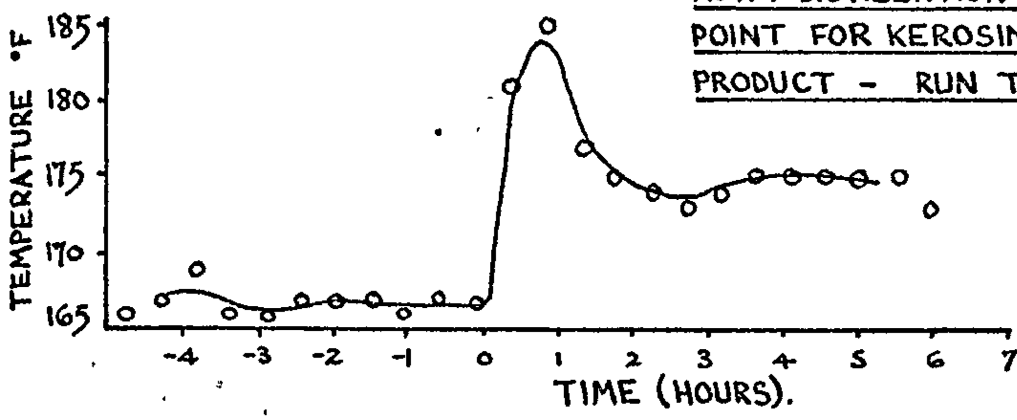


FIG. 5-37.

ASTM DISTILLATION 90% POINT FOR KEROSINE PRODUCT - RUN TR3.

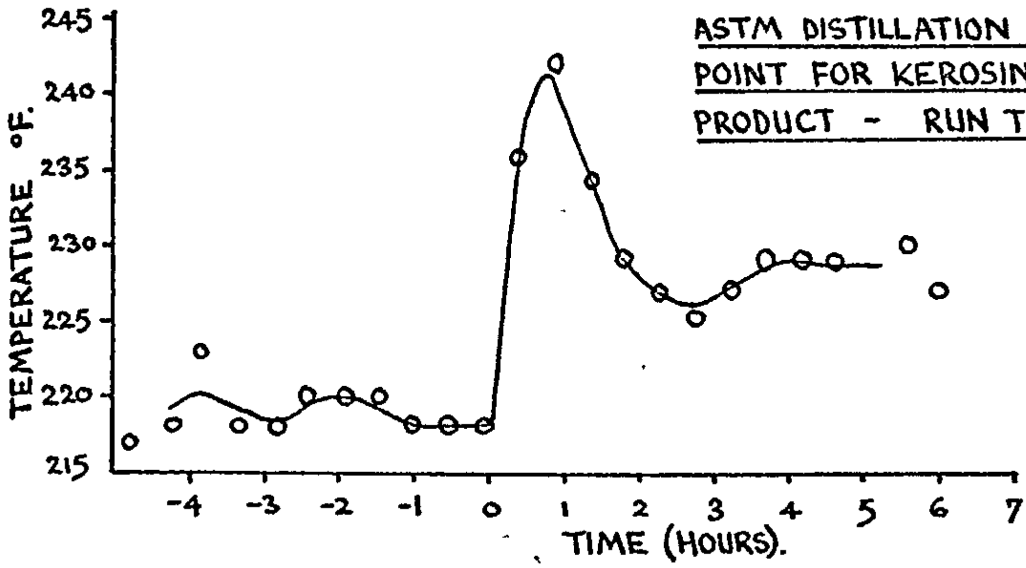


FIG. 5-38.

KEROSINE PRODUCT CLOUD POINT - RUN TR3.

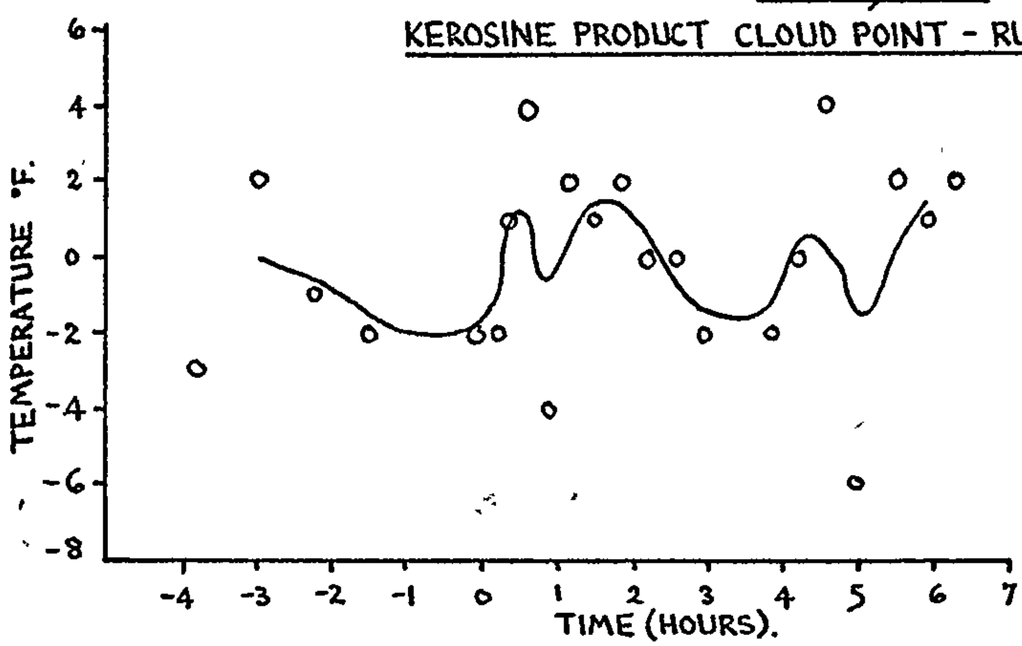


FIG. 5-39.

LIGHT GAS OIL PRODUCT
CLOUD POINT - RUN TR3.

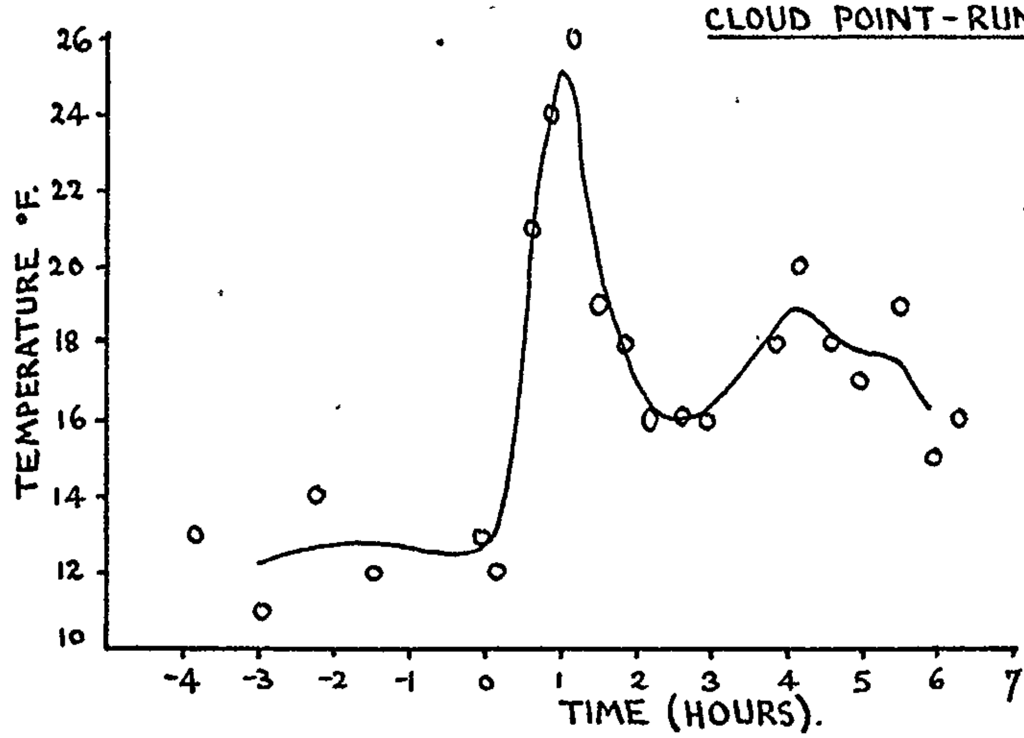
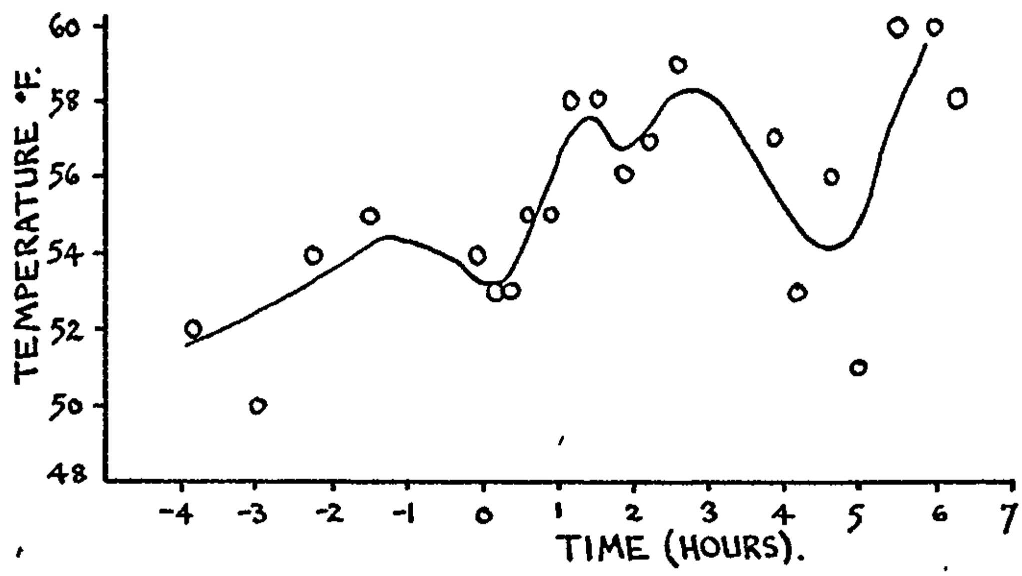


FIG. 5-40.

HEAVY GAS OIL PRODUCT
CLOUD POINT - RUN TR3.



the initial steady state and the peak on the oscillatory response. T2 is the temperature drop from the peak to the final steady state. The times are expressed in hours from the time at which the change was injected.

Tray No.	T1 (^{o}F)	T2	Time of peak
0	17	5	0.40
12	12	1.5	1.10
16	26	16	0.50
30	23	15	0.75
36	22	14	0.90

Fig. 5-42

It is surprising that Fig. 5-42 shows no clearly discernible trends. The times at which the trays begin to swing to their final steady states might be expected to follow some sequential pattern down the column. That they do not might be attributable to the differing effects of the intermediate pumparounds. Further discussion of these results is included in Chapter 7.

5.4.3 Step change experiment on a sidestream - Run TR4.

This experiment was performed whilst the unit was running Crude oil D at maximum throughput and making overheads, kerosine, light and heavy gas oils and residue. The unit was observed for ten hours. Normal operational adjustments were being made during the first four hours. The unit was allowed three hours in which to settle. The light gas oil rate was then reduced using the controller setpoint to give a decrease of 10%. The tray temperature and the automatic distillation analyser results for the kerosine product were then logged for 3½ hours. The results are presented in Figs.5-43 to 5-50. Discussion of the results is included in Chapter 7.

FIG. 5-43.

LIGHT GAS OIL DRAW-OFF TEMPERATURE (EX-TRAY 30) - RUN TR4.

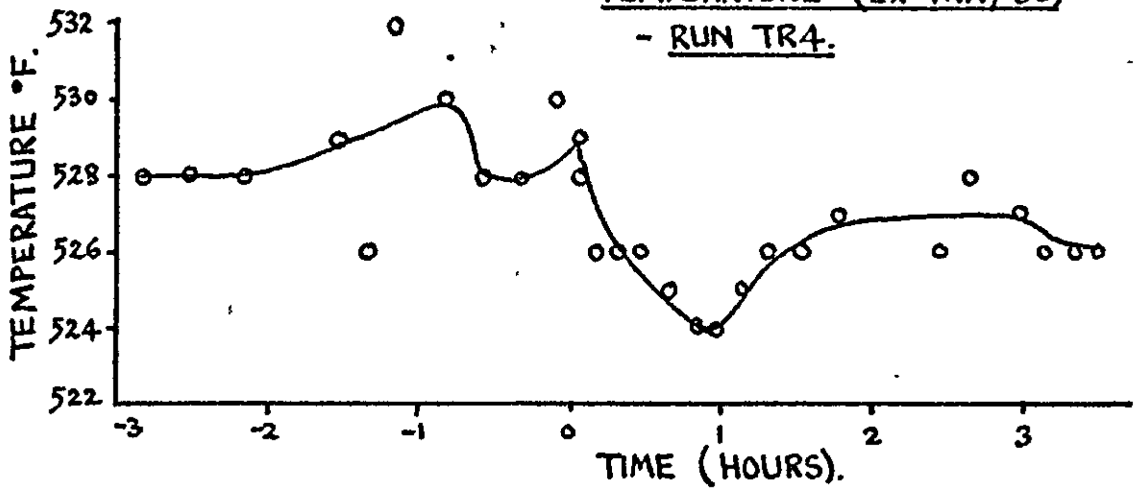


FIG. 5-44.

TEMPERATURE OF LIQUID ON TRAY 31 - RUN TR4.

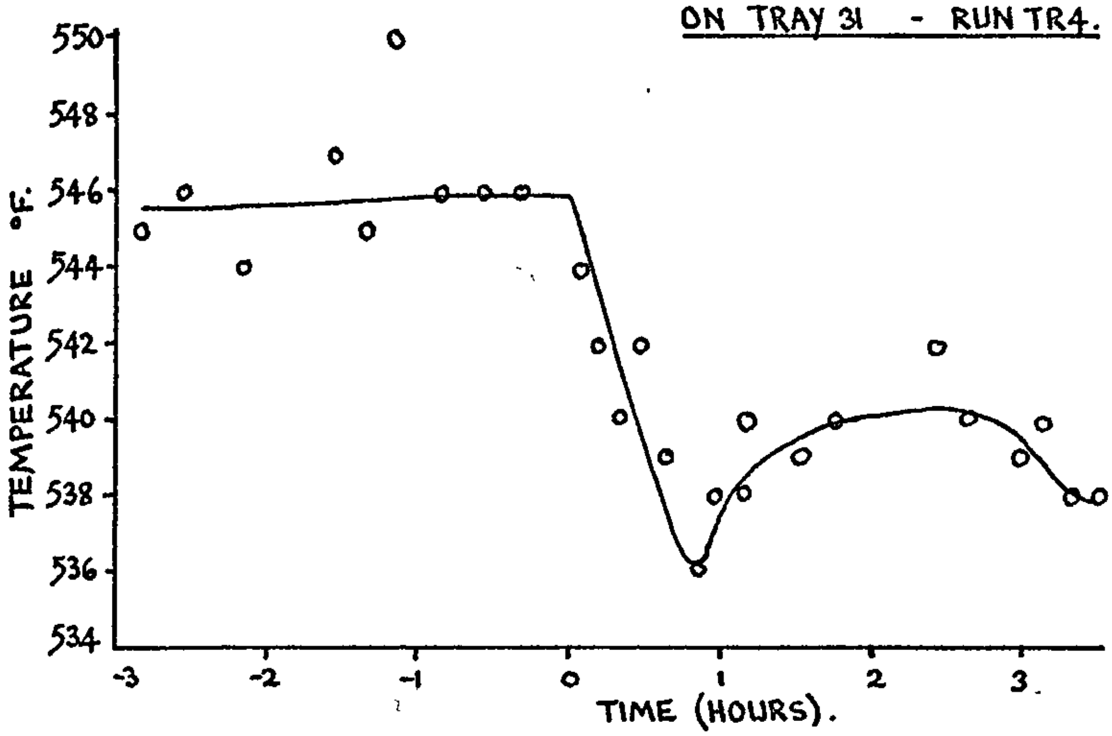


FIG. 5-45.

HEAVY GAS OIL DRAW OFF TEMPERATURE (EX-TRAY 36) - RUN TR4.

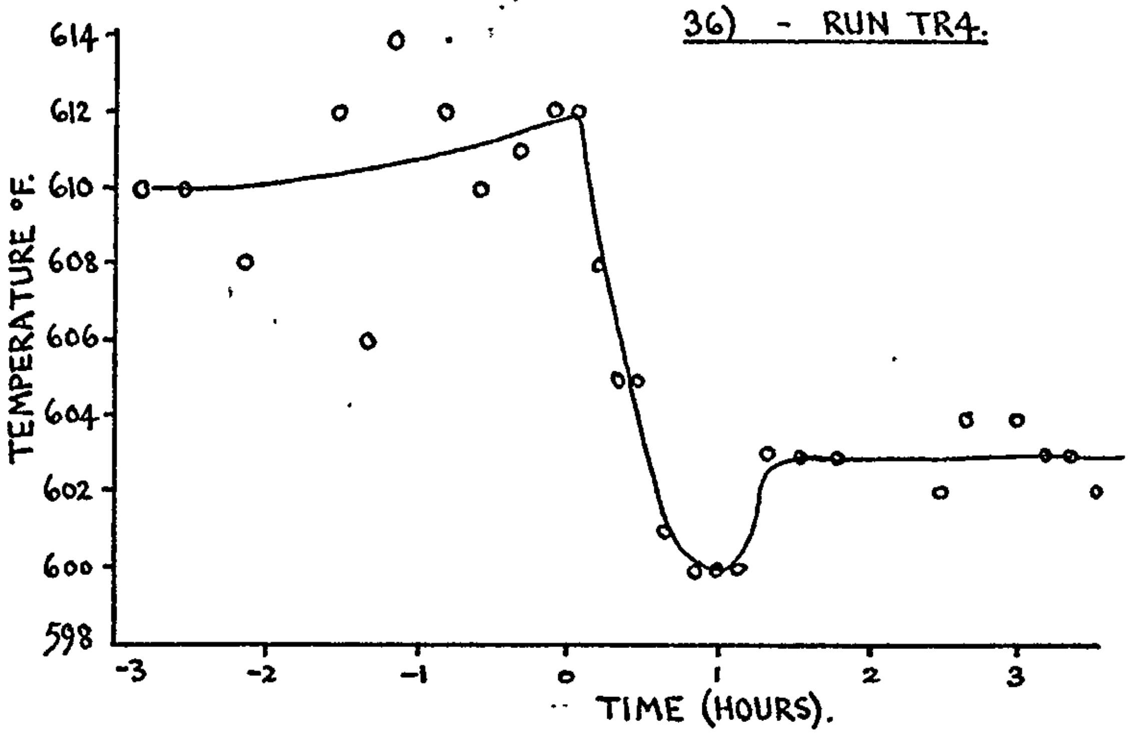


FIG. 5-46.

TEMPERATURE OF LIQUID ON TRAY 37 - RUN TR4.

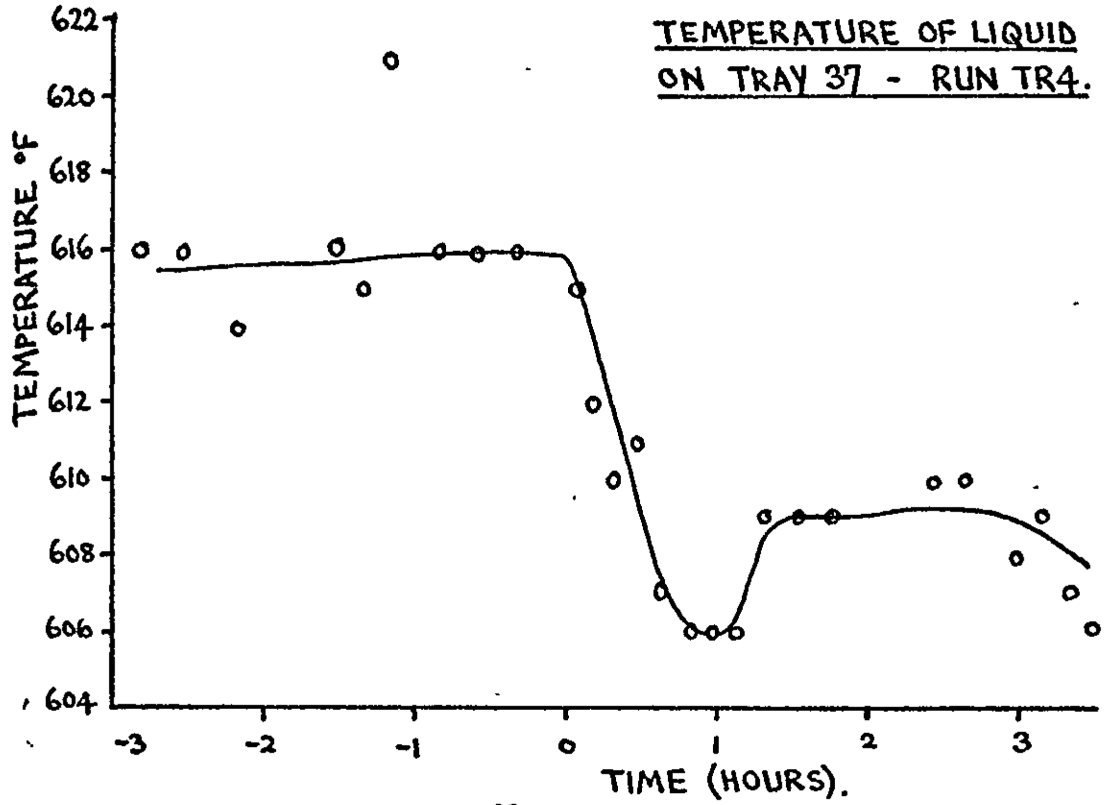


FIG. 5-47.

OVERHEAD VAPOUR TEMPERATURE - RUN TR4.

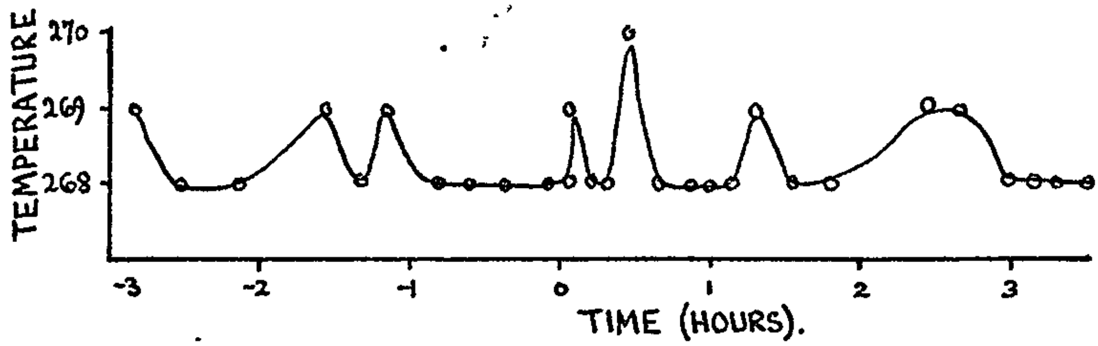


FIG. 5-48.

ASTM DISTILLATION 10% POINT FOR KEROSINE PRODUCT - RUN TR4.

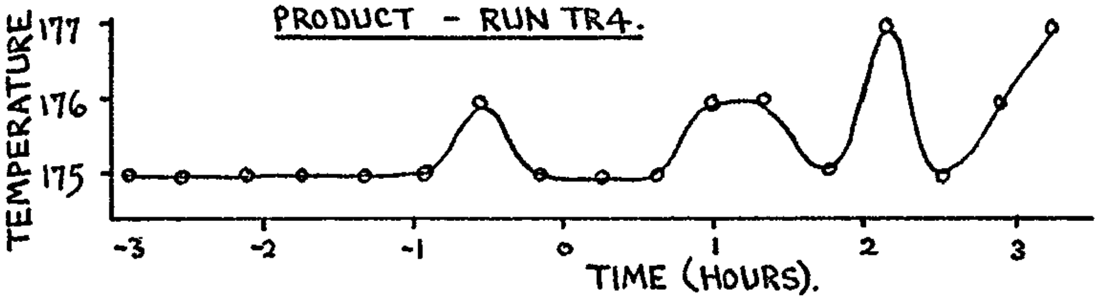
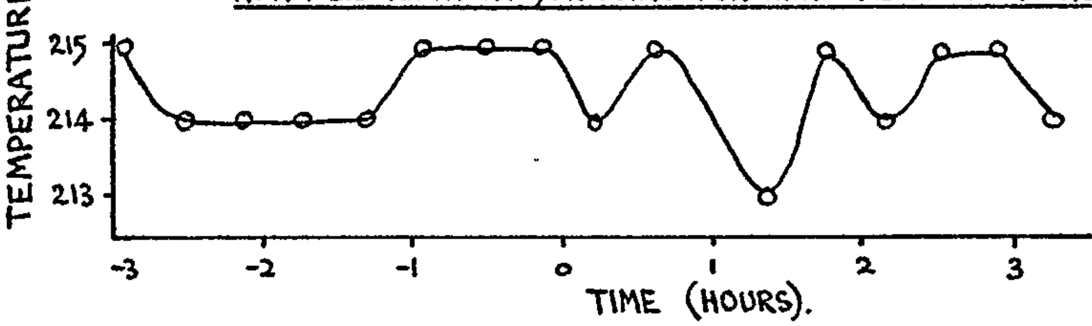


FIG. 5-49.

ASTM DISTILLATION 90% POINT FOR KEROSINE PRODUCT - RUN TR4



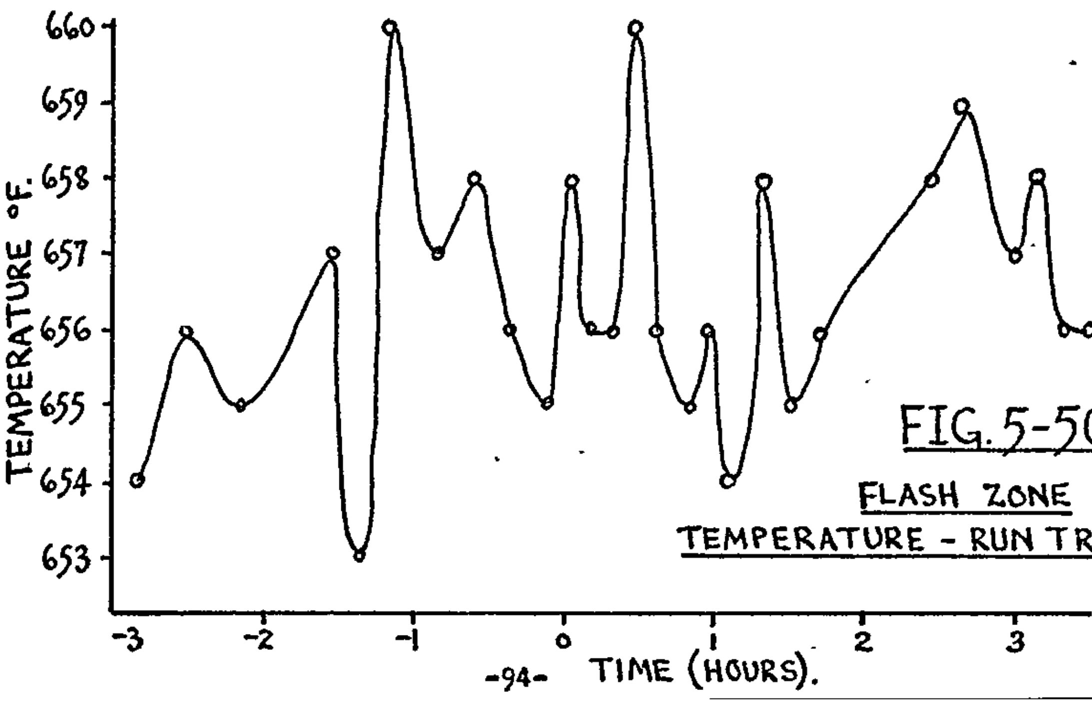


FIG. 5-50.

FLASH ZONE TEMPERATURE - RUN TR4.

5.4.4 Observation of a crude oil change on the unit.

a) Observation run OB1.

The unit was initially operating under steady state conditions refining Crude oil C at maximum flow. Experimental test run TR3 had just been concluded and all flows had been held constant for five hours.

In view of trouble that was anticipated due to water slugs in the feed throughput was dropped by about 4%. The change to Crude oil A was made by first cracking in 50% Crude oil A with Crude oil C. The change to 100% Crude oil A was made thirty minutes later. The main flow and temperatures were logged by the author for two hours and then by the plant operators for a further 24 hours. The results are presented in Figs. 5-51 to 5-61.

b) Observation run OB2.

The unit was running Crude oil C at maximum feed rate. The column variables were logged from 0900 hrs. Crude oil B was blended together with Crude oil C at 0915 hrs in a small unspecified percentage. The switch to 100% Crude oil B was made at 1015 hrs. The sidestream withdrawal rates were maintained constant. The main temperature responses are presented in Figs. 5-62 to 5-65.

c) Observation run OB4.

The unit had been running Crude oil D at near maximum feedrate for about 12 hours. The change to Crude oil B was called for with production of identical products. This necessitated a change in the relative amounts of each sidestream offtake. Also it was required to raise throughput by about 3%.

The change was made at about 1000 hours. At 1015 hrs a rapid fall in the residue flowrate from the unit was noted. This

FIG. 5-51.

TEMPERATURE OF OVERHEAD VAPOUR - RUN OBI.

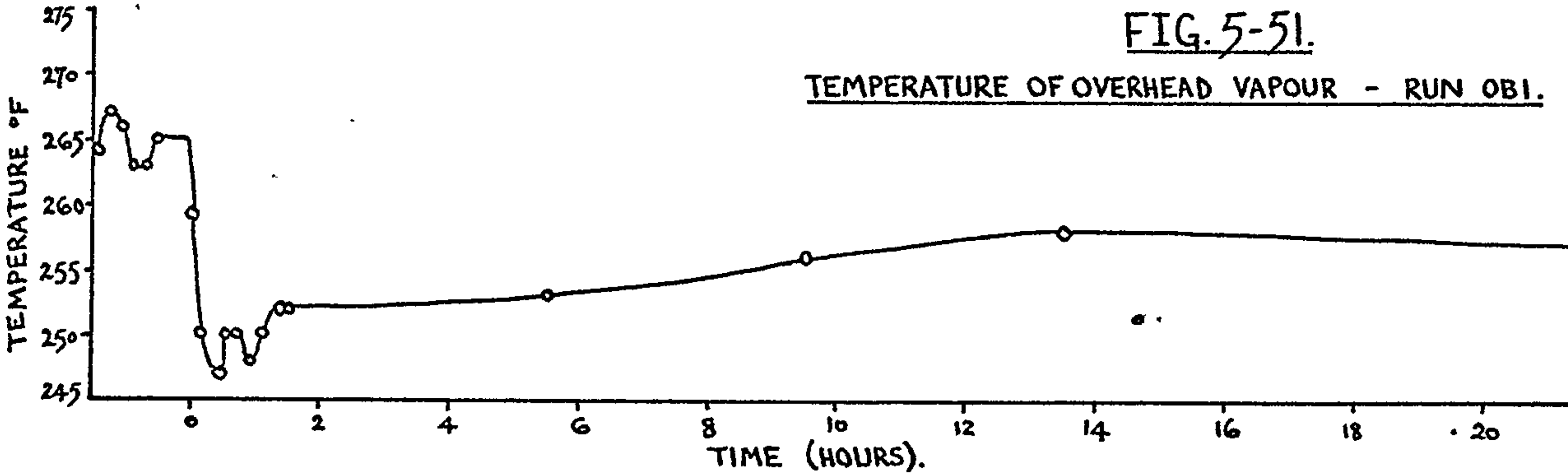


FIG. 5-52

KEROSINE OFF-TAKE TEMPERATURE - RUN OBI.

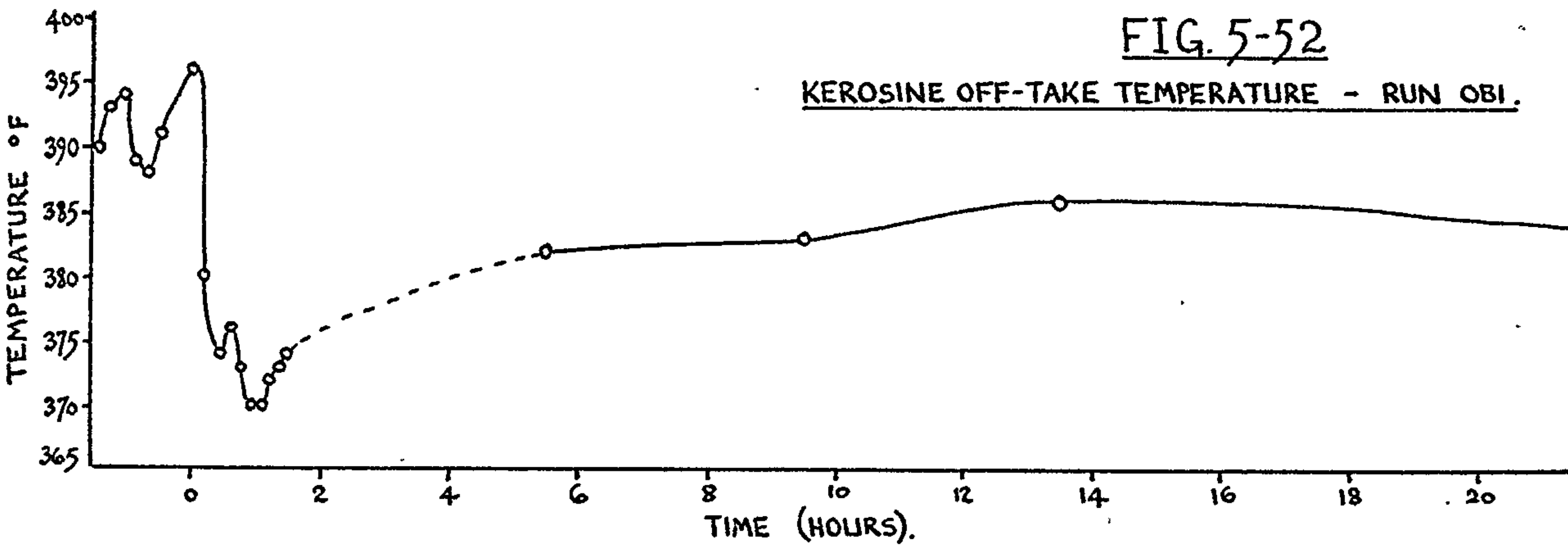


FIG. 5-53.

LIGHT GAS OIL OFF-TAKE TEMPERATURE - RUN OBI.

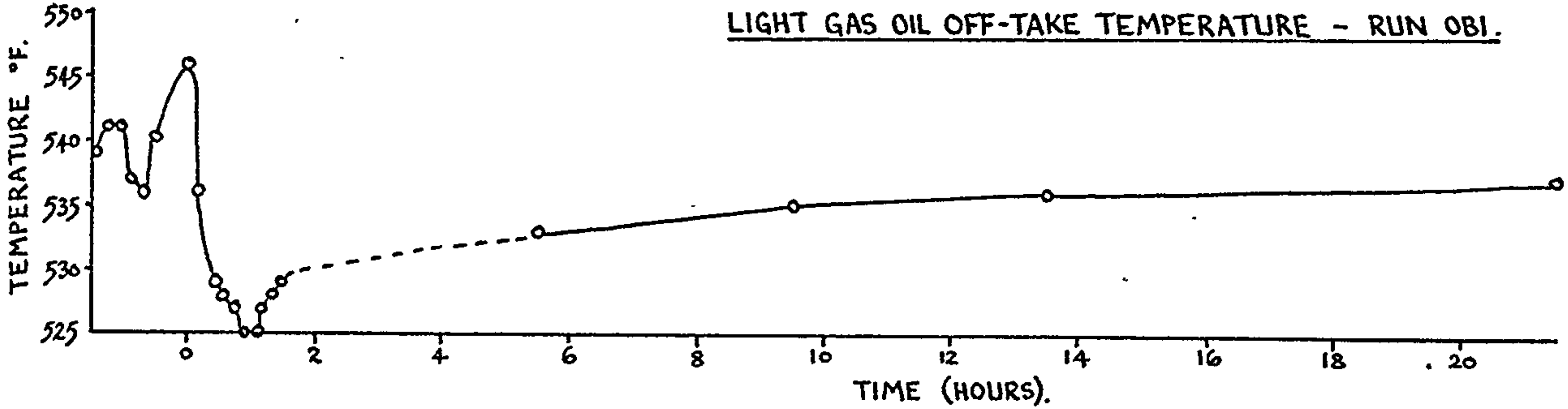


FIG. 5-54.

HEAVY GAS OIL WITHDRAWAL TEMPERATURE - RUN OBI.

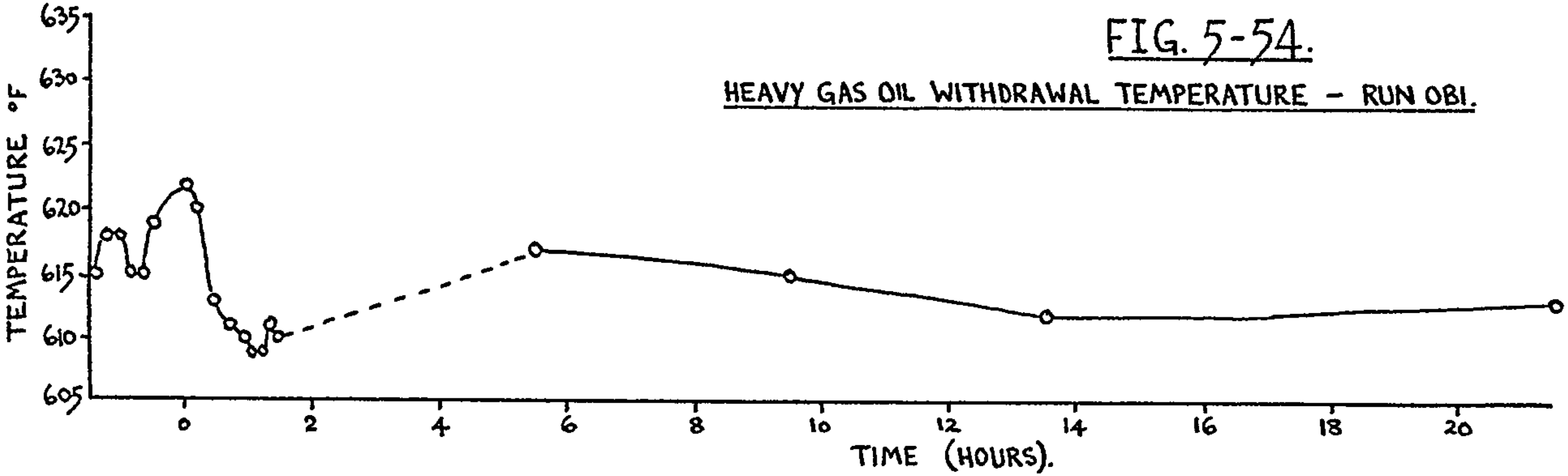


FIG. 5-55.

CRUDE OIL FEEDRATE PER PASS - RUN OBI.

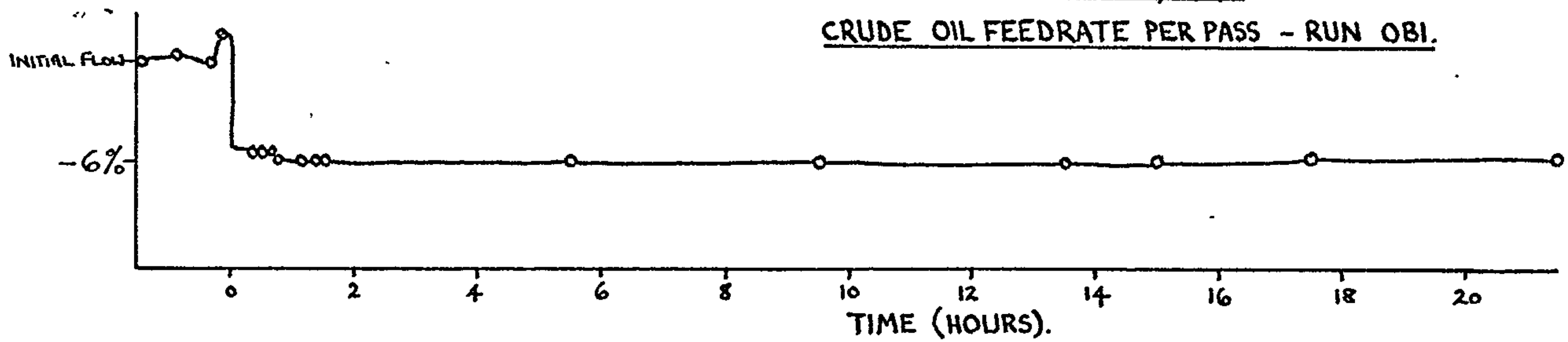


FIG. 5-56.

HEAVY GAS OIL WITHDRAWAL RATE - RUN OBI.

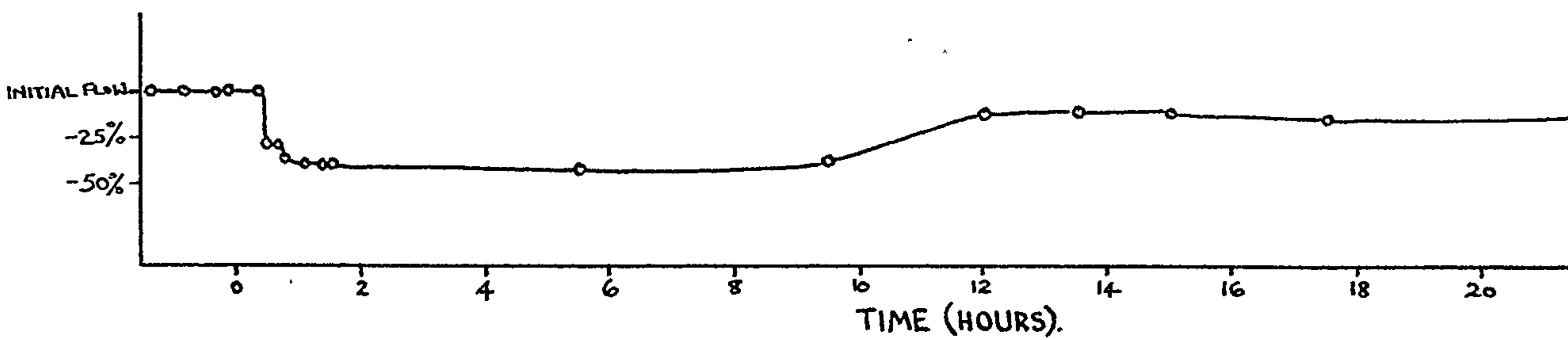


FIG. 5-57.

OVERHEAD REFLUX FLOWRATE - RUN OBI.

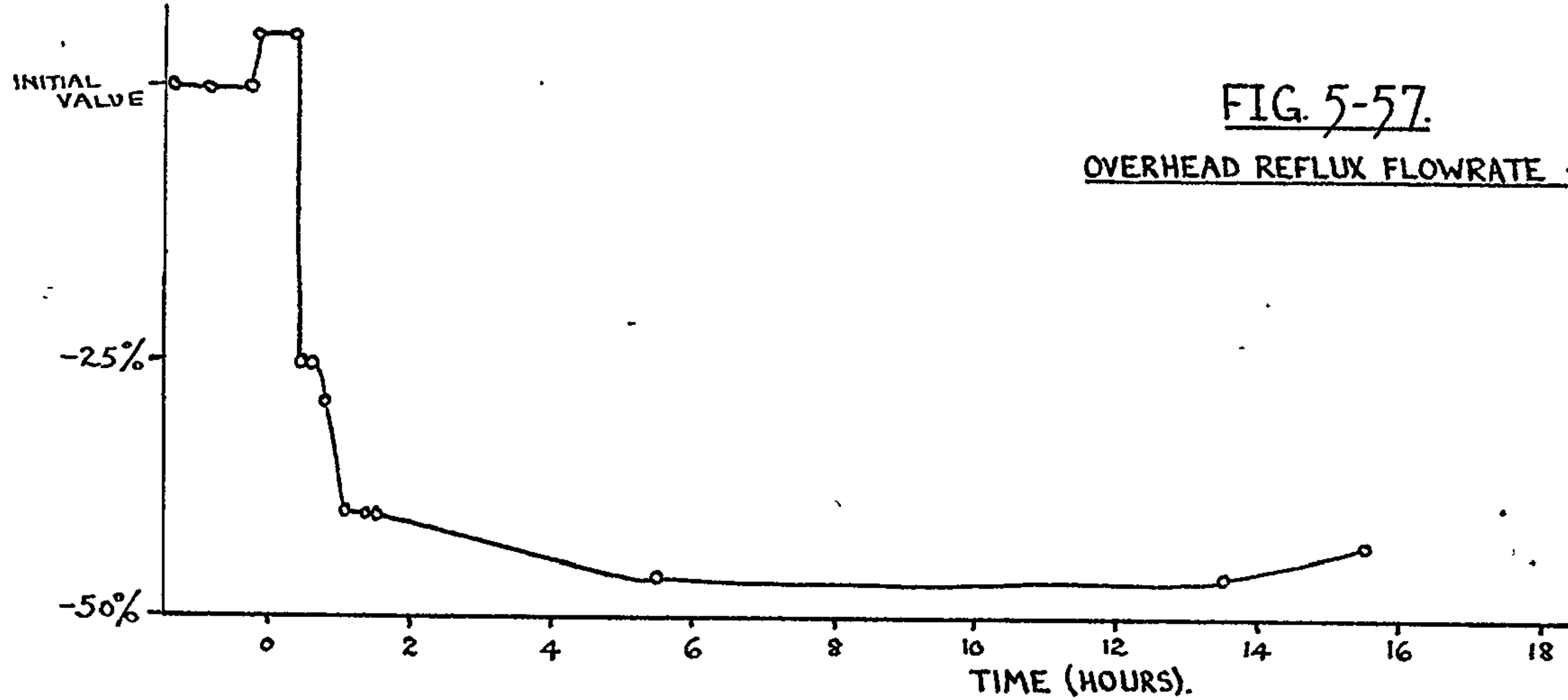
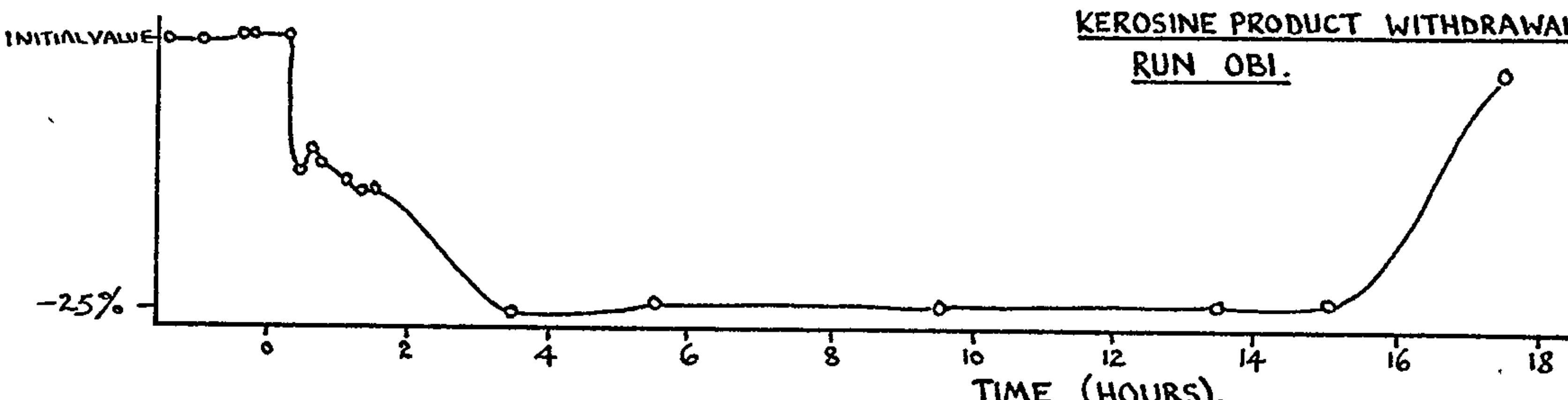


FIG. 5-58.

KEROSINE PRODUCT WITHDRAWAL RATE - RUN OBI.



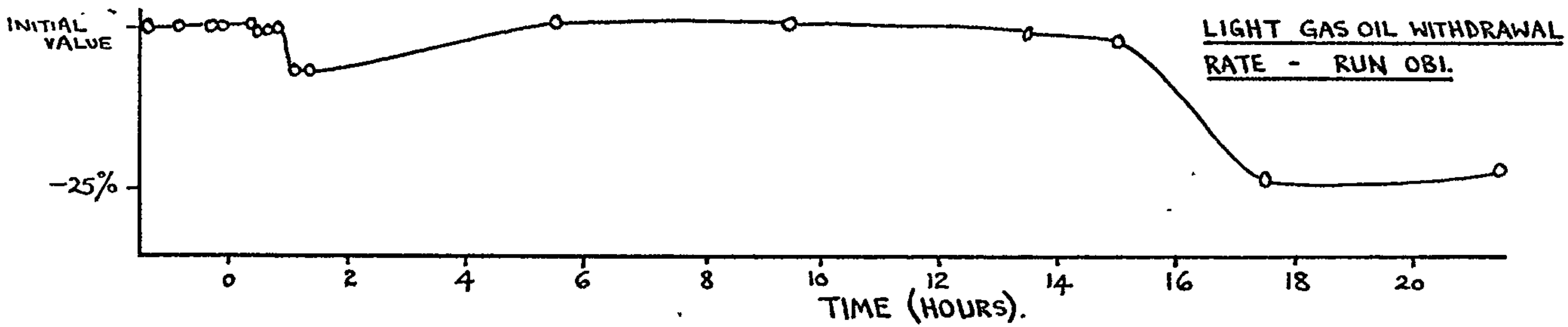


FIG. 5-59.

LIGHT GAS OIL WITHDRAWAL RATE - RUN OB1.

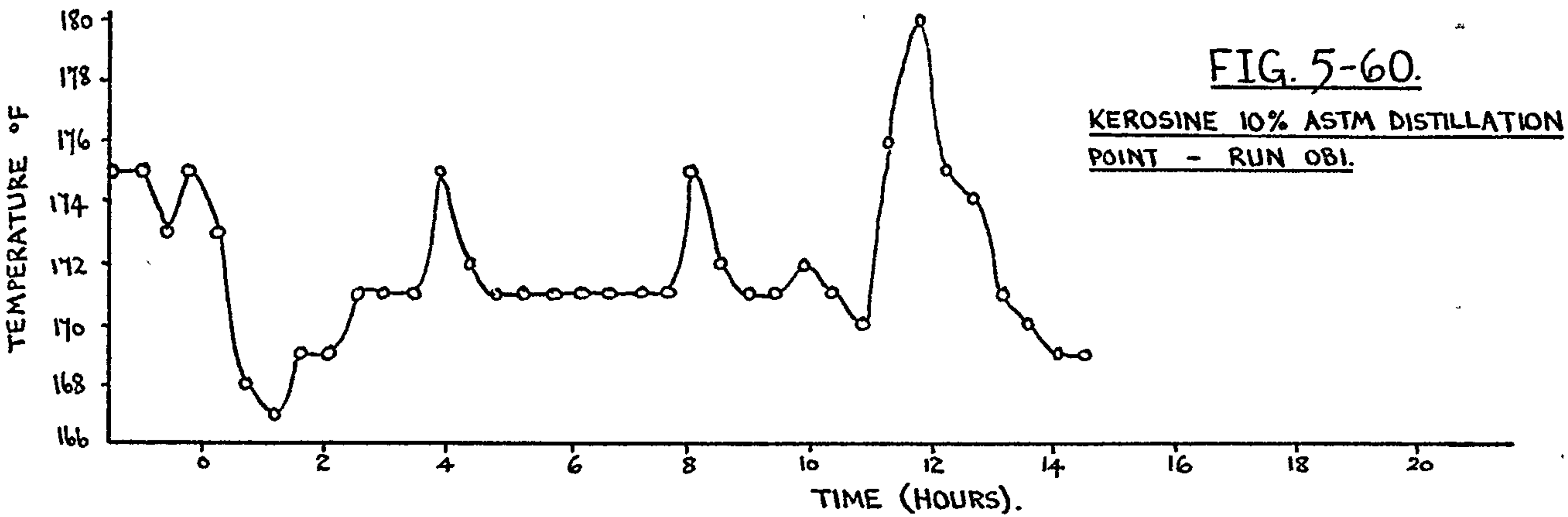


FIG. 5-60.

KEROSINE 10% ASTM DISTILLATION POINT - RUN OB1.

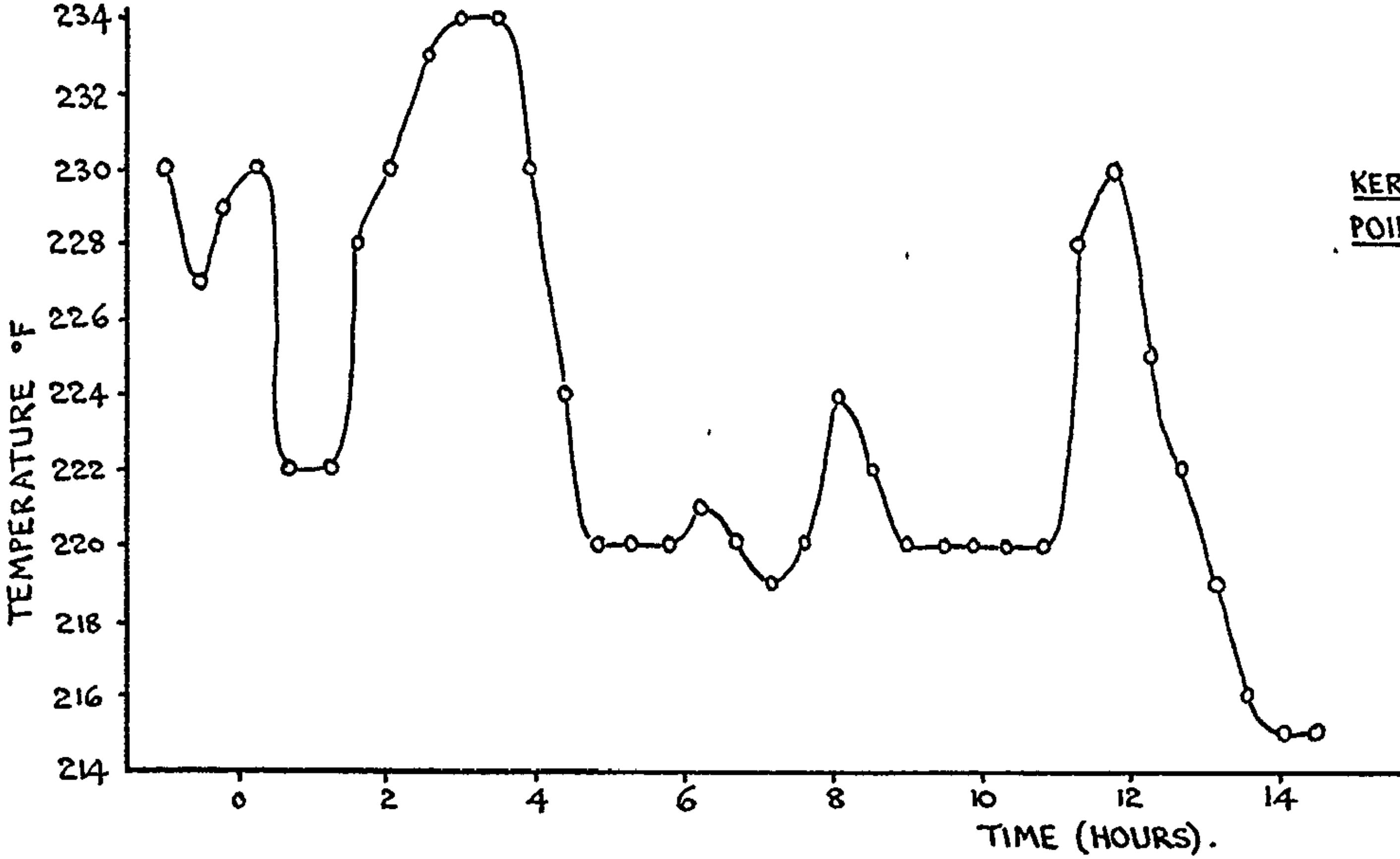


FIG. 5-61.

KEROSINE 90% ASTM DISTILLATION POINT - RUN OBI.

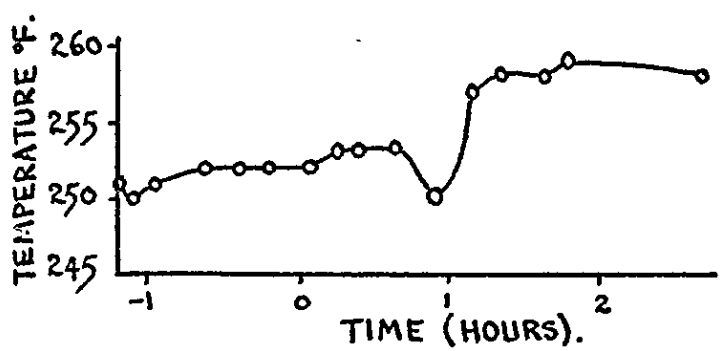


FIG. 5-62.

OVERHEAD VAPOUR TEMPERATURE - RUN OB2.

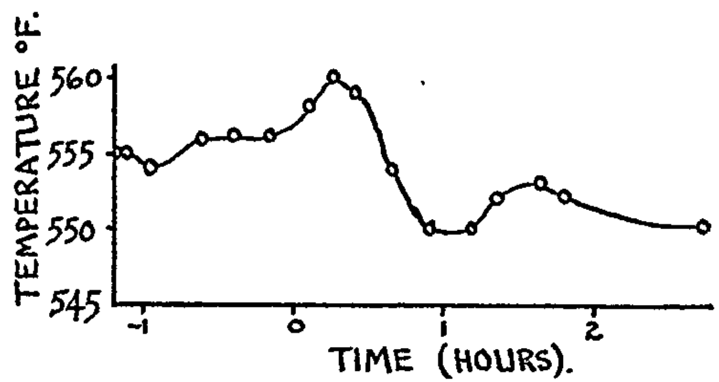


FIG. 5-64.

LIGHT GAS OIL OFFTAKE TEMPERATURE - RUN OB2.

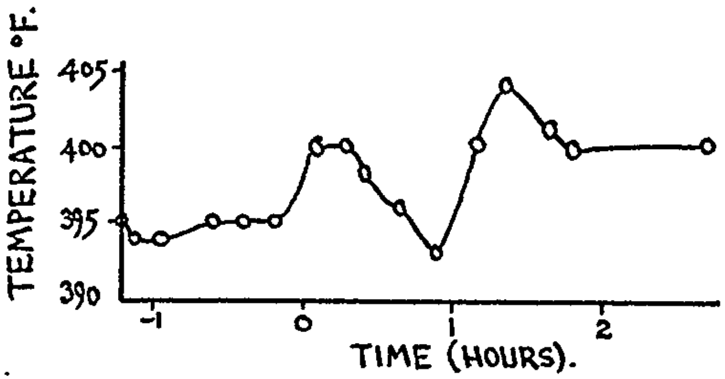


FIG. 5-63.

KEROSINE OFFTAKE TEMPERATURE - RUN OB2.

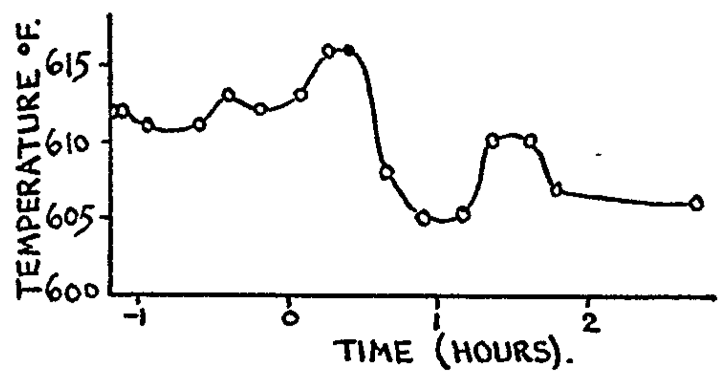


FIG. 5-65.

HEAVY GAS OIL OFFTAKE TEMPERATURE - RUN OB2.

was believed to be due to a slug of light material, possibly water, entering the column. Throughput was cut back then slowly brought back up to 95% maximum over the next 1½ hours, then taken on up to the maximum over the next three hours. The main response curves are shown in Figs. 5-66 to 5-69.

5.4.5 Observation of an activity change on the unit - Run OB3.

This run followed immediately after the crude change, run OB2. The unit was operating steadily and refining Crude oil B. The request was received to change the unit to a yield structure suitable for making a different kerosine. This change is summarised in Fig. 5-70.

Stream	% change
Top product	0
Kerosine	-35
Light gas oil	+57
Heavy gas oil	+12

Fig. 5-70

The changes were made simultaneously, each being a single step. The flows were then held constant. The responses of the main column temperatures are presented in Figs. 5-71 to 5-74. It will be seen that the response dies away rapidly over a period of 1½ hours.

5.4.6 Experiment using a pre-planned control strategy - Run TR5

The characteristic response of many column variables to a step change in the reflux flowrate (with no tower top temperature controller) is as shown in Fig. 5-75.

FIG. 5-66.

KEROSINE WITHDRAWAL TEMPERATURE - RUN OB4.

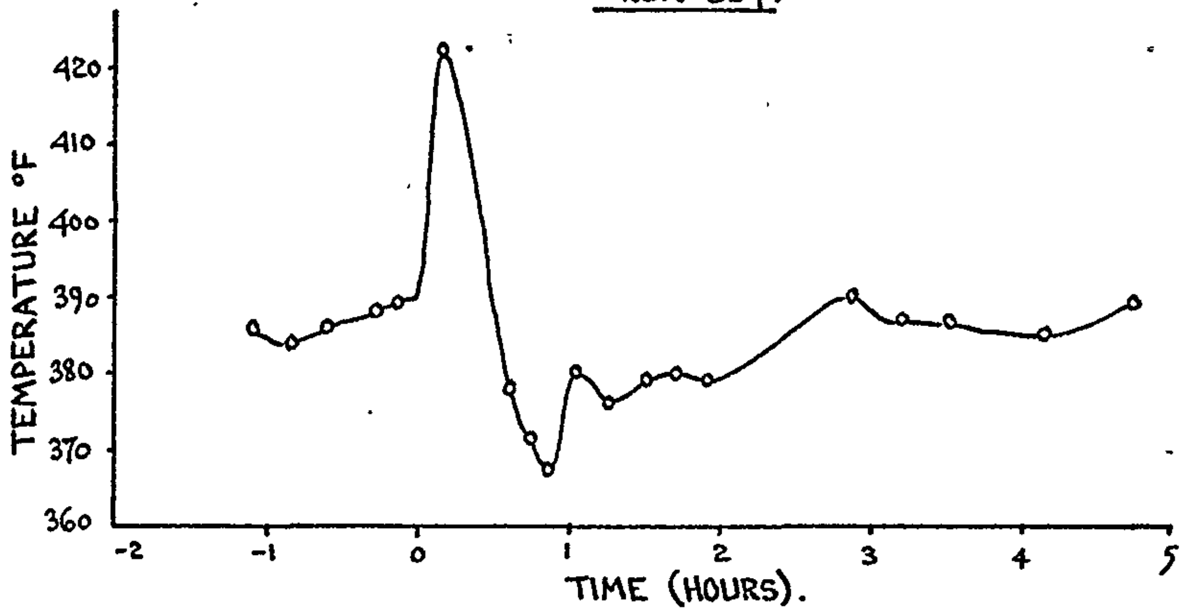


FIG. 5-67.

LIGHT GAS OIL WITHDRAWAL TEMPERATURE - RUN OB4.

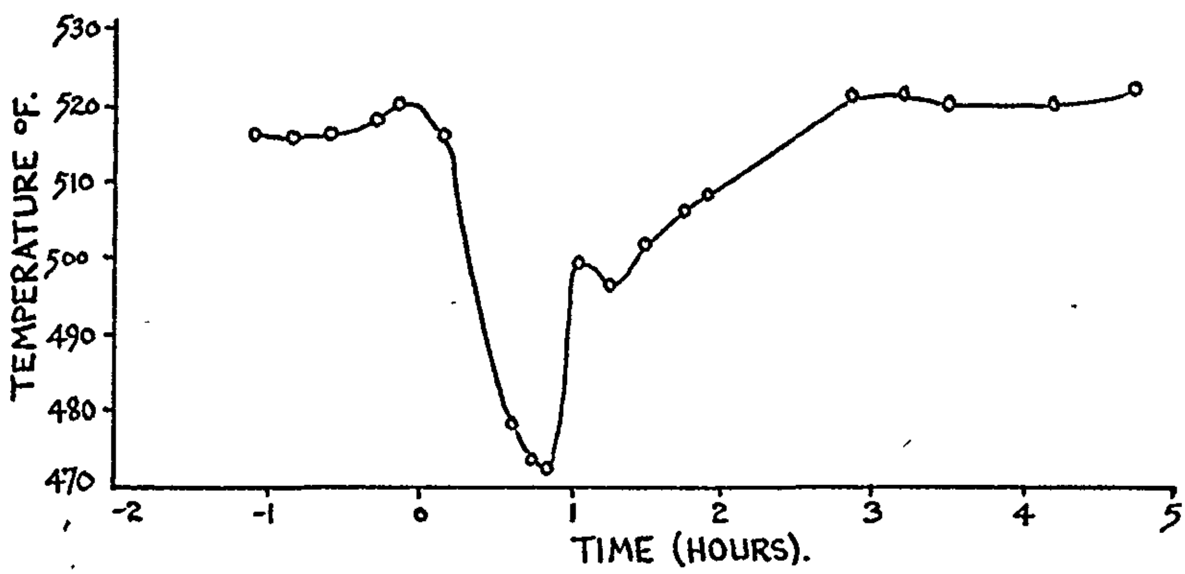


FIG. 5-68.

HEAVY GAS OIL WITHDRAWAL TEMPERATURE - RUN OB4.

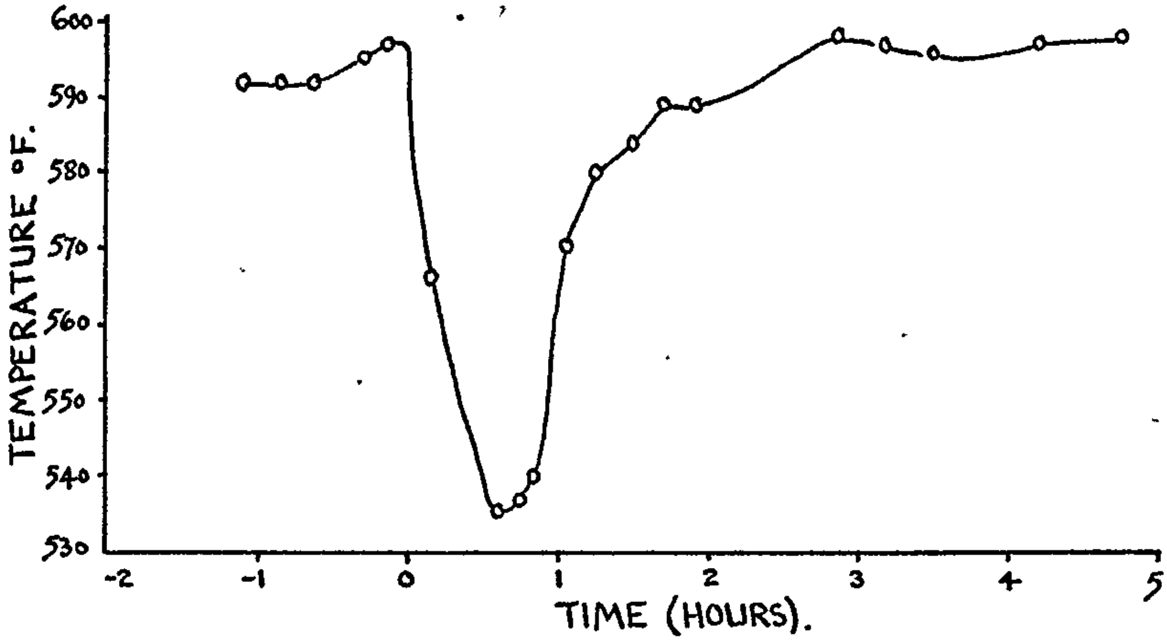
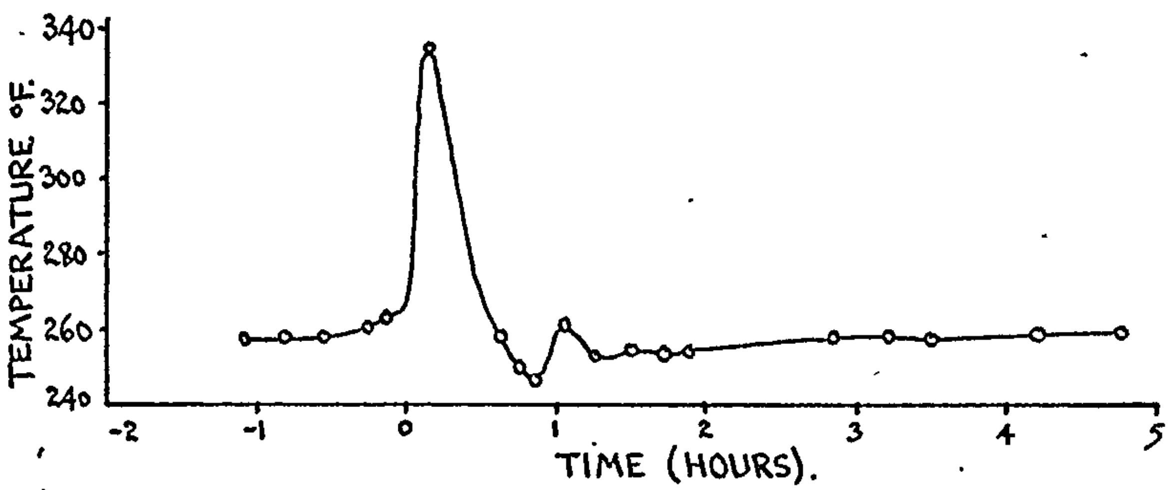


FIG. 5-69.

TOWER TOP TEMPERATURE -RUN OB4.



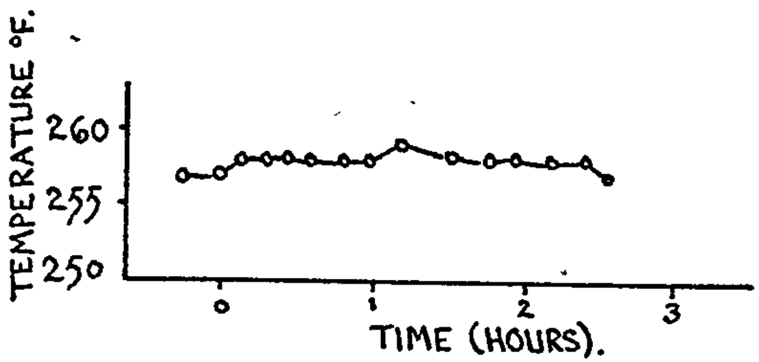


FIG. 5-71.

OVERHEAD VAPOUR TEMPERATURE - RUN OB3.

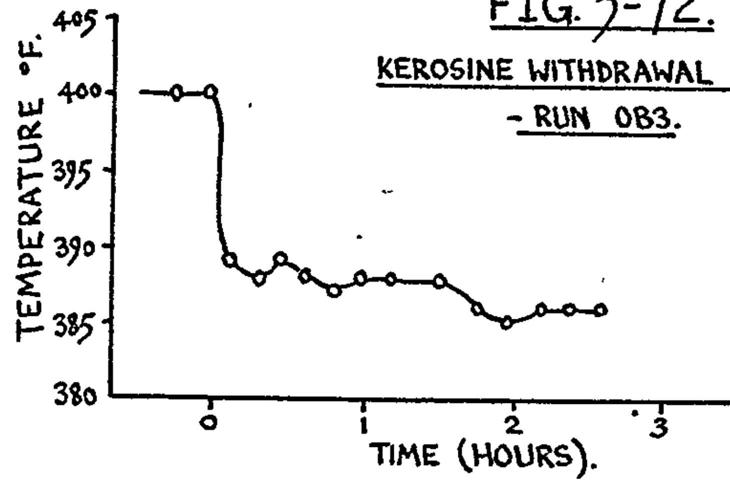


FIG. 5-72.

KEROSINE WITHDRAWAL TEMPERATURE - RUN OB3.

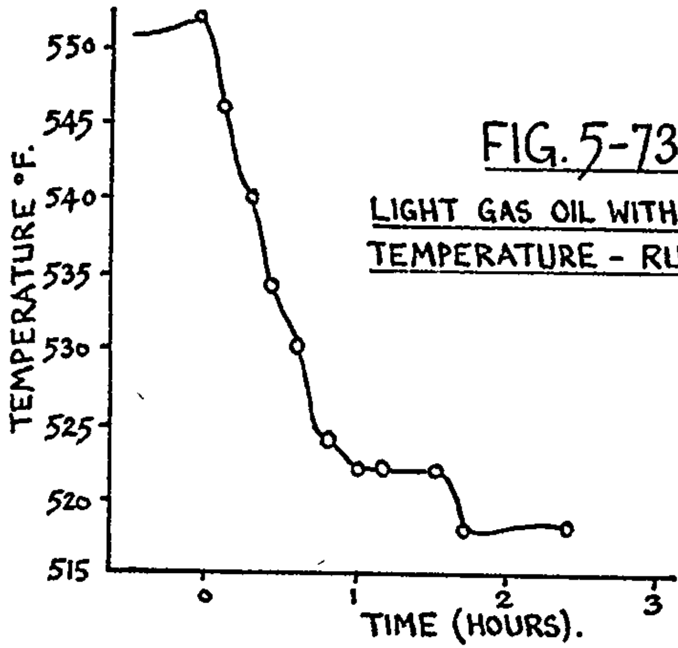


FIG. 5-73.

LIGHT GAS OIL WITHDRAWAL TEMPERATURE - RUN OB3.

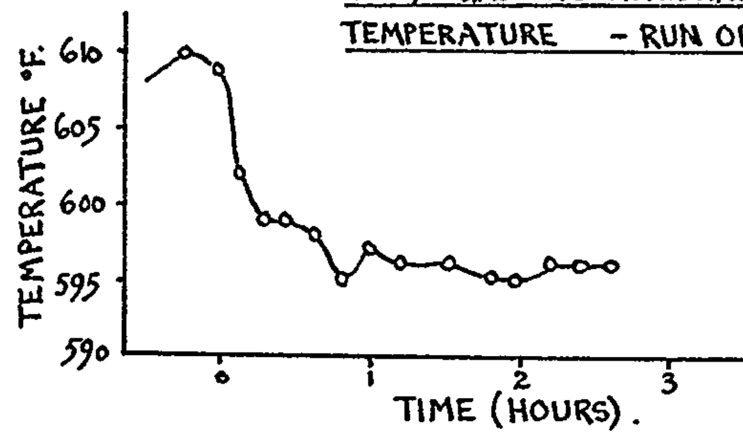


FIG. 5-74.

HEAVY GAS OIL WITHDRAWAL TEMPERATURE - RUN OB3.

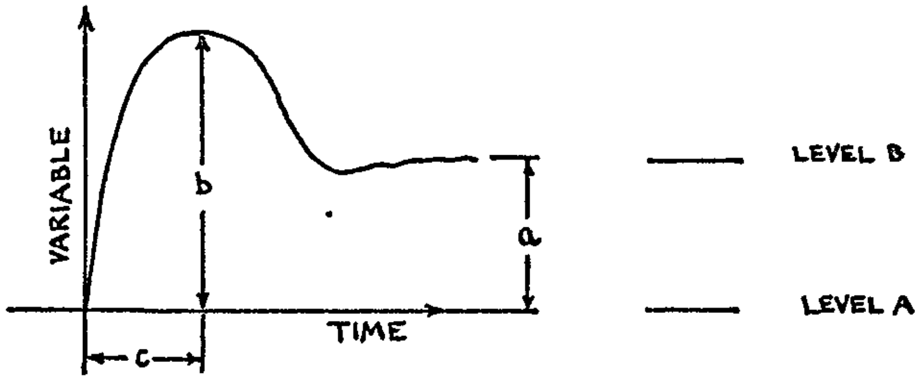


Fig. 5-75

Suppose it is desired to make a change in the overhead reflux during normal operation with no tower top temperature controller. This will result in tray temperatures and product properties moving from level A to level B in Fig. 5-75. A means is required of eliminating the large oscillation (the peak height of which is between 1.5 and 3 times the steady state difference depending on position in the column or product property selected). One approach would be to measure a and b for the overhead reflux temperature response. At time zero fraction a/b of the desired change is stepped in. This is held for a time c hours at which time the peak is reached. The remainder of the change is then ramped in (a ramp being approximated to by a period of small steps over a period (2-c) hours. This should then give a response of the type shown in Fig. 5-76. Steady state would then be achieved

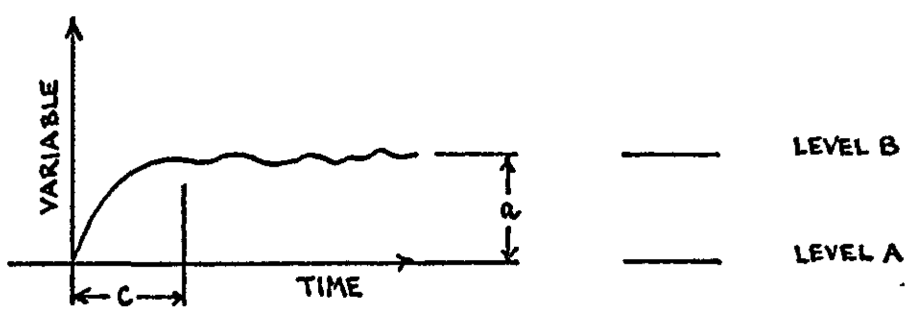


Fig. 5-76.

in less than half the time taken by the step change method, since c is in general less than one hour and the response normally occupies two hours.

The above experiment was carried out on the unit whilst refining Crude oil B at maximum throughput. The results were almost up to expectations and are presented in Figs. 5-77 to 5-81. Because of the small size of the permitted step some difficulty was experienced with the final ramp. This was reduced to two small steps but even so the overall change was greater than planned. Had this difficulty not arisen it may be appreciated that the final steady state would have been achieved even earlier than it actually was. The postulated open loop response is also shown superimposed on the results and is based on the experimental reflux step change responses obtained on run TR3. The times of the peaks, the shapes and the (peak height) : (steady state change) ratio are the key parameters copied from the reflux step change response curves to reconstruct these open loop response curves. If a criterion of performance is taken as the time taken for the draw-off temperature to approach and remain within $3^{o}F$ of the final steady state result then the table shown in Fig. 5-82 can be drawn up.

Variable Temperature	Time to approach within $3^{o}F$ and remain there		Improvement due to control	
	Open loop (minutes)	With control (minutes)	(minutes)	% on open loop time
Tower top temp.	66	49	17	26
Kerosine offtake temp.	75	37	38	51
Light gas oil offtake temp.	90	49	41	46
Heavy gas oil offtake temp.	80	31	49	61

Fig. 5-82

Further discussion on all the experimental results is presented in Chapter 7.

FIG. 5-77.

OVERHEAD REFLUX FLOWRATE - RUN TR5.

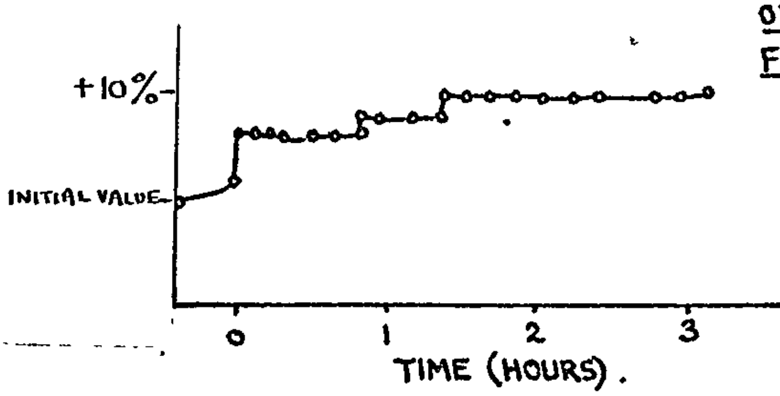


FIG. 5-78.

TOWER TOP TEMPERATURE -RUN TR5.

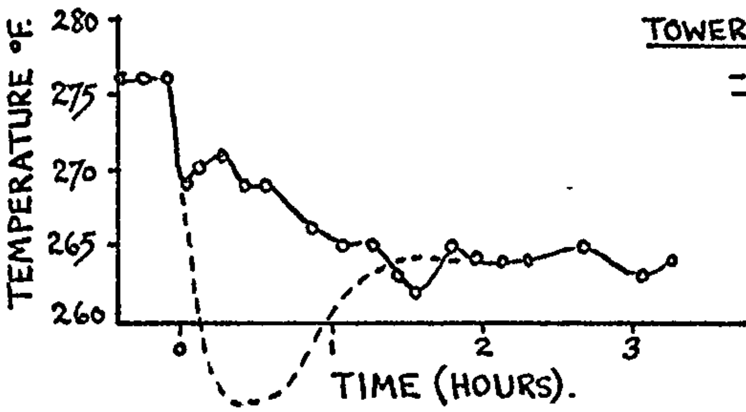


FIG. 5-79.

KEROSINE WITHDRAWAL TEMPERATURE - RUN TR5.

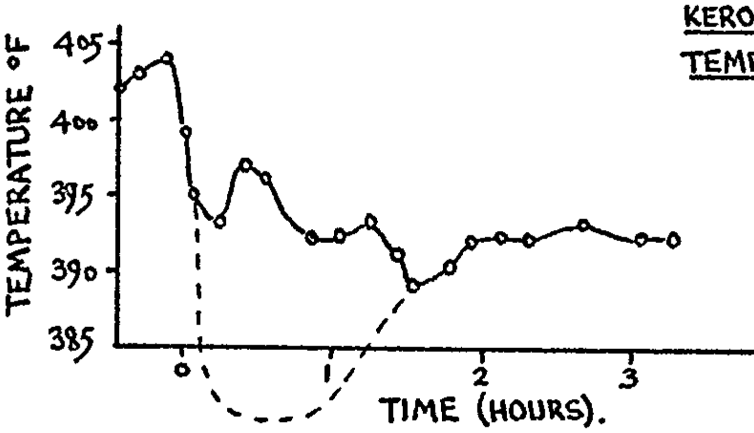


FIG. 5-80.

LIGHT GAS OIL WITHDRAWAL TEMPERATURE - RUN TR5.

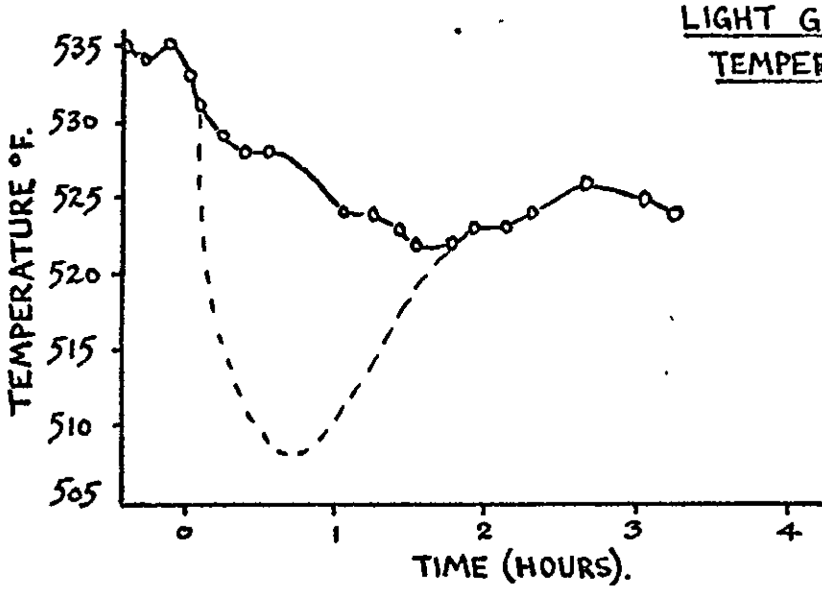
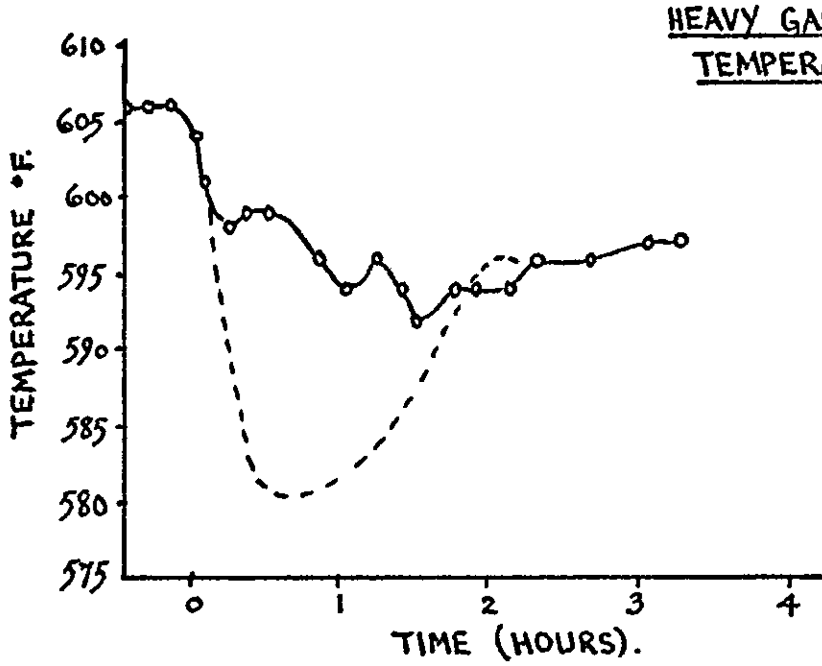


FIG. 5-81.

HEAVY GAS OIL WITHDRAWAL TEMPERATURE - RUN TR5.



CHAPTER 6. EXPERIMENTS ON THE SINGLE SIEVE PLATE UNIT.

6.1 Introduction.

The mathematical model of a crude oil distillation unit described in Chapter 4 relies heavily on the validity of the correlations for estimating froth height and for predicting the flow of froth over the outlet weir. If these correlations are not true at least qualitatively then any enhancement of a model of this type of multistage system by the use of such a detailed mathematical description is nullified. A paper by Bernard and Sargent (6) is so condemnatory of many of the standard design correlations as to cast serious doubts on their validity under any general conditions. It was therefore thought essential that an attempt be made to assess the validity of two of the correlations in a dynamic situation using a laboratory rig.

6.2 Objectives.

The mathematical model of the crude unit described in Chapter 4 uses the froth height correlation of Thomas and Campbell (9) and the Francis weir formula (2). The correlation published by Thomas and Campbell relates the height of the froth on a sieve plate to the liquid and vapour rates. The modified Francis weir formula relates the flow over the outlet weir to the mean density of the froth and the head of froth over the weir. The modification to the basic Francis weir formula was to assume that the froth flowing over the weir behaved as a liquid of density FDxDL where

FD = liquid fraction in froth

DL = clear liquid density.

The objectives of the experiments described in this section were to compare the observed response for a single sieve plate with that predicted by a mathematical model which used the above correlations.

6.3 The apparatus.

The single sieve plate rig is shown in Fig. 6-1. Water from a supply tank was pumped via a rotameter to the rectangular sieve plate. It passed over a small inlet weir (which assisted equal distribution over the width of the plate) and across the plate. The froth from the plate passed over an outlet weir into an intermediate tank. The drain from this ran back into the supply tank. Water which wept through the holes in the sieve plate itself also ran back into the supply tank. This line had a U-bend in it to form a liquid seal to prevent air leakage. The liquid flow was regulated by a valve in the line between the pump and the rotameter. Hence the liquid circuit was a closed system.

The supply tank stood on a weighing machine so that the holdup of water might be continuously monitored. The intermediate tank was fitted with a sight glass for the same reason.

Air was blown through the sieve plate by a centrifugal blower. The air left the system via a wire mesh de-entrainment screen. An orifice plate was fitted at the air inlet. The downstream pressure was led to a water manometer, the other side of which was open to atmosphere. This enabled an estimate of the air flowrate to be made. The air flow was regulated by a gate valve situated between the blower and the sieve plate.

6.4 Experimental work.

The supply tank was filled with water until the weighing maching registered its maximum reading, about 740 lbs. The centrifugal blower was started followed by the water pump. Water weeping through the tray rapidly produced the required seal in the

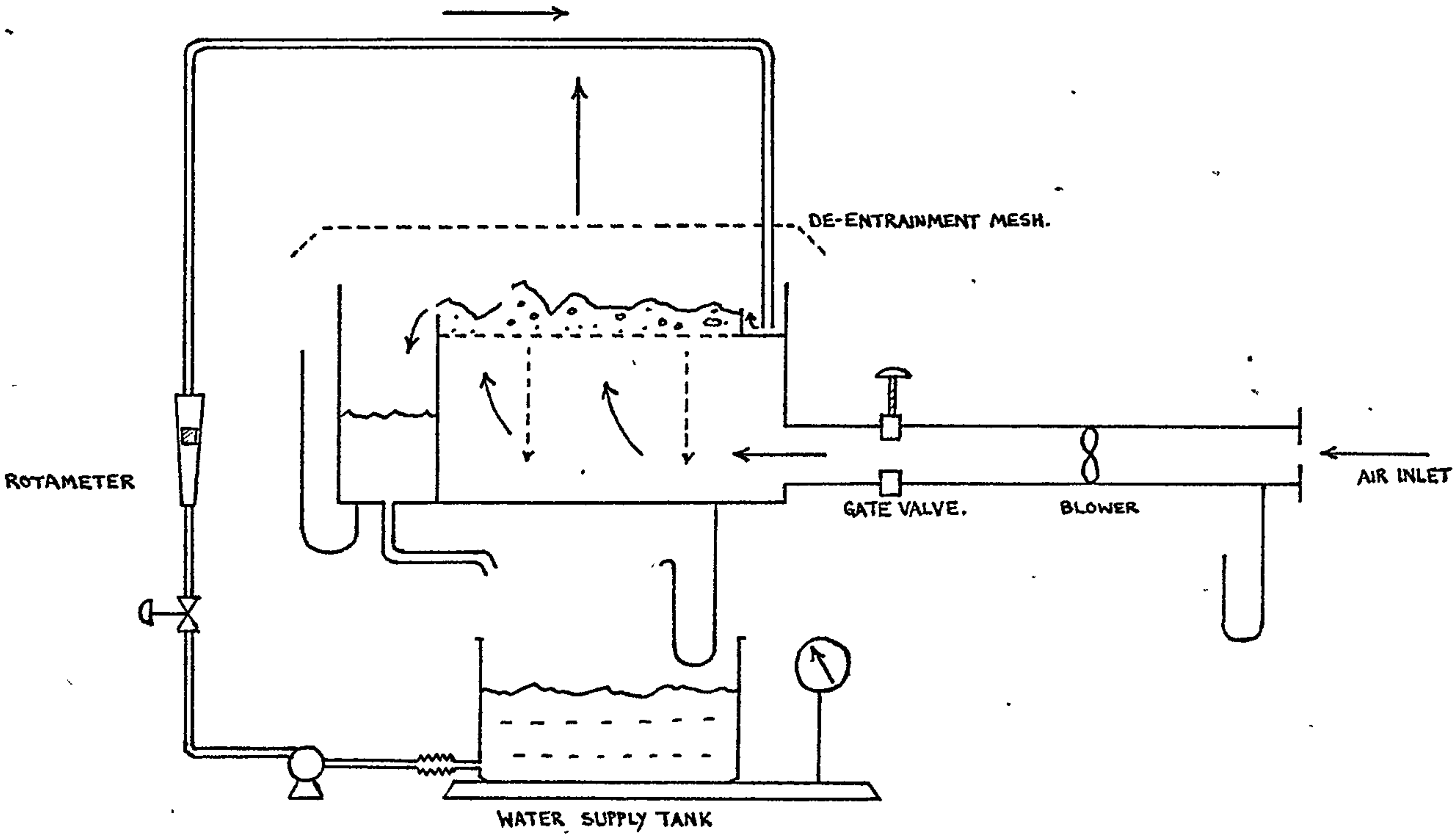


FIG. 6-1.

DIAGRAM SHOWING LAYOUT OF SINGLE SIEVE PLATE UNIT.

U-bend in the weepage drain line and the apparatus was ready for use.

6.4.1 Liquid rate step change response.

Several runs were performed. For each one the air and water rates were set at noted values and the unit was allowed to come to steady state. This took less than ten minutes. The liquid rate was then changed manually by rapid movement of the valve in the liquid line. The reading on the intermediate tank sight glass and on the weighing machine were then monitored until no further change was detectable. The final values of the air and water flows were noted. A tabulated set of results for these experiments is given in Appendix 5. A typical response curve for the liquid holdup is given in Fig. 6-2.

6.4.2 The vapour rate step change response.

The same procedure as for the liquid step change response was followed. Full tabulated results are also given in Appendix 5. A typical response curve for the liquid holdup is given in Fig. 6-3.

6.4.3 Determination of the discharge coefficient for the intermediate tank.

The exit pipe was blocked using a rubber bung. The intermediate tank was filled to nearly the full depth. The rubber bung was removed. A stop watch was started when the water in the sight glass passed a reference mark h_1 and was stopped when the level fell to the reference mark h_2. The experiment was repeated several times and a mean value of the time was taken.

If the head of liquid in the end tank is denoted by h, then

$$dh/dt = -C_7 x(2Gxh)^{\frac{1}{2}} xAE/AX$$

Integrating both sides gives :-

$$\int_{h_1}^{h_2} h^{-\frac{1}{2}}\, dh = -C_7 x 2G^{\frac{1}{2}} \int_{t_1}^{t_2} dt \; AE/AX$$

$$\left[2h^{\frac{1}{2}} \right]_{h_1}^{h_2} = C_7 2G^{\frac{1}{2}} t \; AE/AX$$

The experimental results gave

$h_2 = 17/12$ ft; $h_1 = 29/12$ ft; $t = 7.8$ seconds.

From which $\underline{C_7 = 0.80}$

6.4.4 Sources of experimental inaccuracy.

a) The weighing machine was probably accurate in absolute terms to about 5%. However, in these experiments the main concern was with deviation from a steady state of 15-50 lbs. The major error is therefore likely to have been that of reading the scale. This can be read to the nearest 1 lb division so that a maximum error of ½ lb in 15 lbs or about 3% is possible.

b) The liquid and vapour step changes were injected manually by valve adjustment. This took about one second in the case of the liquid and about two seconds in the case of the vapour. This could well have introduced appreciable error since it would tend to lower any oscillatory peak on a response curve and will also displace slightly the time axis. (This could be a two second displacement in the case of the vapour change.)

c) The rotameter was calibrated at the start of the experiments by recording the time taken to collect a measured amount of liquid under steady state conditions. This calibration was estimated to have an accuracy within 1/10th lb/sec. or say 35 gph in 1200 gph - i.e. about 3%. The rotameter also oscillated about a mean position by ±5%. However, observation of the float for a short period of time did enable a confident mean to be estimated so that it was not felt that any significant error was involved.

d) The water control valve leaked about 1 lb in a two hour period. This was emptied back into the supply tank at regular intervals so that no cumulative error was produced.

e) During the experiments in which the water rate was varied the resultant change in pressure drop across the plate produced a variation in the air rate of up to 5%.

f) At high liquid and low vapour rates up to 5% of the entering liquid wept through the holes in the plate instead of flowing over the outlet weir.

GLOSSARY OF NOMENCLATURE USED IN CHAPTER 6.

Name	Meaning	Units.
AE	Cross-sectional area of the exit pipe from the intermediate tank.	ft^2
AP	Total area of perforations (i.e. free area for vapour passage.)	ft^2
AT	Total bubbling area.	ft^2
AV	Average liquid flowpath width.	ft
AX	Cross-sectional area of intermediate tank.	ft^2
C_1-C_7	Constants.	-
DELV	Change in vapour rate.	lb/sec.
DL	Liquid density.	lb/ft^3.
DV	Vapour density.	lb/ft^3.
E1,E2	Groups of variables defined by equations (6-8) and (6-11)	-
F_A	F-factor for vapour on perforated area of plate.	$(ft/sec)(lb/ft^3.)^{1/2}$
FD	Liquid fraction of the froth.	-
G	Acceleration due to gravity.	$ft.sec^2$.
HF	Depth of froth on the plate.	ft.
HL	Head of liquid in the intermediate tank.	ft
HW	Exit weir height.	ft
L	Liquid flow rate.	lb/sec.
V	Vapour flow rate.	lb/sec.
W	Weir height.	ft
WL	Hold up on tray.	lb
WT	Hold up in intermediate tank.	lb

Fig. 6-4

6.5 A mathematical model of the unit.

A simplified diagram of the unit showing some of the variables used in the model is given in Fig. 6-5.

6.5.1 The equations.

A glossary of nomenclature is given in Fig. 6-4. The equations are :-

a) The mass balance for the tray:

$$d/dt(WL) = L_1 - L_2 \qquad \text{....(6-1)}$$

b) The hold up on the tray :

$$WL = FD \times DL \times AT \times HF \qquad \text{....(6-2)}$$

c) The modified Francis formula for the flow of froth over a weir :

$$L_2 = C_1 \times AV \times FD \times DL \times (HF - HW)^{3/2} \qquad \text{....(6-3)}$$

d) The froth height correlation of Thomas and Campbell (9):

$$HF = C_2V + C_3L_1 + C_4HW + C_5V^2 + C_6 \qquad \text{....(6-4)}$$

e) The mass balance for the intermediate tank:

$$d/dt(WT) = L_2 - L_3 \qquad \text{....(6-5)}$$

f) The flow from the end tank:

$$L_3 = C_7 + DL \times AE \sqrt{(2G \times HL)} \qquad \text{....(6-6)}$$

g) The hold up in the end tank:

$$WT = AX \times DL \times HL \qquad \text{....(6-7)}$$

Hence there are seven equations in seven unknowns - L_3, HF, FD, WL, WT, HL, L_2.

6.5.2 The assumptions.

a) There is negligible mass transfer by which water is carried from the plate in to the vapour stream. (This was found to be a valid assumption by running the unit for a two-hour period. The reading on the weighing machine before start-up was noted and found to differ from that after shutdown by only $1\frac{1}{2}$ lbs.)

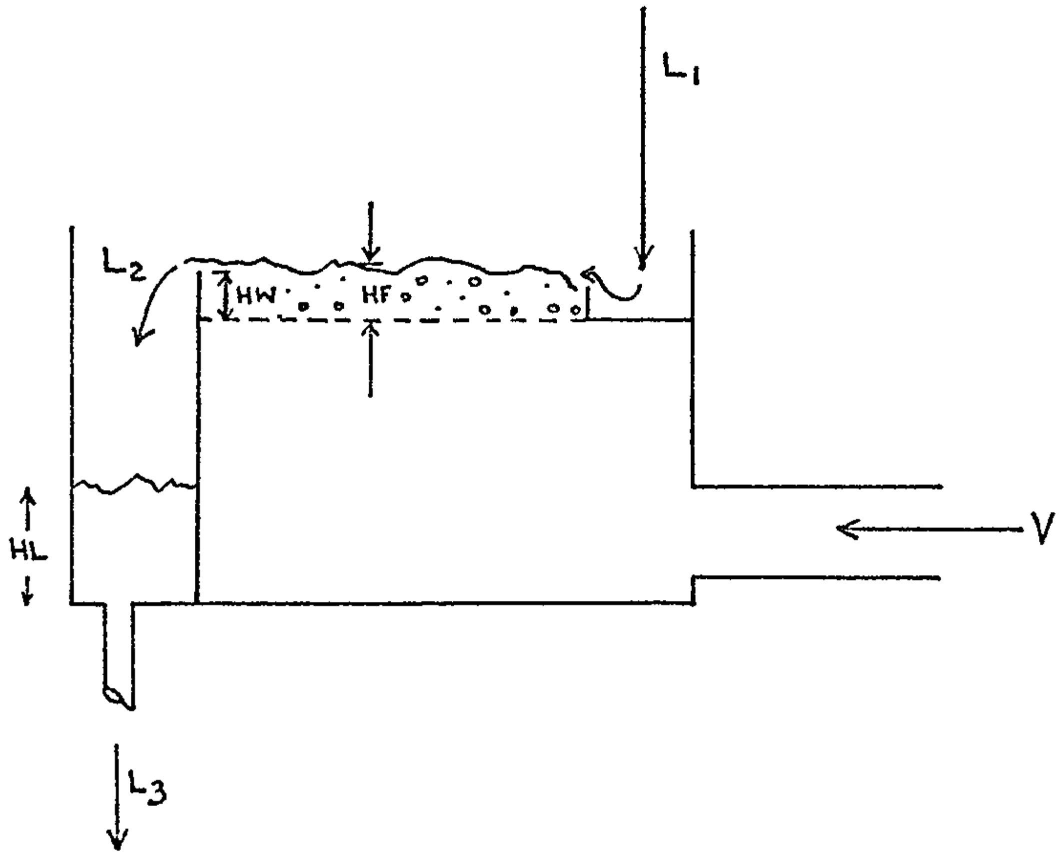


FIG. 6-5.

b) Equations (6-3) and (6-4) are valid. It was to check this assumption that this experimental work was performed.

6.5.3 The solution.

Define a new variable E1 such that

$$E1 = 1/(C_1 \times AV \times DL \times (HF - HW)^{3/2}) \qquad \text{....(6-8)}$$

Then equation (6-3) becomes :

$$L_2 = FD/E1 \qquad \text{....(6-9)}$$

Substitute for FD from equation (6-9) into equation (6-2) to obtain :

$$WL = E1 \times L_2 \times DL \times AT \times HF \qquad \text{....(6-10)}$$

Define $\quad E2 = E1 \times DL \times AT \times HF$

$$= (AT \times HF)/(C_1 \times AV \times (HF - HW)^{3/2}) \qquad \text{....(6-11)}$$

So that equation (6-10) becomes :

$$WL = E2 \times L_2 \qquad \text{....(6-12)}$$

Differentiate both sides of equation (6-12) with respect to time to obtain :

$$d/dt(WL) = E2\ d/dt(L_2) \qquad \text{....(6-13)}$$

(since $d/dt(HF) = 0$ then $d/dt(E2)=0$ also.)

Now substitute $d/dt(WL)$ from equation (6-13) into equation (6-1) to obtain :

$$E2\ d/dt(L_2) = L_1 - L_2 \qquad \text{....(6-14)}$$

Separating the variables and integrating both sides gives :

$$E2 \int_{t=o}^{t=\tau} \frac{dL_2}{(L_1 - L_2)} = \int_{t=o}^{t=\tau} dt$$

L_1 is fixed constant throughout for a step change. Hence :

$$E2 \left[-\log_e(L_1 - L_2) \right]_{t=o}^{t=\tau} = \tau$$

therefore $\quad \log_e \left\{ \frac{L_1 - L_2(\tau)}{L_1 - L_2(o)} \right\} = -\tau/E2 \qquad \text{....(6-15)}$

where $L_2(o)$ and $L_2(\tau)$ denote the values of L_2 at time zero and time τ respectively. Hence

$$L_2(\tau) = L_1 - (L_1 - L_2(o))\exp(-\tau/E2) \qquad \text{....(6-16)}$$

Now consider the equations for the intermediate tank. The hold up is given by :

$$WT = AX \times DL \times HL \qquad \text{....(6-7)}$$

Differentiating both sides with respect to time yields :

$$d/dt(WT) = AX \times DL \times d/dt(HL) \qquad \text{....(6-17)}$$

Substituting $d/dt(WT)$ from equation (6-17) into equation (6-5) gives :

$$AX \times DL \times d/dt(HL) = L_2 - L_3 \qquad \text{....(6-18)}$$

Substituting L_2 from equation (6-16) and L_3 from equation (6-6) into equation (6-18) gives :

$$AX \times DL \times d/dt(HL) = L_1 - (L_1 - L_2(o))\exp(-\tau/E2) - E3 \times HL^{\frac{1}{2}} \qquad \text{....(6-19)}$$

where E3 is defined by :

$$E3 = C_7 \times DL \times AE \times \sqrt{(2G)} \qquad \text{....(6-20)}$$

Integrating equation (6-19) by Euler's method gives :

$$HL(\tau) = HL(\tau-\Delta t) + \frac{\left(L_2\ (\tau-\Delta t) - E3 \times HL(\tau-\Delta t)^{\frac{1}{2}}\right)\Delta t}{(AX \times DL)} \qquad \text{....(6-21)}$$

Now $$L_3(\tau) = E3 \times HL\ (\tau)^{\frac{1}{2}} \qquad \text{....(6-22)}$$

Hence $$WT(\tau) = WT(\tau - \Delta t) + \tfrac{1}{2}\left[L_2(\tau) - L_3(\tau)\right] + \tfrac{1}{2}\left[L_2(\tau-\Delta t) + L_3(\tau-\Delta t)\right] \qquad \text{....(6-23)}$$

The step change in the vapour rate produces an instantaneous change in the froth height, matched by a compatible change in the froth density. This produces an instantaneous change in the liquid rate leaving the plate (but not in the liquid rate leaving the end tank.) Hence the solution to the vapour rate step change is achieved by first calculating this new value of L_2, then using the analysis for the liquid rate step change.

From equation (6-4) :

$$HF(0+) = C_2V + C_3L_1 + C_4HW + C_5V^2 + C_6 \quad ....(6\text{-}24)$$

Since the hold up on the tray is unchanged over the instant the step change is put in, equation (6-2) may be used to yield :

$$FD(0-) \times DL \times AT \times HF(0-) = FD(0+) \times DL \times AT \times HF(0+)$$

Hence $$FD(0+) = FD(0-) \times HF(0-)/HF(0+) \quad ....(6\text{-}25)$$

And so equation (6-3) gives the required initial value of L:

$$\underline{L_2(0) = C \times AV \times FD(0+) \times DL \times (HF(0+) - HW)^{3/2}} \quad ....(6\text{-}26)$$

6.5.4 The computer program.

The method of solution described in section 6.5.3 has been programmed in Fortran for the Argus 108 computer. This program has been used to calculate the responses predicted by the model for the experiments performed on the single sieve plate unit. The program listing and sample data and results are given in Appendix 5.

6.6 A comparison of the responses predicted by the model and those obtained by experiment.

Typical experimental and predicted response curves for the tray liquid hold up following step changes in the liquid and vapour rates are given in Figs. 6-2 and 6-3 respectively.

The predicted response curves produced by a liquid change is a poor match of the peak obtained on the experimental curve, the maximum deviation being 38% of the experimental value. In particular the peak on the experimental response curve indicates the presence of a hold-up or dead time at some point for which the mathematical model does not allow. This could arise for two reasons. No allowance was made in the model for the small distribution channel immediately prior to the tray. It is possible that the

FIG. 6-2.

PREDICTED AND EXPERIMENTAL RESPONSE CURVES FOR THE VARIATION IN TRAY HOLD UP FOLLOWING A STEP CHANGE IN LIQUID RATE.

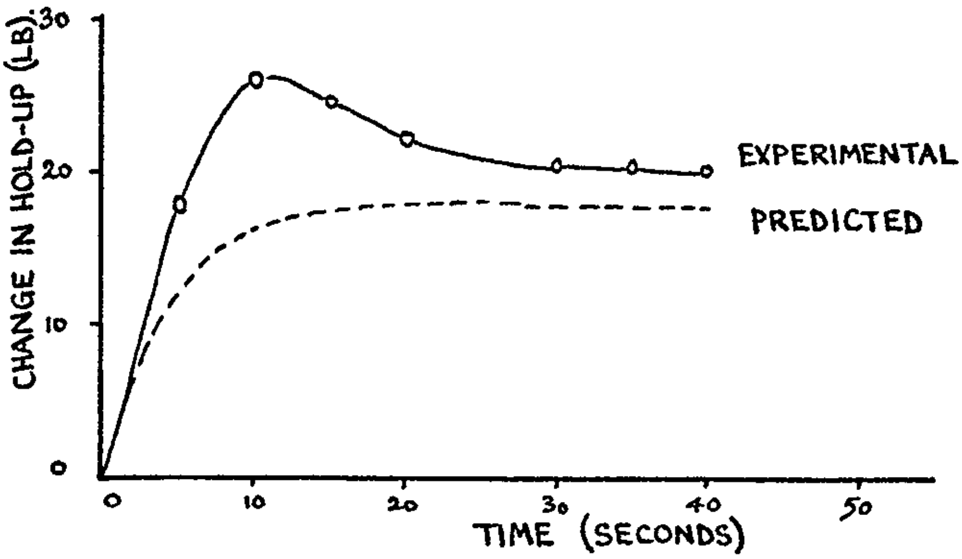
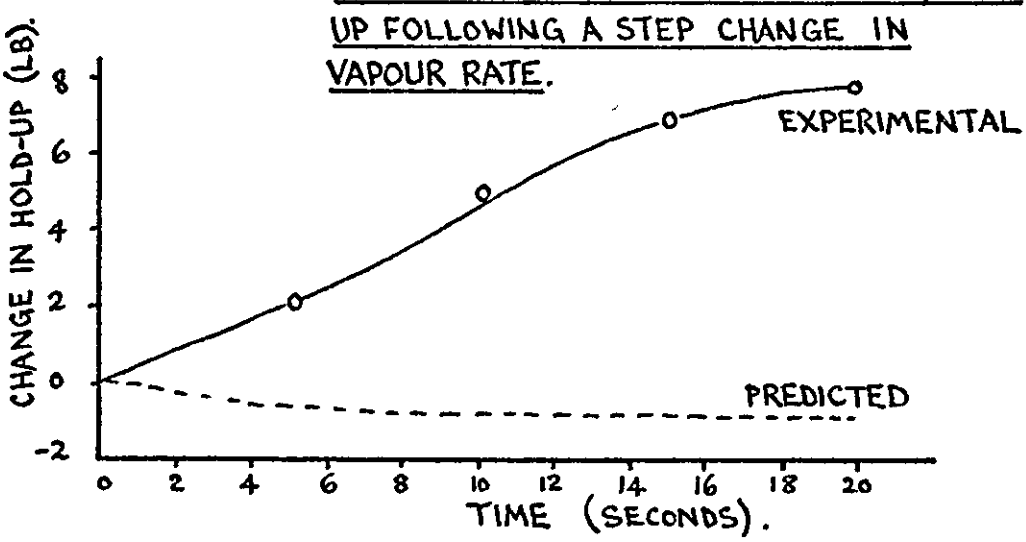


FIG. 6-3.

PREDICTED AND EXPERIMENTAL RESPONSE CURVES FOR THE VARIATION IN TRAY HOLD UP FOLLOWING A STEP CHANGE IN VAPOUR RATE.



hold-up in this increased appreciably with increasing liquid rate. Also no allowance was made for the time taken for the liquid surge to cross the plate immediately after the step was injected. It is felt likely that the peak on the experimental curve is mainly attributable to these causes. The overall time to achieve the steady state and the final steady state value for the tray hold up are predicted to within 20% and 12% respectively of the experimental values.

The response curves for the vapour change bear little resemblance to each other. The predicted time to achieve steady state differs by 50% of the experimental result. The model predicts a fall in the tray hold up of 0.75 lbs. The experimental result indicates a rise in tray hold up of 7.8 lbs.

6.7 Conclusions.

The correlations used produce a model which is moderately good as far as liquid flow changes are concerned but which is inadequate for vapour rate changes. Hence in the mathematical model of the crude unit described in Chapter 4 some confidence may be felt for its predictions with regard to holdup changes brought about by liquid flow changes, but little confidence can be placed upon results that include appreciable vapour rate changes. However, the experimental work at Llandarcy was not concerned with vapour flowrate changes as primary forcing functions, so that this discrepancy is not regarded as being particularly serious.

- - - - -

CHAPTER 7. OPERATION OF A CRUDE OIL DISTILLATION UNIT.

7.1 Introduction.

Although the majority of the work described in this thesis has been carried out at Loughborough University of Technology the project has a strong industrial bias. In view of this an attempt has been made in this chapter to draw together features from the results which have a direct bearing on the operation of a crude oil distillation unit.

7.2 Deductions based on the step-change experiments on the industrial unit.

The experimental work on the industrial unit is described in Chapter 5. The responses of the tray temperatures and product properties to step changes in the overhead reflux return and in the product offtake rates are described. One of the most interesting features to emerge from these results is the characteristic shape of many of the response curves, as shown in Fig. 5-41. This section considers the underlying reasons for this shape of curve.

The following effects may be expected to play a part :-

(i) The reduction in cold reflux entering the column will cause tray temperatures to rise by a simple heat transfer effect.

(ii) The hydrodynamic effect will result in heavy liquid being held higher in the column. This will boil at a higher temperature than the liquid it replaces.

(iii) Less cooling reflux will result in higher vaporisation at the top of the column giving a heavier vapour.

(iv) Higher vapour rates and hotter vapour will strip out more light ends from the top few trays causing these to become heavier. This in turn gives rise to higher vapour temperatures lower in the unit.

(v) As the heavier vapour condenses and mixes in the reflux drum the gravity of the reflux will rise. Thus at the top of the column less vaporisation will occur and more cooling reflux will pass onto the trays below.

(vi) As less vaporisation occurs the gravity of the vapour will fall off a little.

(vii) The mass transfer (fractionation) driving forces finally drive the system to equilibrium.

It may be appreciated that all of the above effects fit into the overall picture. A probable explanation is as follows :

During the first few minutes after the step change the tray temperatures rise by (i) the heat transfer effect and (ii) the hydraulic disturbance. The fall in reflux will also cause (iii) higher vaporisation to occur in these first few minutes. The rather slower fractionation effect of (iv), the hotter vapour at higher flowrate stripping out more light ends probably accounts for the next 20 minutes of the effect. The peak on the overhead vapour temperature curve occurs after only about 12 minutes and is then flat for about 30 minutes. The other peaks lower down the column occur at later intervals of time.

As the heavier vapour condenses in the reflux drum a slightly heavier reflux then passes into the column. The vapour coming up the column will now strip out rather less of this liquid allowing more cooling reflux to go onto the trays below. Thus the overhead vapour will probably become a little lighter and the greater cooling effect of the reflux in the rectification section will probably result in a lower overhead vapour temperature.

The flat peaks which occur on several of the response curves (e.g. overhead vapour temperature) are probably due to a balancing of the two effects at the top of the column: hotter vapour at a higher rate is coming up the column as a result of the (i), (ii), (iii) and (iv) effects occurring lower in the column; this is counteracted by the heavier reflux effect.

A similar explanation for the responses to a step change in the light gas oil offtake rate is envisaged:

As soon as the disturbance is first made the hydraulic response must be a general dumping of additional cold liquid down the lower half of the column. This will drive the tray temperatures rapidly downwards. In addition the heat transfer effect will be to reduce the vapour rate going up the column. Indeed the vapour leaving the light gas oil take-off tray should be lighter and at a lower flowrate. This should then allow the increase in the liquid flows leaving the trays above the light gas oil take off, without noticeably affecting tray temperatures in this area. Hence the first part of the response curve is a combined hydraulic and heat and mass transfer effect. The reverse swing occurs as the constant conditions in the flash zone gradually cause the increase in tray temperatures by the normal mass and heat transfer process.

7.3 Comments on the effectiveness and usefulness of the simple control strategy tried out on the industrial unit.

This experiment is described in section 5.4.6. In essence it consists of achieving a desired flowrate change by an initial step which is held for a certain period, followed by a ramp. A simple method is suggested for estimating optimum step size and starting time and slope of the ramp. These estimates are based on the response curves for a step change in the flowrates under consideration.

The first point of note is that the experiment achieved its objective - a smooth change in the response curves of the major column variables. This does not justify any sweeping conclusions of course, but the results do suggest a potential general method. Although the oscillation in the response curves has a different peak time and shape for each variable the method seems to produce a universal smoothing effect.

The parameters for the strategy were estimated from step response curves obtained when a different crude was being run. Some degree of generality is therefore indicated. However, the changes achieved in each case were each a similar percentage decrease in the reflux.

The method is probably sufficiently simple for operator usage, although the difficulty of manually inserting a ramp is significant. The method used in the experiment of approximating a ramp by a series of steps seems quite suitable. It may be that for many changes a standard set of parameters (size of the initial step, length of time for which this is held and the slope of the final ramp) may produce adequate results.

The method has only limited use for the initial problem posed by BP and described in section 2.1. This sets the objective of minimisation of period of upset following a major change in operating condition. The new steady state is approached very closely in perhaps half an hour as opposed to two hours. However, the main variables must still be adjusted for two hours and the 'steady state' will probably vary slightly during these adjustments. Some improvement will be gained from the smoothness of the change and the products can be expected to be within specification for the final one and a half hours.

The obvious major use for this type of programmed valve control will arise in a system employing direct digital control. In such a case the relevant parameter for the strategy would be stored in the computer memory and the step and the ramp would be input accurately.

The experiment described in Chapter 5 was carried out for a change in a single flowrate. Many changes on a crude unit involve simultaneous changes in process streams. To obtain the open loop response curves for all possible combinations is not practical. However, some simplification is possible. Suppose that the prime variables in the rectifying section are taken to be the temperature of the overhead vapour and the temperatures of each of the four sidestream withdrawals. Let these be denoted by the vector $\underline{w}$. The side control variables may be taken to be the five flowrates - the top reflux return and each of the sidestream withdrawal rates. Let these be denoted by the vector $\underline{x}$. Then for small deviations in $\underline{x}$, we may write :

$$\Delta \underline{w} \doteq J \Delta \underline{x} \qquad \text{....(7-1)}$$

$$\text{i.e.} \quad \Delta \underline{w} \doteq \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{bmatrix} \Delta \underline{x} \qquad \text{....(7-2)}$$

where $\quad a_{ij} = \partial w_i / \partial x_j$

i.e. J isthe Jacobian matrix.

Now it is well known that changing a sidestream withdrawal rate has a significant effect on the withdrawals below it but negligible effect on those above. Hence many elements in the Jacobian approximate to zero and equation (7-2) becomes:-

$$\Delta \underline{w} \doteq \begin{bmatrix} a_{11} & & & & \\ a_{21} & a_{22} & \cdot & & \\ a_{31} & a_{32} & a_{33} & & \\ a_{41} & a_{42} & a_{43} & a_{44} & \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{bmatrix} \Delta \underline{x} \quad \ldots.(7\text{-}3)$$

Now normally an equation such as (7-3) would be constructed to calculate the overall change in the steady state variables $\underline{w}$. However, there is no reason why it should not be constructed to estimate the heights of the peaks on the oscillatory step response curves. This assumes the principle of superposition and also that the peak times are approximately coincident. The justification for these quite coarse assumptions lies in the encouraging results obtained for the single experiment performed.

7.4 Deductions based on the results from the mathematical model.

The response curves predicted by the mathematical model for a step change in top reflux rate on a 15-plate column are given in Chapter 4. For this unit 3-4 minutes appears adequate for the flow rate responses to decay and very little longer is required for the temperature responses to die out. The results suggest that the flow oscillations would be smoothed by merely ramping in small flow changes rather than inputting a step. A ramp spread over perhaps 5-10 minutes would have a beneficial effect. This may well have a cumulative improvement on the mass transfer transient. An improvement of this type for minor flow changes would complement the simple control strategy for major changes discussed elsewhere.

7.5 Deductions based on the results of the single sieve plate experiments.

The results from these experiments described in Chapter 6 indicate that time constants of up to thirty seconds can be obtained with a laboratory sieve plate. Hence it is reasonable to expect time constants of this size and larger to be present in the industrial unit. This gives support to the discussion in section 7.2 which relied partly on the large times required for changes to move both up and down the industrial column.

7.6 Conclusions.

7.6.1 Use of the tower top temperature controller.

The crude unit at Llandarcy is normally operated with the overhead reflux on tower top temperature control. The overhead product rate is then set manually to keep the level in the reflux drum constant. The reflux drum then provides a buffer tank to allow the reflux rate to vary adequately for control purposes. The reflux step change experiments at Llandarcy were performed with the tower top controller disconnected to avoid interaction. It is suggested that, whilst this controller is desirable when the column is running under steady conditions, during major changes temperature stability should be achieved using planned flow control rather than by varying the reflux continually. The effects on product properties of varying amounts of light material can be large and are almost certainly non-linear.

7.6.2 Application of the simple valve control strategy.

The simple control strategy described in section 5.4.6. is probably best suited to DDC systems. Considerable work is required before this is a practical scheme for major complex changes but the results described indicate a potentially useful method.

7.6.3 Use of the mathematical model.

This indicates that liquid flow changes on a crude unit can produce appreciable oscillation and should be input gradually or in some pre-planned way. Although the flow and heat transfer transients decay in a few minutes liquid surges moving through the column could lead to composition imbalance requiring appreciable time for equilibration by the mass transfer driving forces.

CHAPTER 8. MATHEMATICAL MODELS FOR BINARY AND MULTICOMPONENT SYSTEMS.

8.1 Introduction.

The two basic methods for constructing a multicomponent distillation model are described in sections 8.2 and 8.3. The fundamental differences in the results obtained using each formulation are discussed in section 8.4. Section 8.5 contains a description of a distillation system used to demonstrate many of the methods in subsequent chapters. The basic requirements for equivalent simple systems to replace multicomponent systems are discussed in section 8.6.

8.2 The formulation of Mah et al.

Mah, Michaelson and Sargent (23) describe a matrix formulation for a multicomponent distillation system. They use the basic equation that for each component i on plate n (where x and y are absolute values and not deviation variables):-

$$\frac{d}{dt}\left\{H_n x_{ni} + h_n y_{ni}\right\} = L_{n-1}x_{n-1,i} - L_n x_{ni} + V_{n+1}y_{n+1,i}$$
$$-V_n y_{ni} - l_n x_{ni} - v_n y_{ni} + F_n x_{Fni} \qquad \ldots(8\text{-}1)$$

A stepwise solution procedure is proposed such that over each small time interval the approximation

$$y_{ni} = K_{ni}\, x_{ni}$$

is adequate. The differential term on the left hand side of equation (8-1) is based on the average composition over the time step.

In general the mole fractions calculated at the end of a time step do not sum to unity. Mah et al (23) avoid this difficulty by normalisation - that is each mole fraction is divided by the sum of all the mole fractions for the plate.

Neglecting vapour hold-up equation (8-1) may be written in matrix form :

$$\frac{d}{dt}\,\underline{x} = A\,\underline{x} + C$$

where $\underline{x}$ is a vector of liquid concentrations and C is a vector of forcing functions of the form

$$(F_n x_{Fni})/H_n$$

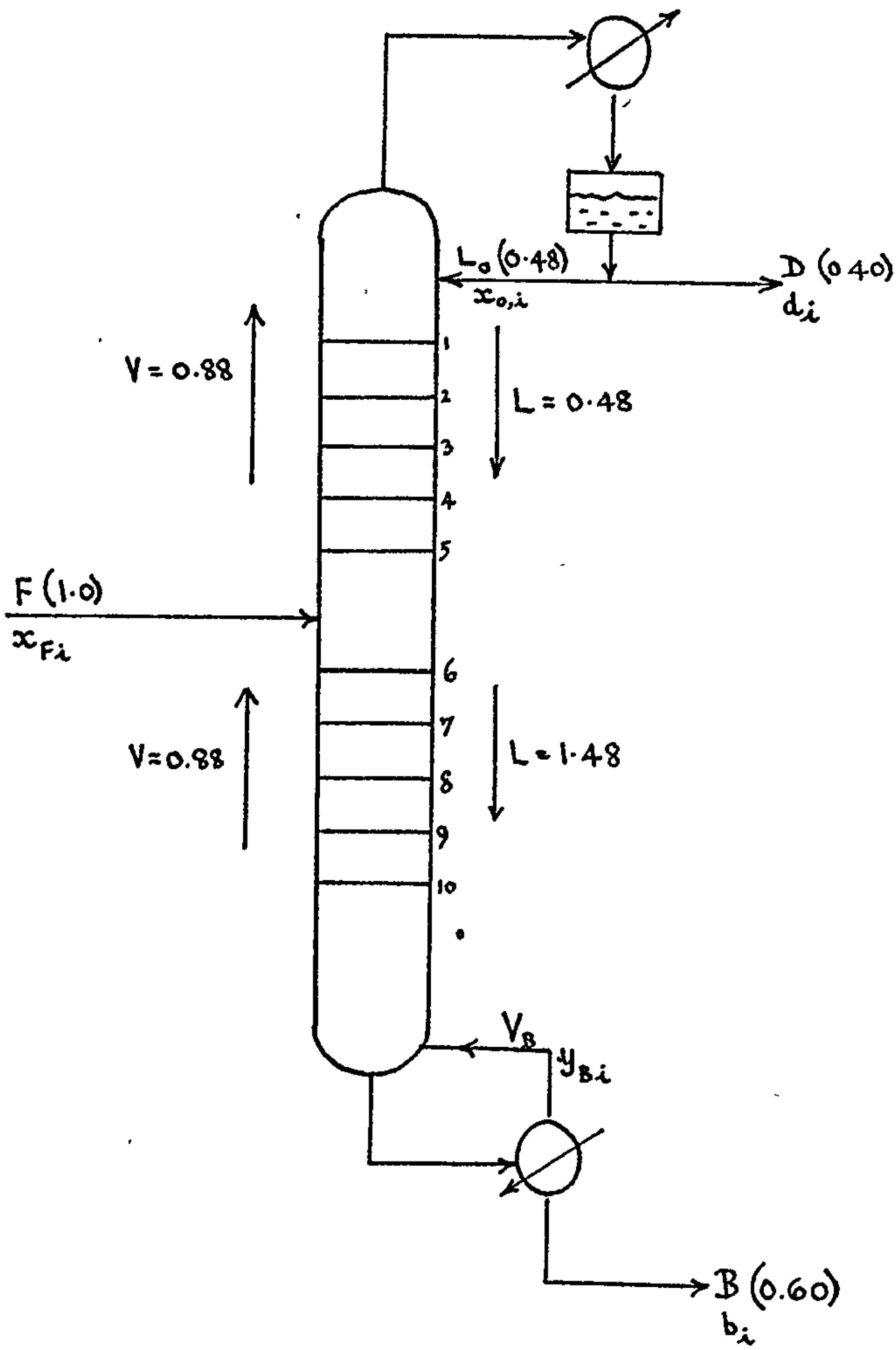


FIG. 8-1.

THE DISTILLATION COLUMN MODELLED.

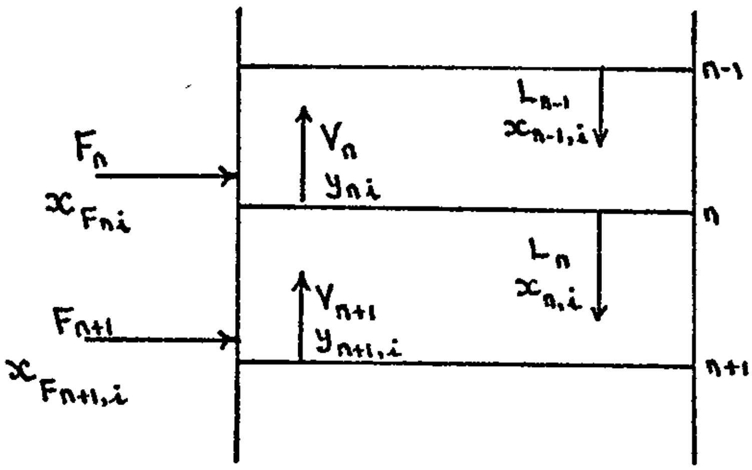


FIG. 8-2.
THE GENERAL PLATE.

GLOSSARY OF NOMENCLATURE FOR CHAPTER 8.

A	system matrix.
B	bottoms rate (moles/hour).
b_i	flowrate of component i in the bottoms (moles/hour).
C	forcing vector.
d	differential operator.
D	distillate rate (moles/hour).
d_i	flowrate of component i in the overheads (moles/hour).
f	function operator.
F	feed rate (moles/hour).
g	a function equivalent to the equilibrium constant.
H	tray liquid holdup (moles).
h	vapour holdup per tray (moles).
J	Jacobian matrix.
K	equilibrium constant.
L	Liquid rate (moles/hour).
l	deviation liquid rate (moles/hour).
N	total number of plates.
r	total number of components.
R	diagonal matrix of tray holdups.
S	square matrix.
t	time (hours).
T	forcing vector.
v	deviation vapour rate (moles/hour).
V	vapour rate (moles/hour)
x	liquid mole fraction.
y	vapour mole fraction.

Subscripts

i component i.

n plate n.

F feed.

B, $N+1$ reboiler

C condenser

Notes :

(i) A bar above the sum of two variables denotes that it is the average value over the time increment that is referred to. e.g. $\overline{V + v}$.

(ii) A bar above a single variable denotes that it is the steady state value that is referred to.

For one component in a system this leads to a tri-diagonal form for matrix A :

$$A = \begin{bmatrix} -\frac{1}{H_1}(L_1+l_1+v_1 \cdot K_1) & V_2K_2/H_1 & & & \\ L_1/H_2 & -\frac{1}{H_2}(L_2+l_2+K_2\overline{V_2+v_2}) & V_3K_3/H_2 & & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{L_{n-1}}{H_n} & -\frac{1}{H_n}(L_n+l_n+K_n\overline{V_n+v_n}) & V_{n+1}K_{n+1}/H_n & & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & \frac{L_{N-1}}{H_N} & -\frac{1}{H_N}(l_N+K_N\overline{V_N+v_N}) \end{bmatrix} \quad \ldots.(8\text{-}4)$$

For all three components in a ternary system the form of the above equation becomes :

$$A = \begin{bmatrix} x & o & o & x & o & o & & & & & & \\ o & x & o & o & x & o & & & & & & \\ o & o & x & o & o & x & & & & & & \\ x & o & o & x & o & o & x & o & o & & & \\ o & x & o & o & x & o & o & x & o & & & \\ o & o & x & o & o & x & o & o & x & & & \\ & & & x & o & o & x & o & o & x & o & o \\ & & & o & x & o & o & x & o & o & x & o \\ & & & o & o & x & o & o & x & o & o & x \end{bmatrix} \text{etc.} \quad \ldots.(8\text{-}5)$$

i.e. A is a matrix composed of a tridiagonal band of submatrices, each sub-matrix being diagonal. The significance of this will be seen when it is compared with the formulation of Wood (25) described in the next section.

8.3 The formulation of Wood.

Wood (25) describes a formulation of the unsteady state distillation mass balance which differs somewhat from equation (8-1). (A bar above the upper case variables denotes steady state values. x, y, l, v denote deviations from the steady state values of the liquid and vapour compositions and liquid and vapour molar flowrates respectively.) :-

$$\bar{L}_{n-1}x_{n-1,i} - (\bar{L}_n+g_{ni}\bar{V}_n)\,x_{n,i} + g_{n-1,i}\bar{V}_{n-1}x_{n-1,i} + F_n x_{Fni}$$

$$= \bar{H}_n \frac{dx_{n,i}}{dt} + h_n \frac{dy_{n,i}}{dt} - l_{n+1}(\bar{x}_{n+1,i} - \bar{x}_{n,i})$$

$$+ v_{n-1}\,(\bar{y}_{n,i} - \bar{y}_{n-1,i}) \qquad \ldots.(8\text{-}6)$$

The essential difference between equations (8-6) and (8-1) lies in the function g. Mah et al use the approximation of equation (8-2) to relate vapour composition to liquid composition over a small time interval. The function g in equation (8-6) is a function of the amounts of each component on the plate. It is given by equations (3-24) to (3-27) in Chapter 3, section 3.2.

Thus as Wood points out whereas in binary distillation the g_{ni} are constant for a particular mole fraction of component i on plate n, in multicomponent distillation g_{ni} is the slope of a line in vector space. Hence all compositions play a part.

By writing down the terms for g_{ni} for an r component mixture it may be demonstrated that the formulation of Wood gives :

$$\sum_{i=1}^{r} y_{n,i} = \sum_{i=1}^{r} g_{n,i}\,x_{n,i} = 0 \qquad (8\text{-}7)$$

This is a significant advantage of Wood's method over that of Mah et al which relied on normalisation of the mole fractions at the end of each time step.

Consider now a three component mixture and use equations (3-24) to (3-27) to replace the g_{ni} in equation (8-6). Neglecting vapour hold-up and considering composition changes only yields for the general plate :

$$\bar{H}_n \frac{dx_{ni}}{dt} = \bar{L}_{n-1} x_{n-1,i} - \left[\bar{L}_n x_{ni} + \bar{V}_n \left(\frac{\partial f_{ni}}{\partial \bar{x}_{n1}} x_{n1} + \frac{\partial f_{ni}}{\partial \bar{x}_{n2}} x_{n2} + \frac{\partial f_{ni}}{\partial \bar{x}_{n3}} x_{n3} \right) \right]$$

$$+ V_{n+1,i} \left(\frac{\partial f_{n+1,i}}{\partial \bar{x}_{n+1,1}} x_{n+1,1} + \frac{\partial f_{n+1,i}}{\partial \bar{x}_{n+1,2}} x_{n+1,2} + \frac{\partial f_{n+1,i}}{\partial \bar{x}_{n+1,3}} x_{n+1,3} \right)$$

$$+ F_n x_{Fni} \qquad \ldots.(8\text{-}8)$$

By the assumption of equimolal overflow :

$$\bar{L}_n = \bar{L}_{n-1} = L \text{ say.}$$

and

$$\bar{V}_n = \bar{V}_{n+1} = V \text{ say.}$$

(Note: The simplifying assumptions made are for the sake of simplicity only and are not essential to the basic formulation.)

so that dividing equation (8-8) by $\bar{L}_n$ yields :

$$\frac{\bar{H}_n}{L} \frac{d}{dt} \underline{x}_n = \underline{x}_{n-1} - \left[\underline{x}_n + \left(\frac{V}{L}\right) J_n \underline{x}_n \right] + \left(\frac{V}{L}\right) J_{n+1} \underline{x}_{n+1} + F_n \underline{x}_{Fn}$$

$$\ldots.(8\text{-}9)$$

where $\underline{x}_n = \begin{bmatrix} x_{1n} \\ x_{2n} \\ x_{3n} \end{bmatrix}$, and the elements of the 3 x 3 Jacobian matrix J may be seen from equation (8-8).

Clearly the value of V/L at and below the feed plate will differ from that above since L will vary at this point. Let (V/L) for the upper section be denoted $(V/L)^u$ and for the lower section $(V/L)^L$.

The condenser equation is obtained by application of the mass balance around the condenser - see Fig. 8-3.

$$\bar{V}_1 g_{1i} x_{1i} - (\bar{L}_o + \bar{D})\, x_{oi} = \bar{H}_o \frac{dx_{oi}}{dt} \qquad \ldots.(8\text{-}10)$$

but $\bar{V}_1 = \bar{L}_o + D$

$$\text{so that } (V/L)^u g_{1i} x_{1i} - \left(\frac{V}{L}\right)^u x_{oi} = \frac{\bar{H}_o}{L} \frac{dx_{oi}}{dt} \qquad \ldots.(8\text{-}11)$$

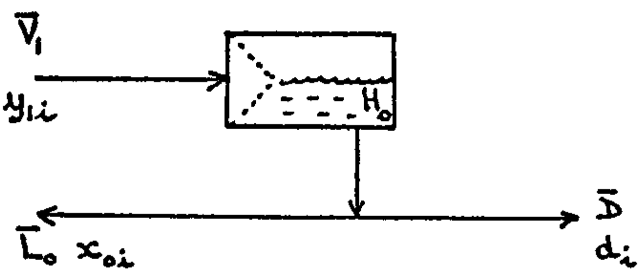


Fig. 8-3

And similarly for the reboiler :

$$\bar{L}_N x_{N,i} - (\bar{V}_{Bi} g_{Bi} x_{Bi} + \bar{B} x_{Bi}) = \bar{H}_B \frac{dx_{Bi}}{dt} \qquad \ldots.(8\text{-}12)$$

$$\text{giving } x_{N,i} - \left[\left(\frac{V}{L}\right) g_{Bi} + \left(\frac{B}{L}\right)\right] x_{Bi} = \frac{\bar{H}_B}{L} \frac{dx_{Bi}}{dt} \qquad \ldots.(8\text{-}13)$$

Application of equation (8-9) to the three component distillation model mentioned earlier yields a state variable model of the following form :

$$
\begin{bmatrix}
x\;o\;o & x\;x\;x & & & \\
o\;x\;o & x\;x\;x & \text{(condenser)} & & \\
o\;o\;x & x\;x\;x & & & \\
1\;o\;o & x\;x\;x & x\;x\;x & & \\
o\;1\;o & x\;x\;x & x\;x\;x\;\;\text{(plate 1)} & & \\
o\;o\;1 & x\;x\;x & x\;x\;x & & \\
 & 1\;o\;o & x\;x\;x & x\;x\;x & \\
 & o\;1\;o & x\;x\;x & x\;x\;x & \\
 & o\;o\;1 & x\;x\;x & x\;x\;x & \\
 & & \ddots & \ddots & \\
 & & & 1\;o\;o & x\;x\;x \\
 & & & o\;1\;o & x\;x\;x \\
 & \text{(reboiler)} & & o\;o\;1 & x\;x\;x
\end{bmatrix}
\begin{bmatrix} x_{o1} \\ x_{o2} \\ x_{o3} \\ x_{11} \\ x_{12} \\ x_{13} \\ x_{21} \\ x_{22} \\ x_{23} \\ \vdots \\ x_{B1} \\ x_{B2} \\ x_{B3} \end{bmatrix}
= \frac{d}{dt}
\begin{bmatrix} x_{o1} \\ x_{o2} \\ x_{o3} \\ x_{11} \\ x_{12} \\ x_{13} \\ x_{21} \\ x_{22} \\ x_{23} \\ \vdots \\ x_{B1} \\ x_{B2} \\ x_{B3} \end{bmatrix}
\qquad \ldots\text{(8-14)}
$$

or

$$
A\underline{x} + C = \frac{d\underline{x}}{dt} \qquad \ldots\text{(8-15)}
$$

8.4 The properties of the eigenvalues.

The characteristic shape of the response of a system to a step perturbation may be deduced from the type and magnitude of the eigenvalues. The main cases are given in Fig. 8-4. In the cases for which an oscillatory response is possible the type and magnitude of the dominant eigenvalues is important. It is quite feasible for the oscillatory contribution to be dwarfed by the contribution of the real negative eigenvalues near to the origin.

Mah et al (23) demonstrate that the eigenvalues of their system matrix for continuous systems are all real negative and distinct. These eigenvalues, the system poles, are shown to form a Sturm sequence, the zeroes interlacing with the poles. This eliminates any possibility of right half plane zeroes. From this it follows that the transient response to perturbation of the system described by equation (8-3)will always be minimum phase and non-oscillatory.

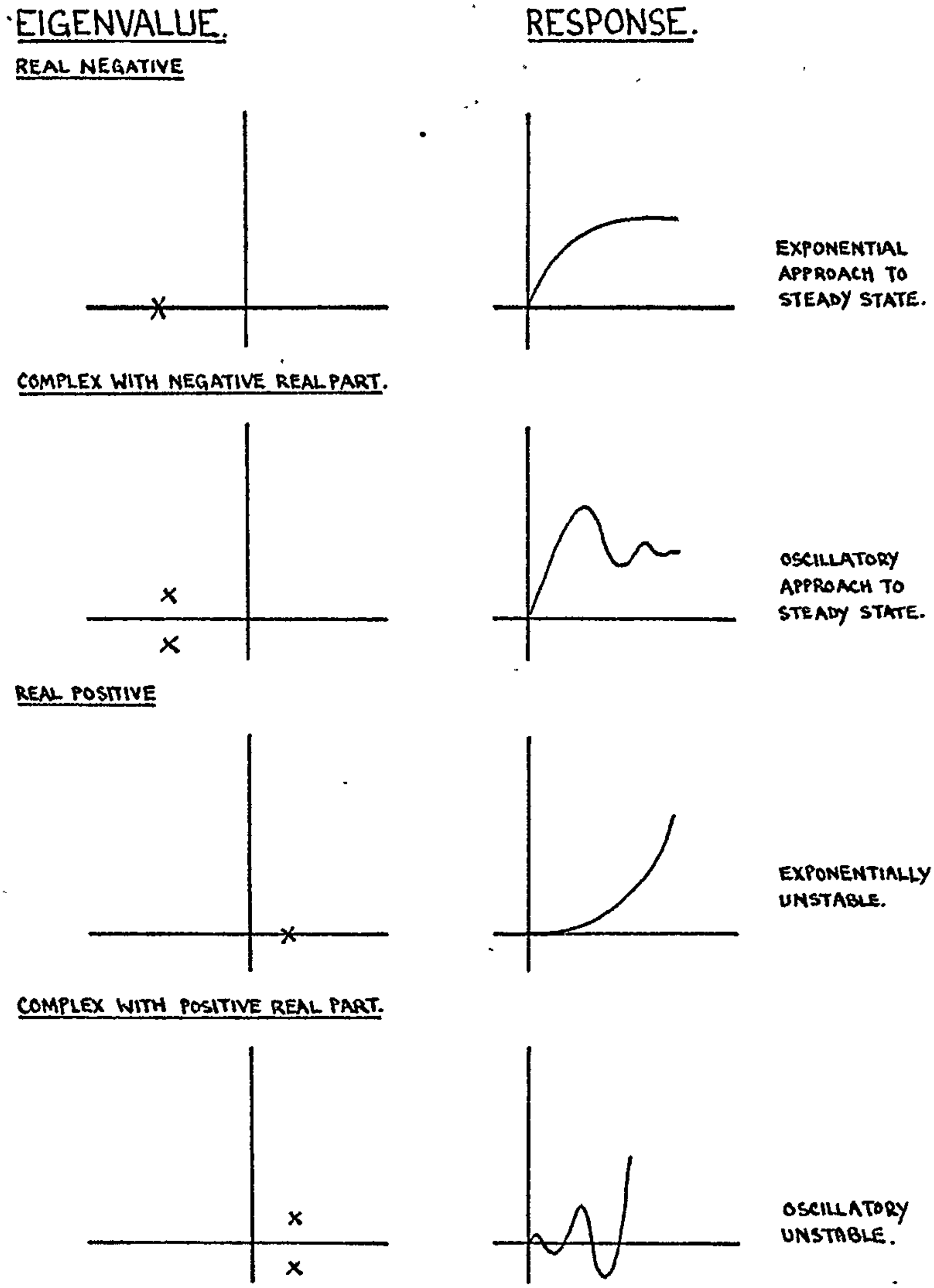


FIG. 8-4.

CHARACTERISTIC SHAPES OF STEP RESPONSE CURVES FOR VARIOUS DOMINANT SYSTEM EIGENVALUES.

The system matrix obtained using Wood's formulation has no such inherent restriction and may well exhibit complex eigenvalues and right half plane zeroes. Indeed it is this very property of Wood's method that leads the author to believe that this is basically a much more sound mathematical description of a system than that proposed by Mah et al. For this reason the distillation model described in the next section has been based on Wood's formulation.

8.5 A distillation model used to demonstrate many ideas in this thesis.

A ten plate column distilling a three component mixture was selected as being a realistically sized vehicle for demonstration purposes. The response of the system to a feed composition perturbation will be considered. The column is shown diagrammatically in Fig. 8-1. The feed used is a liquid at its boiling point of $148^{\circ}F$ and is given in Fig. 8-5.

	BASIC FEED	OVERHEAD PRODUCT	BOTTOMS	NEW FEED	OVERHEAD PRODUCT	BOTTOMS
propane	0.300	0.7337	0.01084	0.350	0.8505	0.01632
n-butane	0.400	0.2657	0.4895	0.350	0.1493	0.4838
n-pentane	0.300	0.0005214	0.4997	0.300	0.0001693	0.4999

Fig. 8-5

Mole fraction composition at steady state of feed and products before and after step-change.

The column is assumed to have a reboiler and a total condenser and operates with a reflux ratio of 1.2. The assumptions of equimolal overflow and unit plate efficiency are also made. The equilibrium data for the three components are assumed to satisfy the following relation for component i at the temperature on plate j, T_j :

$$K_{ji} = \exp\left[A_i - B_i/T_j + C_i T_j\right] \qquad \ldots.(8\text{-}16)$$

The coefficients A, B and C are obtained from Clark (34).

The steady state solution for a distillate rate of 0.4 moles/mole feed has been obtained using a computer program written by Clark (34) for the ICL 1905. This is based on the calculation method recommended by Holland (32) incorporating the Thiele Geddes method of solution speeded by the Theta method of convergence. Clark's program was also used to find the steady state solution to a step change in the feed composition. The steady state results for the products are given in Fig. 8-5, those for all trays being contained in Appendix 6.

Reflux drum, tray and reboiler design is assumed to be such that :

$$(H/L)_0 = 0.5 \text{ hours}$$

$$(H/L)_n = 0.03 \text{ hours} \qquad n = 1,2 \ldots N$$

$$(H/L)_{N+1} = 0.2 \text{ hours}$$

The basic equations for the system are taken from Wood's formulation - equations (8-9), (8-11) and (8-13).

The elements of the submatrices $(V/L).J_n$ were calculated using a computer program written for the Argus 108 computer in the Department of Chemical Engineering at Loughborough University of Technology.

The matrix equation for the complete system may be written :

$$R \frac{d}{dt} \underline{x} = S \underline{x} + T \qquad \text{....(8-17)}$$

where R is a diagonal matrix whose diagonal elements are :

$$\left[H_c/L_u,\ H_c/L_u,\ H_c/L_u,\ H_1/L_u,\ \ldots\ldots H_B/L_L,\ H_B/L_L,\ H_B/L_L \right]$$

Comparison of equations (8-17) and (8-15) indicate that the basic system matrix A is given by :

$$A = R^{-1}S \qquad \text{....(8-18)}$$

and the forcing function C by :

$$C = R^{-1}T \qquad \text{....(8-19)}$$

This is given in full in Appendix 6.

The non-zero elements in the forcing vector C have magnitude Fx_F/H_F where x_F is the change in the feed composition from the steady state value.

$$x_F = 0.05 \qquad F = 1.0$$

$$H_F/L_F = 0.03 \qquad L_F = 1.48$$

Hence $\quad Fx_F/H_F = 1.28$

Hence the forcing vector is :

$$\begin{bmatrix} 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, \\ 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, \\ 1.128, & -1.128, & 0, & 0, & 0, & 0, & 0, & 0, & 0, \\ 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, & 0, \\ 0 \end{bmatrix}^T$$

Various analyses and solutions for this model are contained in Chapters 9, 10 and 11.

8.6 Error introduced by linearisation.

The steady state solution to equation (8-17) is given by :

$$\underline{x} = -(R^{-1} S)^{-1} R^{-1} T$$

If the system were truly linear this should match the final steady state predicted by the distillation design program. The comparison is given in Fig. 8-6. From this it may be seen that the assumption of linearity may produce errors in the change in tray compositions of up to 25%. However, when the discrepancy is expressed as a percentage of the final tray composition the error is much less.

	LIGHT		MIDDLE		HEAVY	
TRAY	(1)	(2)	(1)	(2)	(1)	(2)
Condenser	-0.1168	-0.1155	0.1164	0.1151	0.0003521	0.0003506
1	-0.1655	-0.1478	0.1635	0.1460	0.001995	0.001793
2	-0.1476	-0.1249	0.1423	0.1206	0.005231	0.004340
3	-0.1155	-0.09759	0.1051	0.08943	0.01047	0.008152
4	-0.0916	-0.07946	0.0748	0.06698	0.01685	0.01248
5	-0.0750	-0.06730	0.0562	0.05375	0.0189	0.01355
6	-0.0597	-0.05588	0.0532	0.05125	0.0065	0.004632
7	-0.0509	-0.04644	0.0451	0.04238	0.0058	0.004068
8	-0.03694	-0.03274	0.0323	0.02961	0.0046	0.003129
9	-0.02320	-0.01998	0.0198	0.01783	0.0033	0.002148
10	-0.01258	-0.01040	0.0108	0.009402	0.0018	0.0009947
Reboiler	-0.00548	-0.006296	0.0057	0.006452	-0.0002	-0.0001562

Change in Tray compositions (mole fractions)

(1) distillation obtained by design program of Clark.

(2) steady state solution to linear model.

Fig. 8-6.

8.7 Reduction of multicomponent systems to equivalent simple systems.

Many workers have constructed and solved models of binary distillation systems. They have demonstrated that consideration of one component onlyis quite adequate. In section 8.4 the different characteristics of two types of multicomponent models are discussed. On this basis it appears that reduction of a multicomponent system to anything other than an equivalent ternary system will never produce a model with characteristics similar to those of the complete model.

On this basis the work of Gilbert (36) described in section 3.3 offers one approach to the reduction of systems containing many components such as crude oil. The problem is that the effective absorption factor concept would have to be modified to permit application to more than one component. The best approach would seem to be the use of the cut point component as suggested by Gilbert and in addition the use of a light and a heavy key.

- - - - - - - - - -

CHAPTER 9. TRANSFER FUNCTION REPRESENTATION OF STATE VARIABLE MODELS.

9.1 Introduction.

This section describes the basic differences between the representation of a system by a transfer function and by a state variable model. Different ways of deducing a transfer function from a state variable model are outlined and discussed. Examples are based on the distillation of a ternary mixture in a ten plate distillation column.

9.2 Definitions.

A dynamic system can generally be completely specified by a certain minimum number of variables within the system. These are called the state variables for that system. The vector having these variables for its elements is called the state vector.

9.3 Features of the two types of models.

There may be several sets of variables in a system that together satisfy the definition of state variables. The simplest example is that of a ternary liquid with mole fractions x_1, x_2 and x_3.

$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ $\begin{bmatrix} x_1 \\ x_3 \end{bmatrix}$ or $\begin{bmatrix} x_2 \\ x_3 \end{bmatrix}$ together with $\sum_{i=1}^{3} x_i = 1$ satisfy the above requirement and can be termed state vectors.

A transfer function is rather different. This relates the response of a particular variable to a particular disturbance. The transfer function is the Laplace transform of the response of one variable to one input. Only the location of the input is important (e.g. a particular feed composition disturbance in a distillation column.) The amplitude and frequency do not affect the transfer function.

GLOSSARY OF NOMENCLATURE FOR CHAPTER 9.

A	system matrix.
a_{ij}	element of matrix A.
a_m	coefficient of s^m
$B\underline{u}$	forcing vector.
b_i	element of $B\underline{u}$ vector.
C_m	square matrix of coefficients of s^m occurring in the adjoint matrix.
d	differential operator.
e	extraneous root.
G	transfer function.
H	Bush matrix.
h_{Ni}	bottom row element of Bush matrix.
I	unit matrix.
K	scalar multiplying factor.
p	pole of the transfer function.
R	see equations (9-10) and (9-11).
s	Laplace variable.
T	square matrix of transfer function numerator polynomial coefficients.
t	time
x	liquid mole fraction.
z	zero of transfer function.

Subscript

n	variable n

Superscript

*	defined in section 9.4.2

A transfer function model is often an incomplete representation of a system. It is also important to note that a state variable model can readily be constructed to take account of interaction. This is not usually a simple task with a transfer function model.

9.4 Methods available for constructing a transfer function from a state variable equation.

Consider the basic equation of the general system :-

$$\frac{d}{dt}\underline{x} = A\underline{x} + B\underline{u} \qquad \text{....(9-1)}$$

where $\underline{x}$ = state vector

A = system matrix

$B\underline{u}$ = vector representing the forcing function

Taking the Laplace transform of equation (9-1) gives :-

$$(Is - A)\,\underline{x}\,(s) = B\underline{u}\,(s) \qquad \text{....(9-2)}$$

By Cramer's rule (59) the solution for the nth element in the state vector is given by :-

$$x_n(s) = \frac{|Is - A|_n}{|Is - A|} \qquad \text{....(9-3)}$$

where $|Is - A|$ is the determinant of $(Is - A)$

and $|Is - A|_n$ is the determinant of the matrix formed by replacing the nth column of $(Is - A)$ by $B\underline{u}(s)$.

For an impulse perturbation $B\underline{u}\,(s) = B\underline{u}$

and for a step perturbation $B\underline{u}\,(s) = (1/s).B\underline{u}$

Now the transfer function representation of equation (9-3) is :-

$$\frac{x_n(s)}{r(s)} = G_n(s) \quad \text{where } r \text{ is the input perturbation.}$$

Hence we see that for a unit disturbance :-

$$G_n(s) = \frac{|Is - A|_n}{|Is - A|}$$

The poles of the transfer function are those values of s for which the function $G(s)$ tends to infinity. Clearly these will be given by the solution to the characteristic equation

$$|Is - A| = 0$$

It is well known that the solutions to this equation are the eigenvalues of the matrix A. The problem in deriving the transfer function lies in evaluating the numerator. Four methods are available and are described in succeeding sections.

9.4.1 Transfer function numerator via determinant evaluation.

Consider a third order system. Suppose the elements of $B\underline{u}$ are denoted by $\begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$ then the transfer function for the response x_2 is given by

$$G_2(s) = \begin{vmatrix} s-a_{11} & b_1 & -a_{13} \\ -a_{21} & b_2 & -a_{23} \\ -a_{31} & b_3 & s-a_{33} \end{vmatrix} \Bigg/ |Is - A| \quad \ldots.(9\text{-}4)$$

The determinant may be readily multiplied out by hand for systems of up to fifth order. Above this computer logic could be employed. However, the evaluation of medium sized (say 90) determinants is extremely costly in computation time. At about size 100, years of time on a third generation machine are necessary (ref. Acrivos and Amundsen (67)). Hence this is not suitable as a general method. Hennion (45) gives an algorithm which might prove suitable but results using this for medium sized systems are not given.

9.4.2 Transfer function zeroes via the method of Davison.

The transfer function being considered is :-

$$G_n(s) = \frac{|Is - A|_n}{|Is - A|}$$

Davison (46) showed that the roots of $\left|Is-A\right|_n$ are included in the eigenvalues of $[A]_n^*$. $[A]_n^*$ denotes the system matrix with the nth column replaced by K$B\underline{u}$ where K is a scalar multiplying factor. It is recommended by Davison that K be chosen to be of an order 10^{10} higher than the elements of A. Extraneous roots are produced but these are said to be readily recognisable as they are appreciably larger than the true zeroes. The method is also valid if the nth column of the system is replaced by $B\underline{u}$ but the nth row is multiplied by the factor K. Davison outlines a proof of the method based on the evaluation of the determinants and formation of the characteristic equation :

$$\left|Is - A\right|_n^* = 0 \qquad \ldots.(9\text{-}5)$$

A simpler proof may be constructed by considering the properties of a determinant. The eigenvalues of $[A]_n^*$ are given by the roots of the characteristic equation (9-5). For a 3 x 3 matrix for n=2 this gives :-

$$\begin{vmatrix} s-a_{11} & -Kb_1 & -a_{13} \\ -a_{21} & s-Kb_2 & -a_{23} \\ -a_{31} & -Kb_3 & s-a_{33} \end{vmatrix} = 0 \qquad \ldots.(9\text{-}6)$$

This determinant may be expressed as the sum of two determinants (ref. Kreyszig (59)).

$$\begin{vmatrix} s-a_{11} & -Kb_1 & -a_{13} \\ -a_{21} & -Kb_2 & -a_{23} \\ -a_{31} & -Kb_3 & s-a_{33} \end{vmatrix} + \begin{vmatrix} s-a_{11} & 0 & -a_{13} \\ -a_{21} & s & -a_{23} \\ -a_{31} & 0 & s-a_{33} \end{vmatrix} = 0 \qquad \ldots.(9\text{-}7)$$

i.e.

$$-K \times \begin{vmatrix} s-a_{11} & b_1 & -a_{13} \\ -a_{21} & b_2 & -a_{23} \\ -a_{31} & b_3 & s-a_{33} \end{vmatrix} + \begin{vmatrix} s-a_{11} & 0 & -a_{13} \\ -a_{21} & s & -a_{23} \\ -a_{31} & 0 & s-a_{33} \end{vmatrix} = 0 \qquad \ldots.(9\text{-}8)$$

Clearly for high values of K equation (9-8) will approximate to equation (9-5). For K equal to infinity this approximation becomes exact.

The validity of the Davison row method, in which row n rather than column n is multiplied by K may be seen from equation (9-7). The row method would yield the alternative equation :-

$$\begin{vmatrix} s-a_{11} & -b_1 & -a_{13} \\ -Ka_{21} & -Kb_2 & -Ka_{23} \\ -a_{31} & -b_3 & -a_{33} \end{vmatrix} + \begin{vmatrix} s-a_{11} & 0 & -a_{13} \\ -a_{21} & s & -a_{23} \\ -a_{31} & 0 & s-a_{33} \end{vmatrix} = 0$$

$$\text{i.e. } K \times \begin{vmatrix} s-a_{11} & -b_1 & -a_{13} \\ -a_{21} & -b_2 & -a_{23} \\ -a_{31} & -b_3 & s-a_{33} \end{vmatrix} + \begin{vmatrix} s-a_{11} & 0 & -a_{13} \\ -a_{21} & s & -a_{23} \\ -a_{31} & 0 & -a_{33} \end{vmatrix} = 0$$

$$\text{i.e. } \begin{vmatrix} s-a_{11} & -Kb_1 & -a_{13} \\ -a_{21} & -Kb_2 & -a_{23} \\ -a_{31} & -Kb_3 & s-a_{33} \end{vmatrix} + \begin{vmatrix} s-a_{11} & 0 & -a_{13} \\ -a_{21} & s & -a_{23} \\ -a_{31} & 0 & s-a_{33} \end{vmatrix} = 0$$

which is identical to equation (9-7).

Davison recommends that the value of K be selected to be of order 10^9 to 10^{15} greater than the elements of the matrix. A discussion of the numerical problems associated with this is given later in this chapter.

The importance of the row method, as pointed out by Davison (46), is that it reduces inaccuracy in the first part of the eigenvalue QR routines. This involves transformation of the matrix to upper Hessenberg form. The row or column method is selected so that the large elements fall into the upper Hessenberg part of the matrix. This results in less manipulation of very large and very small numbers which is a major source of numerical error.

It is of importance to note that the structure of equation (9-8) leads to a useful check on the numerical accuracy of the results using Davison's method. The second determinant contains a term $\dot{s}$ on the diagonal. Hence it is not possible for this determinant to contribute to the constant term in the expansion of the left hand side of equation (9-8). Hence this constant term must always be proportional to K. It may be readily obtained in practice as the product of all the eigenvalues obtained by the application of Davison's method.

It is possible to use a further check and also obtain the gain of the transfer function. From the expansion of equation (9-8) and neglecting the second determinant it follows that :

$$- K\, a_m \prod_{i=1}^{m} (s-z_i) = 0$$

from which it may be seen that the constant term is :

$$- K\, a_m \prod_{i=1}^{m} z_i$$

which should approximate to the product of all the eigenvalues obtained by Davison's method.

$$\text{i.e.} \quad - K\, a_m \prod_{i=1}^{m} (z_i) = \prod_{i=m+1}^{n} (e_i) \cdot \prod_{i=1}^{m} (z_i)$$

where e_i are the extraneous roots. Hence since $\prod_{i=1}^{m} z_i$ = constant for large K then

$$a_m = - \prod_{i=m+1}^{n} (e_i)/K.$$

Constancy of this factor provides a second check on the numerical convergence as K is increased. Also it provides a slightly simpler way of obtaining the gain than that proposed by Davison.

If the product of all the eigenvalues and the extraneous root product are each plotted against K then a graph similar to that shown in Fig. 9-9 should be obtained. Correct values of the zeroes will be calculated at values of K for which both curves are horizontal. Experience with the eigenvalue routines on the ICL 1905 showed that both curves normally exhibited a second plateau at high values of K. This should be ignored.

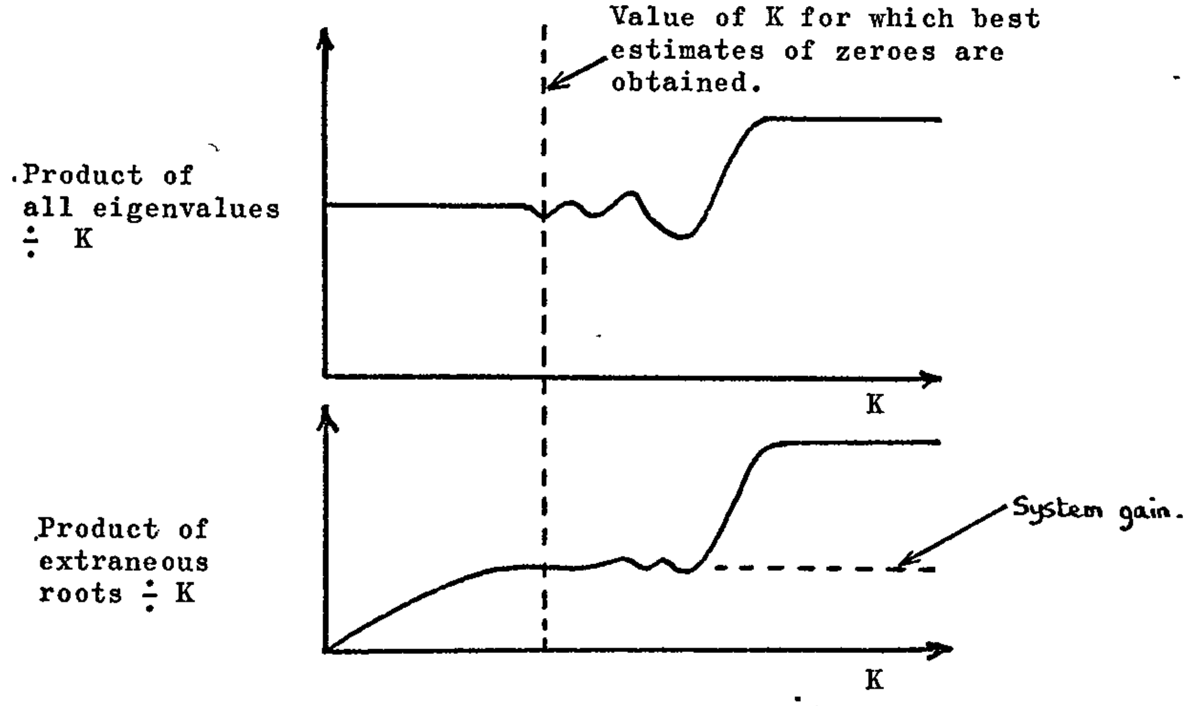


Fig. 9-9

9.4.3 Transfer function zeroes via the root locus.

If the poles of $G_n(s)$ are denoted by p_i and the zeroes by z_j then the transfer function may be written:-

$$k\,G_n(s) = \frac{k\prod_{j=1}^{m}(s-z_j)}{\prod_{i=1}^{\ell}(s-p_i)} \qquad \ldots.(9\text{-}9)$$

for a 3 x 3 problem in which n=2 this is equivalent to:-

$$k\,G_n(s) \;=\; \frac{K\begin{vmatrix} s-a_{11} & b_1 & -a_{13} \\ -a_{21} & b_2 & -a_{23} \\ -a_{31} & b_3 & s-a_{33} \end{vmatrix}}{\begin{vmatrix} s-a_{11} & -a_{12} & -a_{13} \\ -a_{21} & s-a_{22} & -a_{23} \\ -a_{31} & -a_{32} & s-a_{33} \end{vmatrix}} \qquad \ldots.(9\text{-}10)$$

where:

$$K = k \,/\, (\text{coefficient of } s^m) \qquad \ldots.(9\text{-}11)$$

Note of course that m need not necessarily be n-1.

For a closed loop system with negative feedback the characteristic equation for the root locus may be written:-

$$1 + kG_n(s) = 0$$

$$\text{or } K\begin{vmatrix} s-a_{11} & b_1 & -a_{13} \\ -a_{21} & b_2 & -a_{23} \\ -a_{31} & b_3 & s-a_{33} \end{vmatrix} + \begin{vmatrix} s-a_{11} & -a_{12} & -a_{13} \\ -a_{21} & s-a_{22} & -a_{23} \\ -a_{31} & -a_{32} & s-a_{33} \end{vmatrix} = 0 \qquad \ldots.(9\text{-}12)$$

Equation (9-12) gives the path of the roots of the system as K is varied from zero to infinity. It is evident that K equals zero will yield the poles of the system and K equals infinity will yield the zeroes. This is of course in accordance with the properties of the root locus (ref. Chen and Haas (44)). Equation (9-12) may be manipulated using the properties of determinants (ref. Kreyzig (59)). to yield:-

$$\begin{vmatrix} s-a_{11} & -(a_{12} - Kb_1) & -a_{13} \\ -a_{21} & s-(a_{22} - Kb_2) & -a_{23} \\ -a_{31} & -(a_{32} - Kb_3) & s-a_{33} \end{vmatrix} = 0 \qquad \ldots.(9\text{-}13)$$

The roots of (9-13) are clearly the eigenvalues of:-

$$\begin{bmatrix} a_{11} & (a_{12} - K b_1) & a_{13} \\ a_{21} & (a_{22} - K b_2) & a_{23} \\ a_{31} & (a_{31} - K b_3) & a_{33} \end{bmatrix}$$

Hence determination of the eigenvalues of this matrix for high values of K should yield approximations to the zeroes of the original system, together with some extraneous roots. These extraneous roots are points on the locii of the roots that tend to infinity as K tends to infinity and should be recognisable on two criteria. The first is that they should be appreciably larger than the true zeroes. The second is that as K is increased so these should continue to increase, the true zeroes remaining unchanged.

The reader will note the close similarity of this method of zero determination to the method of Davison. In fact if equations (9-13) and (9-6) are compared then there is a value of K above which for computational purposes the methods are identical. If the computer word length permits the storage of a number to 12 decimal digits, then a value of say $-Kb_1$ that is of order 10^{12} greater than a_{12} will be indistinguishable from the value $(a_{12} - Kb_1)$ stored in the same machine.

Further discussion on the numerical problems associated with the choice of K is given later in the chapter.

<u>9.4.4 Transfer function numerator via the method of Bosley et al.</u>

Consider the basic state variable model described by equation (9-1) and the Laplace transform of this, equation (9-2). The solution of equation (9-2) may be written

$$\underline{x}(s) = [Is - A]^{-1} B\underline{u}(s) \qquad \ldots.(9\text{-}14)$$

or

$$\underline{x}(s) = \frac{\text{Adj}\,[Is - A]}{|Is - A|} B\underline{u}(s) \qquad \ldots.(9\text{-}15)$$

Clearly $\mathrm{Adj}[Is - A]B\underline{u}(s)$ is a column vector, each element of which is a polynomial in s of maximum order N-1 where N is the order of the system. Hence, the transfer function $G_j(s)$ relating the response of the jth element in $\underline{x}$ to the perturbation $\underline{u}(s)$ will be the jth element of $\mathrm{Adj}[Is - A]B\underline{u}(s)$ divided by $|Is - A|$. A method is described in a paper by Bosley et al (49) for obtaining a transfer function numerator via the adjoint matrix. The method will be stated then proved.

Write Adj (Is - A) B$\underline{u}$ in polynomial form

$$\begin{bmatrix} (t_{10} + t_{11}\, s + t_{12}\, s \;\ldots\ldots\ldots\; t_{1\,N-1}s^{N-1}) \\ t_{20} + t_{21}\, s + t_{22}\, s \;\ldots\ldots\ldots\; t_{2\,N-1}s^{N-1}) \\ \cdot \\ \cdot \\ \cdot \\ t_{No} + t_{N1}s + t_{N2}s \;\ldots\ldots\ldots\; t_{N\,N-1}s^{N-1}) \end{bmatrix} \qquad \ldots.(9\text{-}16)$$

a column vector

and rearrange the coefficients into a matrix:-

$$T = \begin{bmatrix} t_{10} & t_{11} & t_{12} & \ldots\ldots\ldots\ldots & t_{1\,N-1} \\ t_{20} & t_{21} & t_{22} & \ldots\ldots\ldots\ldots & t_{2\,N-1} \\ \cdot & & & & \\ \cdot & & & & \\ \cdot & & & & \\ t_{No} & t_{N1} & t_{N2} & \ldots\ldots\ldots\ldots & t_{N\,N-1} \end{bmatrix} \qquad \ldots.(9\text{-}17)$$

Clearly if this T matrix can be found, then, as the elements represent the coefficients of the N numerator polynomials, the problem is solved, for it is a simple matter to find the M zeroes of each polynomial by some root searching technique.

Matrix T can in fact be found from the equation

$$TH = AT \qquad \ldots.(9\text{-}18)$$

Equation (9-18) is a similarity transformation for producing the Bush matrix form. As shown below T can be evaluated very simply if the characteristic equation is known.

H is the Bush form of the A matrix:-

$$H = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & & \\ \vdots & & 0 & 1 & \cdots & \\ \vdots & & & & \ddots & 1 \\ h_{N1} & h_{N2} & \cdots & & h_{NN-1} & h_{NN} \end{bmatrix} \qquad \ldots.(9\text{-}19)$$

where the elements $h_{N1} \ldots\ldots h_{NN}$ are simply related to the coefficients of the characteristic equation of A by

$$|sI - A| = a_o + a_1 s \;\ldots\ldots\; + a_N s^N \qquad \ldots.(9\text{-}20)$$

by $\quad h_{Ni} = \dfrac{-a_{i-1}}{a_N} = -a_{i-1} \quad$ as $\quad a_N = 1$

Because of the special form of the Bush matrix, solution of equation (9-18) is easy and may be given by a recursion formula. If T is partitioned into column vectors:-

$$T = \left[\underline{T}_1 \;\vdots\; \underline{T}_2 \;\vdots\; \cdots\cdots \;\vdots\; \underline{T}_N\right]$$

then

$$\begin{aligned} \underline{T}_N &= B\underline{u} \\ \underline{T}_{N-1} &= A\underline{T}_N - B\underline{u}h_{NN} \\ \underline{T}_{N-2} &= A\underline{T}_{N-1} - B\underline{u}h_{N,N-1} \end{aligned} \qquad \ldots.(9\text{-}21)$$

or

$$\underline{T}_i = A\underline{T}_{i+1} - B\underline{u}h_{N,i+1} \qquad \begin{matrix} i+N-1,1 \\ i \neq 1 \end{matrix}$$

The proof of the above method is that usually given for the Cayley Hamilton Theory (59).

$$\left[sI - A\right]\mathrm{Adj}(sI - A) = \left|sI - A\right| . I \qquad ....(9\text{-}22)$$

The characteristic equation of A is equation (9-20)

$$\left|sI - A\right| = a_o + a_1 s + a_2 s^2 .... a_N s^N =$$
$$- (h_{N1} + h_{N2} s .... + h_{NN} s^{N-1} - s^N) \qquad ....(9\text{-}23)$$

Let

$$\mathrm{Adj}\ (sI - A) = C_o + C_1 s + C_2 s^2 .... C_{N-1}\ s^{N-1} \qquad ....(9\text{-}24)$$

where C_i is an NxN matrix.

Substituting equation (9-23) and (9-24) into equation (9-22) gives

$$\left[sI - A\right] (C_o + C_1 s + C_2 s^2 ... C_{N-1} s^{N-1}) = -(h_{N1} + h_{N2} s ... h_{NN} s^{N-1} - s^N).I \qquad ....(9\text{-}25)$$

Equating coefficients of s in equation (9-25) gives

$$\begin{aligned} C_{N-1} &= I \\ C_{N-2} &= AC_{N-1} - h_{NN}.I \\ &\vdots \\ C_1 &= AC_2 - h_{N3}.I \\ C_o &= AC_1 - h_{N2}.I \end{aligned} \qquad ....(9\text{-}26)$$

But from the definitions of the matrix C and the vector T

$$C_i\ B\underline{u} = \underline{T}_{i+1} \qquad ....(9\text{-}27)$$

therefore

$$\begin{aligned} \underline{T}_N &= B\underline{u} \\ \underline{T}_{N-1} &= A\underline{T}_N - B\underline{u}\ h_{NN}.I \\ &\vdots \\ \underline{T}_1 &= A\underline{T}_2 - B\underline{u}\ h_{N2}.I \end{aligned} \qquad ....(9\text{-}28)$$

which agree exactly with equations (9-21)

9.5.1 Application of the zero estimation method of Davison to a distillation model.

International Computers Ltd. supply a standard program package for eigenvalue determination based on the QR algorithm(63). A short program was written for the ICL 1905 at Loughborough University of Technology utilising the above package. This greatly facilitated zero estimation using Davison's method.

The distillation model described in section 8.5 was analysed using the above program. The poles of the system were first determined and are given in Fig. 9-1. The transfer function zeroes for the responses to a feed composition perturbation for the light and middle components in the overheads and for the middle and heavy components in the bottoms were estimated. These values are given in Figs. 9-2 to 9-5.

The results obtained for values of K, the scalar multiplying factor, from 10^4 to 10^{10} for the zeroes of the transfer function for variable 2 (the middle component in the overheads) are given in Appendix 9.

The results of applying the numerical check described in section 9.4.2 to the zeroes for the middle component in the overheads are given below:

VALUE OF K	EIGENVALUE PRODUCT	PRODUCT OF EXTRANEOUS ROOTS
1	$0.12088\ 21209 \times 10^{52}$	-
10^4	$0.12088\ 21197 \times 10^{55}$	6.38×10^8
10^5	$0.12088\ 21745 \times 10^{56}$	1.039×10^{10}
10^6	$0.12088\ 21293 \times 10^{57}$	1.176×10^{10}
10^7	$0.12087\ 00235 \times 10^{58}$	1.181×10^{10}
10^8	$0.12100\ 90752 \times 10^{59}$	-
10^9	$0.12189\ 41707 \times 10^{60}$	-
10^{10}	$0.12117\ 80290 \times 10^{61}$	-

Real part	Imaginary part
-1.52460	
-1.85879	
-2.02705	
-2.83715	
-2.94350	
-3.66659	
-6.82537	
-25.0033	
-27.6544	
-39.9679	
-50.1617	
-54.0308	
-60.7625	
-70.7888	
-75.0031	
-75.7139	
-87.2083	
-104.425	
-118.867	
-149.354	
-159.399	
-202.595	
-10.3525	0.900363
-10.3525	-0.900363
-19.2155	0.540479
-19.2155	-0.540479
-26.7046	4.70554
-26.7046	-4.70554
-30.3429	7.31836
-30.3429	-7.31836
-34.6086	7.72156
-34.6086	-7.72156
-38.4875	5.95289
-38.4875	-5.95289
-40.9188	2.33033
-40.9188	-2.33033

Product of eigenvalues = $0.10501054873 \times 10^{52}$

The system poles.

Fig. 9-1.

Davison's Column method. ($K = -10^7$)	Davison's Row method. ($K = 10^7$)	Matrix root locus method. ($K = 10^8$)
-1.85772	-1.85772	-1.85609
-2.02705	-2.02704	-2.02690
-2.90159	-2.90151	-2.90325
-3.66660	-3.66659	-3.66661
-3.77424	-3.77427	-3.77419
-7.49138	-7.49145	-7.49080
-11.4283	-11.4291	-11.4289
-16.9951	-16.9874	-16.9921
-20.0416	-20.0585	-20.0417
-26.7905	-26.8837	-27.7601
-28.3744	-39.5716	-32.1306
-49.5002	-49.4995	-49.4994
-56.9909	-56.9899	-56.9904
-60.0403	-60.0425	-60.0406
-70.7446	-70.7456	-70.7463
-75.5386	-75.5373	-75.5354
-87.2046	-87.2051	-87.2065
-105.858	-105.858	-105.856
-148.587	-148.588	-148.589
-28.4978 ± 3.68029i	-27.8401 ± 2.40240i	-29.6048 ± 1.33384i
-31.0947 ± 5.61594i	-30.1647 ± 4.94546i	-31.1646 ± 3.58377i
-35.1737 ± 5.42005i	-33.5978 ± 5.76127i	-33.9570 ± 4.27926i
-37.9038 ± 3.45005i	-36.8453 ± 4.50157i	-36.5788 ± 3.26876i
-39.6325 ± 0.557516i	-38.8041 ± 1.42251i	-39.2364 ± 0.213976i

Extraneous roots

-369.904	197.250	-488.179
170.817 ± 115.522i	91.8927 ± 209.133i	274.890 ± 158.294i
-21.1305 ± 258.821i	-147.060 ± 259.162i	4.75572 ± 354.297i
-262.032 ± 206.704i	-340.755 ± 114.691i	-334.686 ± 282.094i

Eigenvalue product

$0.12124995043 \times 10^{58}$	$-0.12123317411 \times 10^{58}$	$0.12120181046 \times 10^{59}$

Transfer function zeroes for the response of the light component in the overheads to a feed composition perturbation.

Fig. 9-2.

Davison's Column method. ($K = -10^8$)	Davison's Row method. ($K = 10^7$)	Matrix root locus method. ($K = 10^9$)
-1.85749	-1.85772	-1.85902
-2.02670	-2.02706	-2.02577
-2.90746	-2.90741	-2.90741
-3.66532	-3.66646	-3.66637
-3.77465	-3.77336	-3.77323
-7.47605	-7.47592	-7.47603
-11.4242	-11.4244	-11.4218
-16.9961	-16.9948	-17.0001
-20.0359	-20.0377	-20.0515
-27.5877	-27.2816	-27.8876
-27.6201	-39.6824	-40.1803
-49.4897	-49.4907	-49.4920
-56.9901	-56.9916	-56.9621
-60.0392	-60.0362	-60.0833
-70.7330	-70.7411	-70.6379
-75.5505	-75.5424	-75.6407
-87.2025	-87.2042	-87.1869
-105.859	-105.859	-105.858
-148.588	-148.587	-148.591
-28.7194 ± 3.44096i	-27.7074 ± 2.21698i	-26.4396 ± 1.88188i
-31.5325 ± 5.34509i	-30.1258 ± 4.94533i	-28.4874 ± 5.70998i
-34.8094 ± 5.51862i	-33.5740 ± 5.75141i	-32.5929 ± 7.73910i
-37.9096 ± 3.86035i	-36.8139 ± 4.51563i	-37.6237 ± 7.02565i
-39.9037 ± 0.915939i	-38.7744 ± 1.52901i	-41.2916 ± 3.00264i
Extraneous roots		
302.915	-369.779	444.170
157.207 ± 293.671i	170.788 ± 115.426i	246.174 ± 416.004i
-170.960 ± 365.476i	-21.2575 ± 258.781i	-201.871 ± 514.315i
-435.025 ± 162.401i	-261.961 ± 206.736i	-565.542 ± 229.171i
Eigenvalue product		
$-0.12085080725 \times 10^{59}$	$0.12087002351 \times 10^{58}$	$-0.12088890058 \times 10^{60}$

Transfer function zeroes for the response of the middle component in the overheads to a feed composition perturbation.

Fig. 9-3.

Davison's Column method. ($K = -10^6$)	Davison's Row method. ($K = 10^6$)	Matrix root locus method. ($K = -10^7$)
-1.20711	-1.20660	-1.20699
-1.60595	-1.60636	-1.60601
-2.02707	-2.02708	-2.02707
-2.95131	-2.95131	-2.95131
-3.66659	-3.66658	-3.66656
-5.52722	-5.52707	-5.52701
-13.3031	-13.3030	-13.3031
-24.5227	-24.4176	-24.4966
-27.8723	-28.0043	-27.9354
-39.4919	-39.4592	-39.8735
-43.2140	-43.2502	-42.9677
-55.4799	-55.4795	-55.4796
-69.9255	-69.9253	-69.9255
-76.5684	-76.5682	-76.5681
-87.0471	-87.0477	-87.0473
-103.515	-103.519	-103.517
-155.096	-155.162	-155.126
-199.406	-201.451	-200.788
-18.6470 ± 2.93262i	-18.6446 ± 2.93291i	-18.6540 ± 2.93327i
-25.7705 ± 6.39065i	-25.7151 ± 6.42441i	-25.7813 ± 6.36286i
-31.2970 ± 10.8197i	-31.2886 ± 10.8678i	-31.2872 ± 10.7927i
-38.8319 ± 10.8446i	-38.8554 ± 10.8756i	-38.8167 ± 10.8104i
-42.9469 ± 6.39079i	-42.9762 ± 6.39008i	-42.8689 ± 6.35936i
-58.4098 ± 19.3403i	-58.5044 ± 19.3981i	-58.4855 ± 19.3663i
Extraneous roots		
86.9521	67.5058 ± 64.0707i	147.638
-216.761	-60.7313 ± 125.314i	-275.376
13.9157 ± 109.994i	-193.672 ± 60.9298i	43.0836 ± 168.815i
-136.972 ± 107.172i		-168.254 ± 167.474i
Eigenvalue product		
$-0.67756251035 \times 10^{55}$	$0.67748444116 \times 10^{55}$	$-0.67753609346 \times 10^{56}$

Transfer function zeroes for the response of the middle component in the bottoms to a feed composition perturbation.

Fig. 9-4.

Davison's Column method.[7] ($K = -10^7$)	Davison's Row method.[6] ($K = 10^6$)	Matrix root locus method.[8] ($K = -10^8$)
-0.0733656	-0.0733593	-0.0734020
-1.59551	-1.59536	-1.59077
-2.02693	-2.02700	-2.03110
-3.00239	-3.00260	-3.00239
-3.66679	-3.66663	-3.66563
-4.51241	-4.51258	-4.51290
-14.0104	-14.0104	-14.0084
-27.3679	-27.2710	-25.2078
-40.2896	-40.3051	-41.0143
-55.2364	-55.2368	-55.2356
-69.2908	-69.2915	-69.2956
-88.7079	-88.6842	-88.7055
-103.310	-103.329	-103.310
-155.075	-155.331	-155.095
-199.494	-202.288	-200.412
-18.6651 ± 3.48046i	-18.6648 ± 3.48098i	-18.6587 ± 3.48209i
-25.2371 ± 3.38843i	-25.2752 ± 3.39974i	-25.6825 ± 4.18008i
-28.7821 ± 8.69525i	-28.7932 ± 8.68915i	-29.0183 ± 8.83036i
-35.5344 ± 10.3723i	-35.5340 ± 10.3651i	-35.6254 ± 10.4452i
-41.9251 ± 8.04316i	-41.9193 ± 8.04166i	-41.9513 ± 8.06226i
-42.9137 ± 3.49467i	-42.9102 ± 3.49929i	-42.8397 ± 3.61121i
-79.4660 ± 3.96196i	-79.4503 ± 3.95692i	-79.4639 ± 3.96103i
Extraneous roots		
-216.824	57.0012	-268.124
80.1005 ± 59.6618i	15.3692 ± 73.7369i	128.080 ± 84.1545i
-22.3082 ± 132.647i	-80.4904 ± 87.8642i	-11.2848 ± 190.578i
-153.457 ± 103.449i	-165.949 ± 34.7570i	-187.853 ± 150.696i
Eigenvalue product		
$0.16400168165 \times 10^{55}$	$-0.16394453285 \times 10^{54}$	$0.16352276283 \times 10^{56}$

Transfer function zeroes for the response of the heavy component in the bottoms to a feed composition perturbation.

Fig. 9-5.

Even with the various aids and checks it was still difficult to select the best set of zeroes from runs with various values of K. The criterion adopted was to use the largest value of K consistent with the product of all the eigenvalues agreeing to four significant figures with the product obtained with $K=10^4$. On this basis the zeroes obtained using $K=10^7$ were chosen as the best estimates and are presented in Fig. 9-3. The overall system gain is then 1.181×10^{10}.

9.5.2 Application of the numerator calculation method of Bosley et al to a distillation model.

The distillation model described in section 8.5 was analysed using the method of Bosley et al(49). The calculations were performed using a computer program written by M.J. Bosley in the Department of Chemical Engineering at Loughborough University of Technology. The coefficients for the numerator polynomials of the transfer functions for the responses of each of the elements in the state vector to a perturbation in the feed composition were obtained. The coefficients relating to the light and middle components in the overheads and to the middle and heavy components in the bottoms are given in Fig. 9-6. The program also calculates the denominator polynomial coefficients, these being identical for all the transfer functions of course.

Inspection of the coefficients obtained by the method of Bosley et al revealed several changes of sign per row and high numerical values. Numerical inaccuracy was suspected and since the method depends on a recursion formula this inaccuracy was expected to be greatest in the last values calculated, namely the first elements in each row. (These are the constant terms in the numerator polynomial.) Calculation of the steady state gain confirmed this suspicion since it failed to tally with the results of the steady state calculation presented in Chapter 8.

Denominator.

-0.1050105487E52	-0.3809739408E52	-0.6209356714E52	-0.6045981131E52
-0.3949589632E52	-0.1845364702E52	-0.6428319004E51	-0.1720558031E51
-0.3622329799E50	-0.6114268769E49	-0.8406781408E48	-0.9541540600E47
-0.9039736096E46	-0.7215944002E45	-0.4890980047E44	-0.2832881983E43
-0.1409365723E42	-0.6046959099E40	-0.2244337649E39	-0.7220894045E37
-0.2016377275E36	-0.4888518717E34	-0.1028419201E33	-0.1874615832E31
-0.2953465631E29	-0.4007483321E27	-0.4660257225E25	-0.4614704471E23
-0.3858496820E21	-0.2094410287E19	-0.1548789463E17	-0.7186753627E14
-0.2619827523E12	-0.7208593988E09	-0.1404607824E07	-0.1723878717E04

Numerator - row 1.

-0.1143859583E65	0.5646170939E62	-0.2787008444E60	0.1375708401E58
-0.6790639402E55	0.3356474525E53	-0.1547608073E51	0.2820638227E49
0.2890654185E48	0.3420824194E47	0.3230697076E46	0.2504914075E45
0.1609400761E44	0.8035525415E42	0.3892032089E41	0.1479360840E40
0.4753566383E38	0.1292305680E37	0.2970098731E35	0.5756517714E33
0.9367650929E31	0.1271471873E30	0.1425912713E28	0.1304016074E26
0.9547842289E23	0.5452204362E21	0.2334935440E19	0.7040192381E16
0.1329936816E14	0.1181516442E11	0.0 0.0 0.0 0.0 0.0 0.0	

Numerator - row 2.

0.1142510347E65	-0.5639511027E62	0.2783721051E60	-0.1374085700E58
0.6782629889E55	-0.3352506519E53	0.1545995314E51	-0.2813501778E49
-0.2881954645E48	-0.3410967196E47	-0.3221718343E46	-0.2498208278E45
-0.1605252125E44	-0.8614091534E42	-0.3882728680E41	-0.1475954141E40
-0.4743016497E38	-0.1289540286E37	-0.2963967698E35	-0.5745049128E33
-0.9349629357E31	-0.1269108592E30	-0.1423350615E28	-0.1301749629E26
-0.9531779736E23	-0.5443319612E21	-0.2331246823E19	-0.7029400843E16
-0.1327956727E14	-0.1179805827E11	0.0 0.0 0.0 0.0 0.0 0.0	

Numerator - row 35.

-0.9641642550E61	0.4757417363E59	-0.2347189695E57	0.1157866525E55
-0.5726009152E52	0.2262300812E50	-0.1619748617E49	-0.2951143668E48
-0.4542812884E47	-0.5489922591E46	-0.5321754634E45	-0.4201172271E44
-0.2733825970E43	-0.1480359495E42	-0.6718867987E40	-0.2569493347E39
-0.8309108377E37	-0.2276400718E36	-0.5285477535E34	-0.1038788836E33
-0.1723098589E31	-0.2400705043E29	-0.2789575292E27	-0.2676721130E25
-0.2092187464E23	-0.1307097418E21	-0.6354117265E18	-0.2309471348E16
-0.5886868727E13	-0.9355860144E10	-0.6951419753E07	0.0 0.0 0.0
0.0 0.0			

Numerator - row 36.

-0.1087361300E61	0.5364890561E58	-0.2646638568E56	0.1305515039E54
-0.6390370551E51	0.4861607073E49	0.4627591764E48	0.9880803884E47
0.1530680200E47	0.1854764025E46	0.1774382688E45	0.1368733468E44
0.8627362129E42	0.4488812569E41	0.1942428862E40	0.7027602431E38
0.2132737910E37	0.5430888279E35	0.1163790706E34	0.2087038830E32
0.3122144263E30	0.3870374629E28	0.3938038392E26	0.3245134519E24
0.2125728102E22	0.1077824897E20	0.4065727631E17	0.1070538110E15
0.1749778294E12	0.1331634822E09	0.0 0.0 0.0 0.0 0.0 0.0	

Denominator polynomial coefficients and selected numerator polynomial coefficients by the method of Bosley et al.

(Note: 3.7E11 denotes 3.7×10^{11})

Fig. 9-6.

A remedy suggested by Kropholler(56) was employed. This was to operate the recursion formula of equation (9-21) in reverse. Equating the constant term on both sides of equation (9-25) gives:

$$- AC_o = -h_{N1} \, . \, I$$

From the definition of matrix C and vector T:

$$C_o \, B\underline{u} = T_1$$

Hence $$T_1 = A^{-1} h_{n1} . \, I$$

and $$T_2 = A^{-1} \; T_1 + B\underline{u} \; h_{N2} . I$$

$$\vdots$$

$$T_i = A^{-1} \; T_{i-1} + B\underline{u} \; h_{Ni} . I$$

Application of this formula yielded a second set of coefficients. Comparison of the two sets revealed a match for several coefficients for the middle powers of s - see Figs. 9-6 and 9-7. The coefficients for the high and low powers did not correlate at all. It was thus concluded that accumulation of rounding error was occurring with both processes. Use was made of the fortuitous match for the middle powers of s to obtain a 'best set'. Hence the numerator coefficients for response 2, the middle component in the overheads, are as given in Fig. 9-8. Note also that the coefficient of the highest power of s is 1.180×10^{10} in good agreement with the prediction of the method of Davison. Also there are 30 coefficients in the polynomial indicating the presence of 29 zeroes, again in agreement with the results of Davison's method.

9.5.3 Application of the matrix formulation of the root locus to a distillation model.

The computer program used to calculate the zeroes by the method of Davison was modified slightly to perform the root locus

Row 1.

-0.1212503075E51	-0.3290971509E51	-0.3956629628E51	-0.2803028430E51
-0.1315504639E51	-0.4367207279E50	-0.1071115898E50	-0.2003791291E49
-0.2930978587E48	-0.3418834352E47	-0.3230789395E46	-0.2504948630E45
-0.1609141611E44	-0.8052567944E42	-0.3780158729E41	-0.2213396228E40
0.4339781080E39	-0.3171225361E39	0.2071171704E39	-0.1358619329E39
0.8910718016E38	-0.5844287803E38	0.3833130010E38	-0.2514078382E38
0.1048948888E38	-0.1081529441E38	0.7093684707E37	-0.4652725633E37
0.3051720044E37	-0.2001627870E37	0.1312874303E37	-0.8011204087E36
0.5648140140E36	-0.3704654075E36	0.2429911133E36	-0.1593799022E36

Row 2.

0.1208821213E51	0.3280630469E51	0.3943888634E51	0.2793884989E51
0.1311210647E51	0.4353104103E50	0.1067725739E50	0.1997618321E49
0.2922231485E48	0.3408979699E47	0.3221810564E46	0.2498242750E45
0.1604993472E44	0.8031104119E42	0.3771043855E41	0.2208776935E40
-0.4332957892E39	0.3166054608E39	-0.2067806951E39	0.1356414685E39
-0.8896267276E38	0.5834812934E38	-0.3826916676E38	0.2510003514E38
-0.1646276355E38	0.1079776590E38	-0.7082188048E37	0.4645185006E37
-0.3046774159E37	0.1998383856E37	-0.1310746543E37	0.8597248596E36
-0.5638986249E36	0.3698649970E36	-0.2425972991E36	0.1591215960E36

Row 35.

0.6775695898E49	0.2286258110E50	0.3328003196E50	0.2777818142E50
0.1494471071E50	0.5539477693E49	0.1480912480E49	0.2957985523E48
0.4542475990E47	0.5489938496E46	0.5321757858E45	0.4201149461E44
0.2733953122E43	0.1479650477E42	0.6757741889E40	0.2353656781E39
0.2037375298E38	-0.6574229644E37	0.3878203796E37	-0.2229053536E37
0.1297718247E37	-0.7642933907E36	0.4553613694E36	-0.2743631855E36
0.1670813871E36	-0.1027650056E36	0.6378335548E35	-0.3991313762E35
0.2515735313E35	-0.1595727382E35	0.1017709432E35	-0.6521052277E34
0.4195008880E34	-0.2707686552E34	0.1752583771E34	-0.1137030284E34

Row 36.

-0.1640242382E48	-0.2655275396E49	-0.6185683707E49	-0.6619928549E49
-0.4140510190E49	-0.1687686234E49	-0.4784016657E48	-0.9873097995E47
-0.1536718180E47	-0.1854761857E46	-0.1774384789E45	-0.1368720741E44
-0.8628146200E42	-0.4484052325E41	-0.1971145353E40	-0.5298192357E38
-0.1256128800E38	0.6254742114E37	-0.3835624787E37	0.2343142637E37
-0.1440385736E37	0.8908959369E36	-0.5544283824E36	0.3471021742E36
-0.2185394940E36	0.1383221493E36	-0.8797257330E35	0.5619399317E35
-0.3603392327E35	0.2318518994E35	-0.1496226410E35	0.9680475229E34
-0.6276979616E34	0.4077732893E34	-0.2653244105E34	0.1728695418E34

Selected numerator polynomial coefficients obtained by Kropholler's modification to the method of Bosley et al.

Fig. 9-7.

(Note: 3.7E11 denotes 3.7×10^{11} etc.)

-0.1208821213E51	-0.3280630469E51	-0.3943888634E51	-0.2793884989E51
-0.1311210647E51	-0.4353104103E50	-0.1067725739E50	-0.1997618321E49
-0.2922231485E48	-0.3408979699E47	-0.3221810564E46	-0.2498208278E45
-0.1605252125E44	-0.8614091534E42	-0.3882728680E41	-0.1475954141E40
-0.4743016497E38	-0.1289540286E37	-0.2963967698E35	-0.5745049128E33
-0.9349629357E31	-0.1269108592E30	-0.1423350615E28	-0.1301749629E26
-0.9531779736E23	-0.5443319612E21	-0.2331246823E19	-0.7029400843E16
-0.1327956727E14	-0.1179805827E11		

Numerator polynomial coefficients for response 2.

Fig. 9-8.

calculation described in section 9.4.3. The results of these runs for light and middle components in the overheads and for the middle and heavy components in the bottoms are given in Figs. 9-2 to 9-5. In the absence of any of the checks associated with Davison's method it was difficult to predict the value of K for which numerical instability became critical. In the absence of a better method the following was used, bearing in mind the close similarity between the matrix root locus method and Davison's method for high values of K. The value of the eigenvalue product for successive values of K was examined and the value closest to the product obtained using Davison's method with $K=10^4$ determined the set of zeroes selected.

The method of the matrix root locus was originally tried in an attempt to overcome the numerical problems which bedevilled the application of Davison's methods. It was hoped that the inherent stability of the root locus calculation would overcome the tendency of the zeroes to deviate from their correct values at high values of K. This did not prove to be the case and the checks for numerical accuracy which have been devised for Davison's method must render this method superior.

CHAPTER 10. SIMPLIFICATION OF POLYNOMIAL RATIO TRANSFER FUNCTIONS USING CONTINUED FRACTIONS.

10.1 Introduction.

A wide range of systems give rise to transfer functions of the type discussed and derived in Chapter 9. In general an nth order system will give rise to a denominator polynomial in s of order n and a numerator polynomial in s of order up to n-1. Clearly for systems larger than third or fourth order some simplification may often be desirable.

10.2 General problems of model selection and parameter estimation.

Most of the simplification methods described in recent papers rely on the selection of a suitable form of model and the subsequent estimation of parameters to give the best fit for the model to the data generated either by experiment or using the exact form of the transfer function. Such models are described by Gibilaro and Lees(68) and Kropholler et al(69).

A novel approach has been adopted by Chen and Shieh(51) and it is this method which is examined in more detail in this chapter. The interesting feature about the method is that it gives several simplified models of successively higher order together with their parameters in a single calculation.

10.3 The simplification method of Chen and Shieh.

10.3.1 The basic principles.

Consider a simple feedback system as shown in Fig. 10.1. The output c is related to the input r by the relation:-

$$\frac{c}{r} = \frac{G}{1 + GH}$$

or

$$\frac{c}{r} = \frac{1}{H + \frac{1}{G}} \qquad \ldots.(10\text{-}1)$$

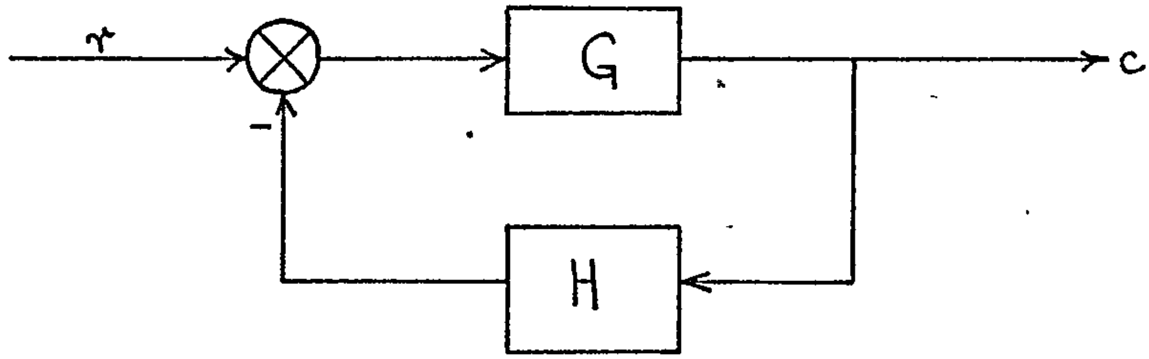


FIG. 10-1.

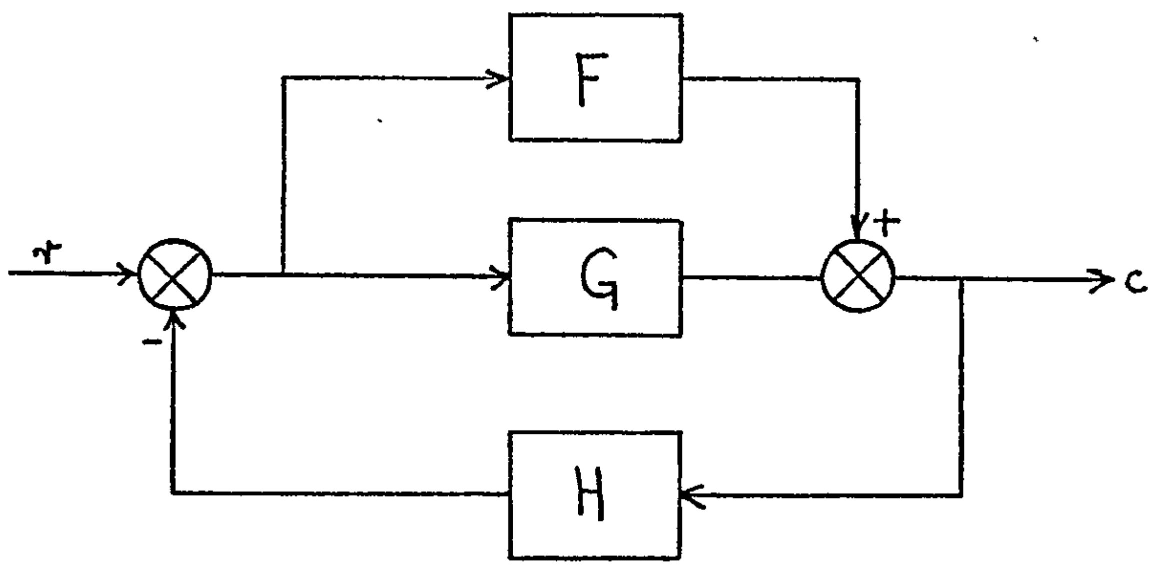


FIG. 10-2.

Equation (10-1) is the simplest continued fraction form of the transfer function equation. If we add a single feedforward loop to the system as in Fig. 10-2 then we obtain:-

$$\frac{c}{r} = \frac{F + G}{1 + (F + G)H}$$

or

$$\frac{c}{r} = \cfrac{1}{H + \cfrac{1}{F + G}} \qquad \text{....(10-2)}$$

Note from equation (10-2) that G could itself be a more complicated system which could be represented by an expression of the form of the right hand side of equation (10-2). It may thus be seen how the continued fraction expansion idea emerges.

Consider the example given below:-

$$G(s) = \frac{3+s}{1 + 2s + S^2} \qquad \text{....(10-3)}$$

Dividing numerator and denominator by 3+s gives

$$G(s) = \cfrac{1}{\frac{1}{3} + \cfrac{s(5/3 + s)}{s+3}}$$

and applying the same procedure to the fraction in the denominator finally gives:-

$$G(s) = \cfrac{1}{\frac{1}{3} + \cfrac{s}{9/5 + \cfrac{(-4/5)s}{(5/3 + s)}}}$$

i.e.

$$G(s) = \cfrac{1}{\frac{1}{3} + \cfrac{s}{9/5 + \cfrac{s}{-25/12 - \cfrac{s}{4/5}}}} \qquad \text{....(10-4)}$$

A more useful form of (10-4) is obtained by removing the s term from the numerator of the subsidiary fractions to give:-

$$G(s) = \cfrac{1}{\frac{1}{3} + \cfrac{1}{\cfrac{9/5}{s} + \cfrac{1}{-25/12 - \cfrac{1}{\cfrac{4/5}{s}}}}} \qquad \text{....(10-5)}$$

Now the block diagram representing equation (10-5) may be constructed using the diagram for equation (10-2) as a guide. This is shown in Fig. 10-3. The general pattern obtained by this transformation now becomes clear. If the ratio

$$G(s) = f(s) / g(s)$$

is first reduced to

$$G(s) = \cfrac{1}{H_1 + \cfrac{1}{\cfrac{H_2}{s} + \cfrac{1}{H_3 + \cfrac{1}{\cfrac{H_4}{s} + \cfrac{1}{H_5 + \cfrac{1}{\cfrac{H_6}{s} + \cdots}}}}}} \qquad \ldots\ldots(10\text{-}6)$$

then this may be represented as in Fig. 10-4. In general there will be 2n H coefficients where n is the order of the denominator polynomial.

The Chen and Shieh method of simplification is basically to truncate the running fraction, equation (10-6), after a term H_j/s where j is even. This is equivalent to removing the inner part of the block diagram, Fig. 10-4. For example truncation of equation (10-6) after H_4/s would reduce the system to that shown in Fig. 10-5.

It is also apparent that truncation of the continued fraction after H_j/s will reduce equation (10-6) to a polynomial ratio with the denominator of order j/2.

10.3.2 Matrix representation of the simplified model.

Equation (10-6) becomes interesting when a suitable state space representation is used. If the input to each integrator in Fig. 10-4 is denoted as an element of the vector Z, which has n elements, then the state equations and the output equation can be written:-

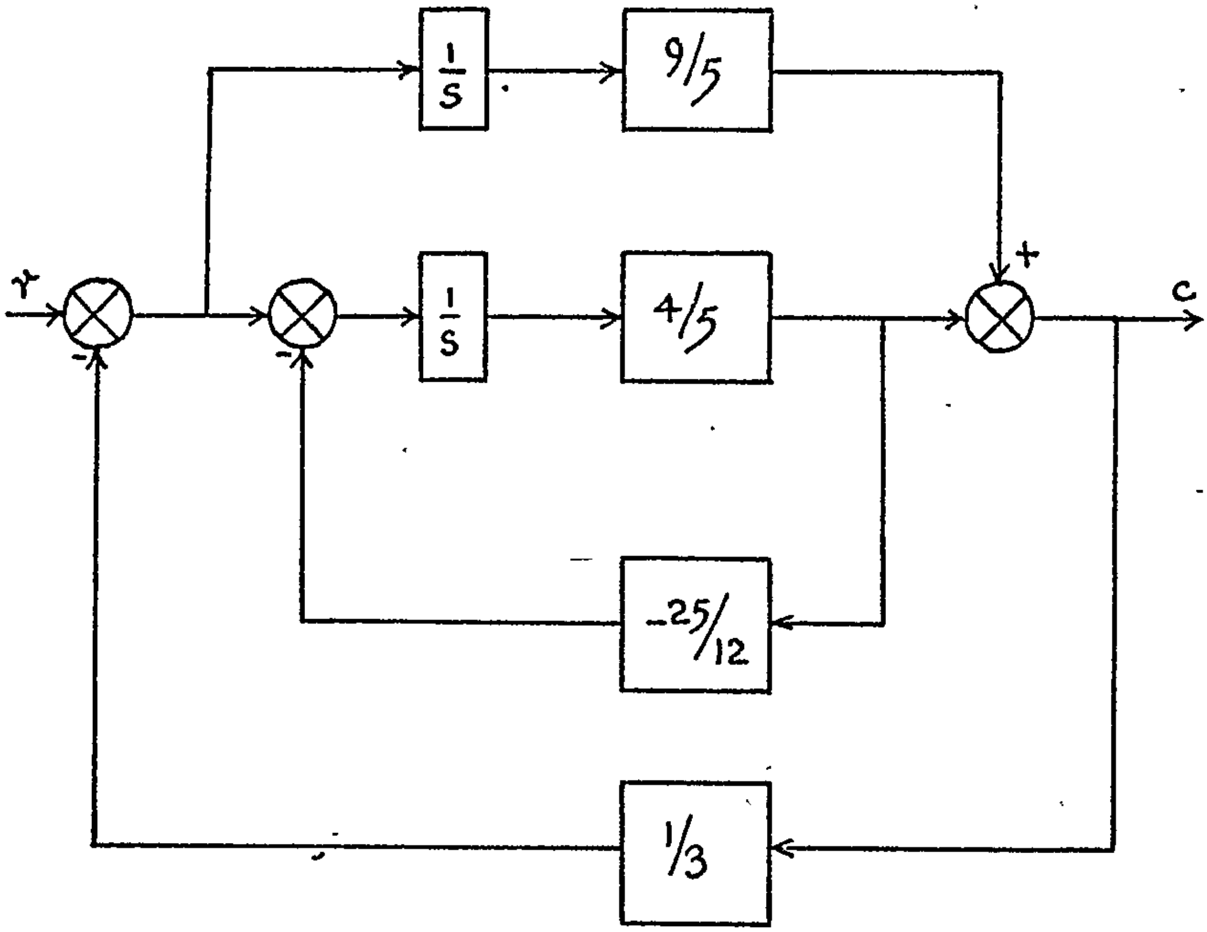


FIG. 10-3.

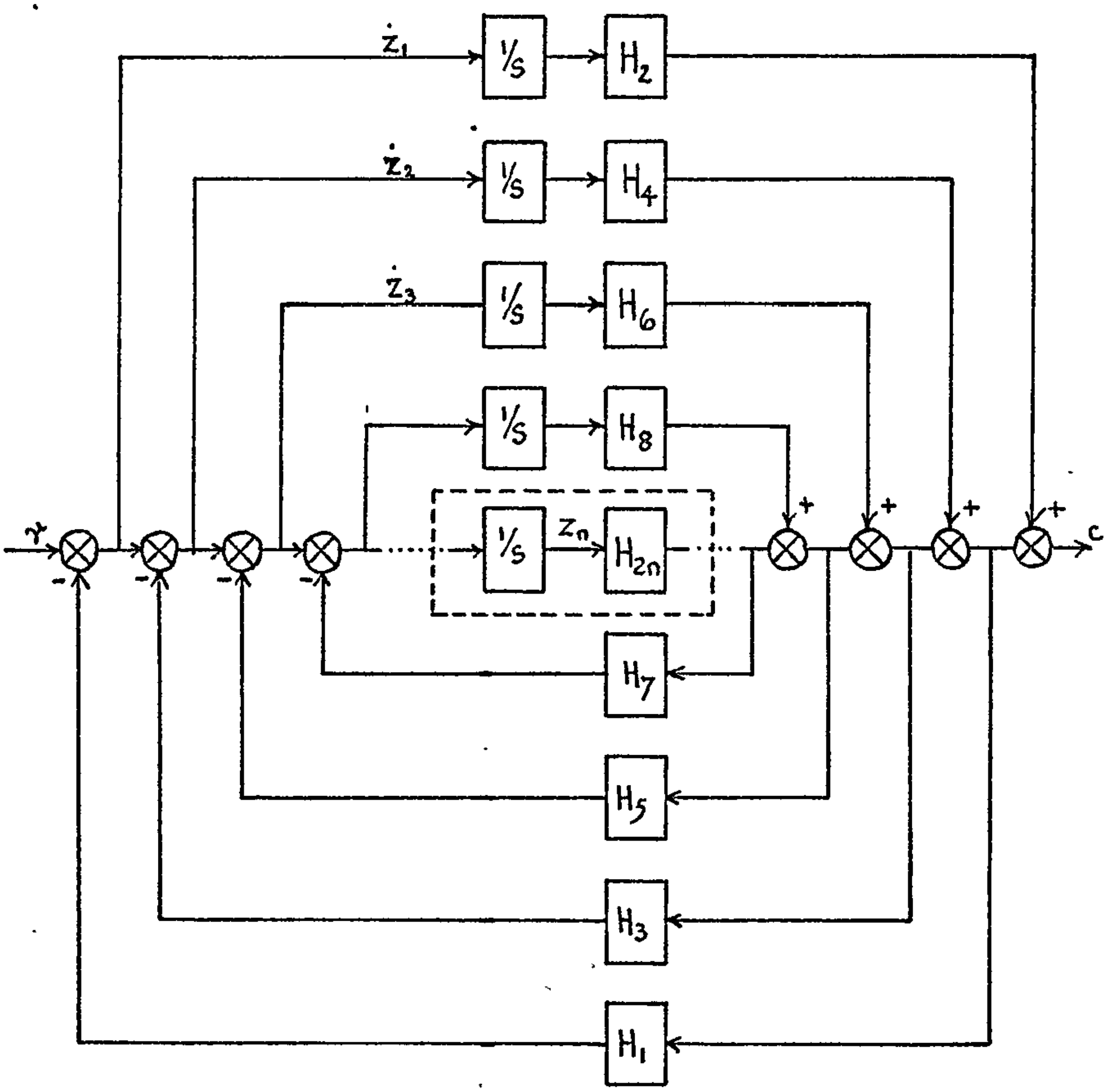


FIG. 10-4.

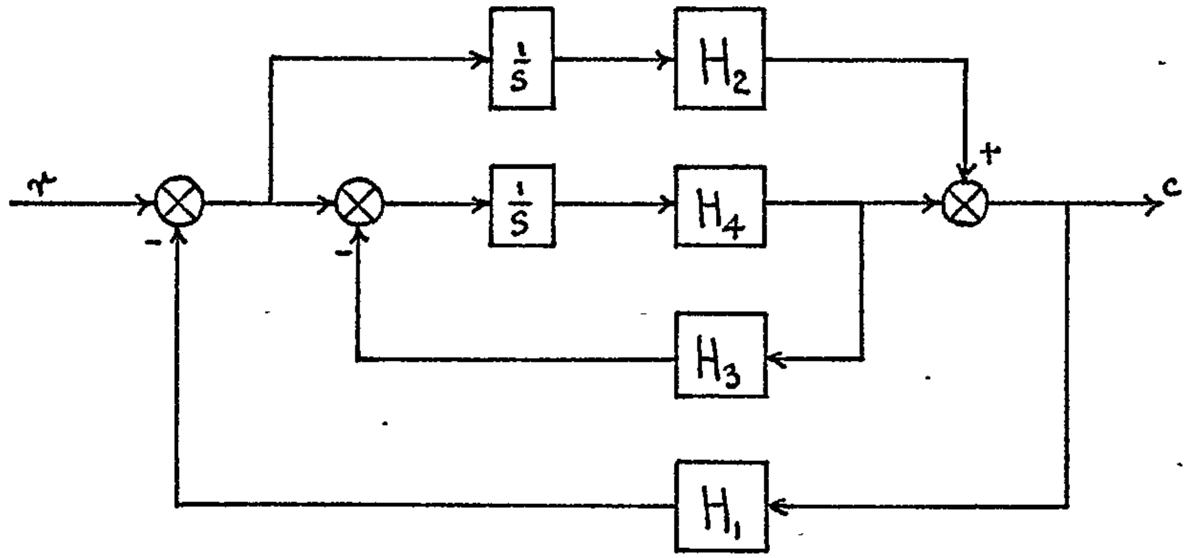


FIG. 10-5.

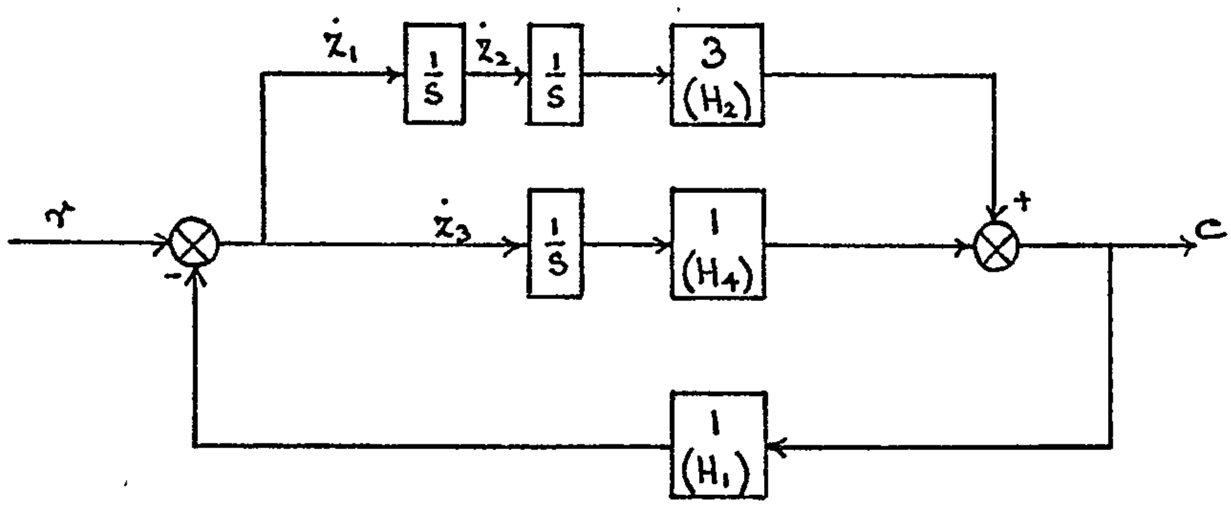


FIG. 10-5a.

$$\frac{d}{dt}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \cdot \\ \cdot \\ z_n \end{bmatrix} = \begin{bmatrix} H_2H_1 & H_4H_1 & H_6H_1 & \cdots & H_{2n}H_1 \\ H_2H_1 & H_4(H_1+H_3) & H_6(H_1+H_3) & \cdots & H_{2n}(H_1+H_3) \\ H_2H_1 & H_4(H_1+H_3) & H_6(H_1+H_3+H_5) & \cdots & H_{2n}(H_1+H_3+H_5) \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ H_2H_1 & H_4(H_1+H_3) & H_6(H_1+H_3+H_5) & \cdots & H_{2n}(H_1+H_3+\ldots H_{2n-1}) \end{bmatrix}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \cdot \\ \cdot \\ z_n \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \\ 1 \\ \cdot \\ \cdot \\ 1 \end{bmatrix} \quad \ldots\ldots(10\text{-}7)$$

$$c = H_2z_1 + H_4z_2 + H_6z_3 + \ldots H_{2n}z_n \quad \ldots\ldots(10\text{-}8)$$

Now suppose a second order approximation is required. The corresponding form of equation (10-7) is:-

$$\frac{d}{dt}\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} H_2H_1 & H_4H_1 \\ H_2H_1 & H_4(H_1+H_3) \end{bmatrix}\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \end{bmatrix} r \quad \ldots\ldots(10\text{-}9)$$

Equation (10-9) is obtainable directly from equation (10-7) by simply partitioning the matrix. In general the nth order model may be obtained by simply using the nxn matrix that forms the top left hand corner of the full matrix. Hence if several models are required for comparison to see which is the lowest order model commensurate with adequate representation, only a single matrix need be calculated. The simpler models can be written down directly from this.

10.3.3 Calculation of the H coefficients.

In section 10.3.1 the calculation of the H coefficients was demonstrated using repeated long division. The method may appear to break down during this process if at any time the remainder term in s goes to zero. For example, consider

$$G(s) = \frac{3+s}{3+s+3s^2} \quad \ldots\ldots(10\text{-}10)$$

$$= \frac{1}{1+\frac{s^2}{3+s}}$$

$$= \frac{1}{1+\frac{s(0+s)}{3+s}}$$

and the process can apparently go no further since division by 0+s is not possible. Although not mentioned by Chen and Shieh the solution is fairly straightforward. Division is continued leaving a term s^2 rather than s in the numerator. Hence the form of equation (10-10) analogous to equation (10-4) is:-

$$G(s) = \cfrac{1}{1 + \cfrac{s^2}{3 + \cfrac{s}{1}}}$$

Removal of s and s^2 from the numerator of the subsidiary fractions then gives:-

$$G(s) = \cfrac{1}{1 + \cfrac{1}{\cfrac{3}{s^2} + \cfrac{1}{s}}}$$

The equivalent block diagram form is then given by Fig. 10-5a, and the state variable equation is:

$$\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 0 & H_2H_1 & H_4H_1 \\ 1 & 0 & 0 \\ 0 & H_2H_1 & H_4H_1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

In a later paper Chen and Shieh(52) describe a method of deriving the H coefficients by a method more suitable for automatic computation. Consider the general polynomial ratio form of the transfer function:-

$$G(s) = \frac{A_{21} + A_{22}s + A_{23}s^2 + \dots A_{2,n}s^{n-1}}{A_{11} + A_{12}s + A_{13}s^2 + \dots A_{1,n+1}\ s^n} \qquad \dots.(10\text{-}11)$$

Performing the division once gives:-

$$G(s) = \frac{A_{11}}{A_{21}} + \frac{\frac{A_{21}A_{12} - A_{11}A_{22}}{A_{21}}s + \frac{A_{21}A_{13} - A_{11}A_{23}}{A_{21}}s^2 + \dots}{A_{21} + A_{22}s + A_{23}s^2 + \dots \cancel{A_{21ns}{}^{n-1}}\ A_{2n}s^{n-1}} \qquad \dots.(10\text{-}12)$$

Define $$\frac{A_{21}A_{12} - A_{11}A_{22}}{A21} = A_{31}$$

$$\frac{A_{21}A_{13} - A_{11}A_{23}}{A_{21}} = A_{32} \qquad \text{....(10-13)}$$

Then equation (10-12) becomes:-

$$G(s) = \cfrac{1}{\cfrac{A_{11}}{A_{21}} + \cfrac{A_{31}s + A_{32}s^2 + A_{33}s^3 + \ldots}{A_{21} + A_{22}s + A_{23}s^2 + \ldots}} \qquad \text{....(10-14)}$$

which yields:-

$$G(s) = \cfrac{1}{\cfrac{A_{11}}{A_{21}} + \cfrac{s}{\cfrac{A_{21}}{A_{31}} + \cfrac{\cfrac{A_{22}A_{31} - A_{32}A_{21}}{A_{31}}s + \ldots}{A_{31} + A_{32}s + \ldots\ldots}}} \qquad \text{....(10-15)}$$

Define again:-

$$\frac{A_{22}A_{31} - A_{32}A_{21}}{A_{31}} = A_{41} \qquad \text{....(10-16)}$$

So that equation (10-15) becomes:-

$$G(s) = \cfrac{1}{\cfrac{A_{11}}{A_{21}} + \cfrac{1}{\cfrac{\frac{A_{21}}{A_{31}}}{s} + \cfrac{1}{\cfrac{A_{31}}{A_{41}} + \cfrac{1}{\vdots}}}} \qquad \text{....(10-17)}$$

The basic coefficients from equation (10-11) and the subsequently derived ones from equations (10-13) and (10-16) may be rearranged into the Routh array:-

$$\begin{array}{cccc} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & \\ A_{41} & A_{42} & A_{43} & \\ A_{51} & A_{52} & & \end{array} \qquad \text{....(10-18)}$$

where

$$A_{j,k} = A_{j+2,k+1} \quad \frac{-A_{j-1,1}\, A_{j-1,k+1}}{A_{j-1,1}} \quad , \quad \begin{array}{l} j=3,4,\ldots.n+1 \\ k=1,2.... \end{array} \qquad \text{....(10-19)}$$

<u>10.4 Application of the method of Chen and Shieh to a distillation model.</u>

In Chapter 9 methods are described for the determination of transfer functions relating product compositions to feed composition perturbations. The methods of Davison(46) and the root locus produce the system zeroes, enabling the numerator polynomial of the transfer function to be written down in factored form. The method of Bosley et al(49) yields the coefficients of the numerator polynomial directly. Simplification of either form is desirable for economic control system design. The method of Chen and Shieh affords a convenient way of achieving this simplification.

A computer program has been prepared for the ICL 1905 at Loughborough University of Technology. This program accepts as data either the poles and zeroes of the transfer function or the numerator and denominator polynomial coefficients. The Chen and Shieh H coefficients and the Chen and Shieh matrix are calculated (see sections 10.3.1 and 10.3.2). The final part of the program utilises a numerical integration routine prepared two years ago by other workers in the Department of Chemical Engineering and described in a paper by Gibilaro et al(58). This section of the program calculates the step response predicted by successively higher order Chen+Shieh models. These models are obtained by partitioning the system matrix of equation (10-7) as described in section 10.3.2.

10.4.1 Simplification of a transfer function in pole-zero form.

The zeroes for response 2 (the middle component in the overheads) calculated by the method of Davison and by the matrix root locus method given in Chapter 9 were presented to the Chen+Shieh computer program mentioned earlier. (In the case of the Davison method the Davison-row method results were employed as recommended by Davison for reasons mentioned in section 9.4.2.)

The step response for 2nd to 5th order Chen+Shieh models is given in Fig. 10-6. Note that the curves are almost identical - going to a 5th order model is no improvement over a 2nd.

10.4.2 Simplification of a transfer function in polynomial ratio form.

The set of numerator polynomial coefficients for response 2 (the middle boiling component in the overheads) calculated by the method of Bosley et al(49) with the modification of Kropholler(56) were presented to the Chen+Shieh program. The results are given in Fig. 10.7. Note again that the 2nd order model is almost coincident with the 5th. Response 35 (the middle boiling component in the bottoms) was treated similarly, the results being given in Fig. 10.8. Here there is some difference between 2nd and 3rd order models but the 4th and 5th are close to the 3rd.

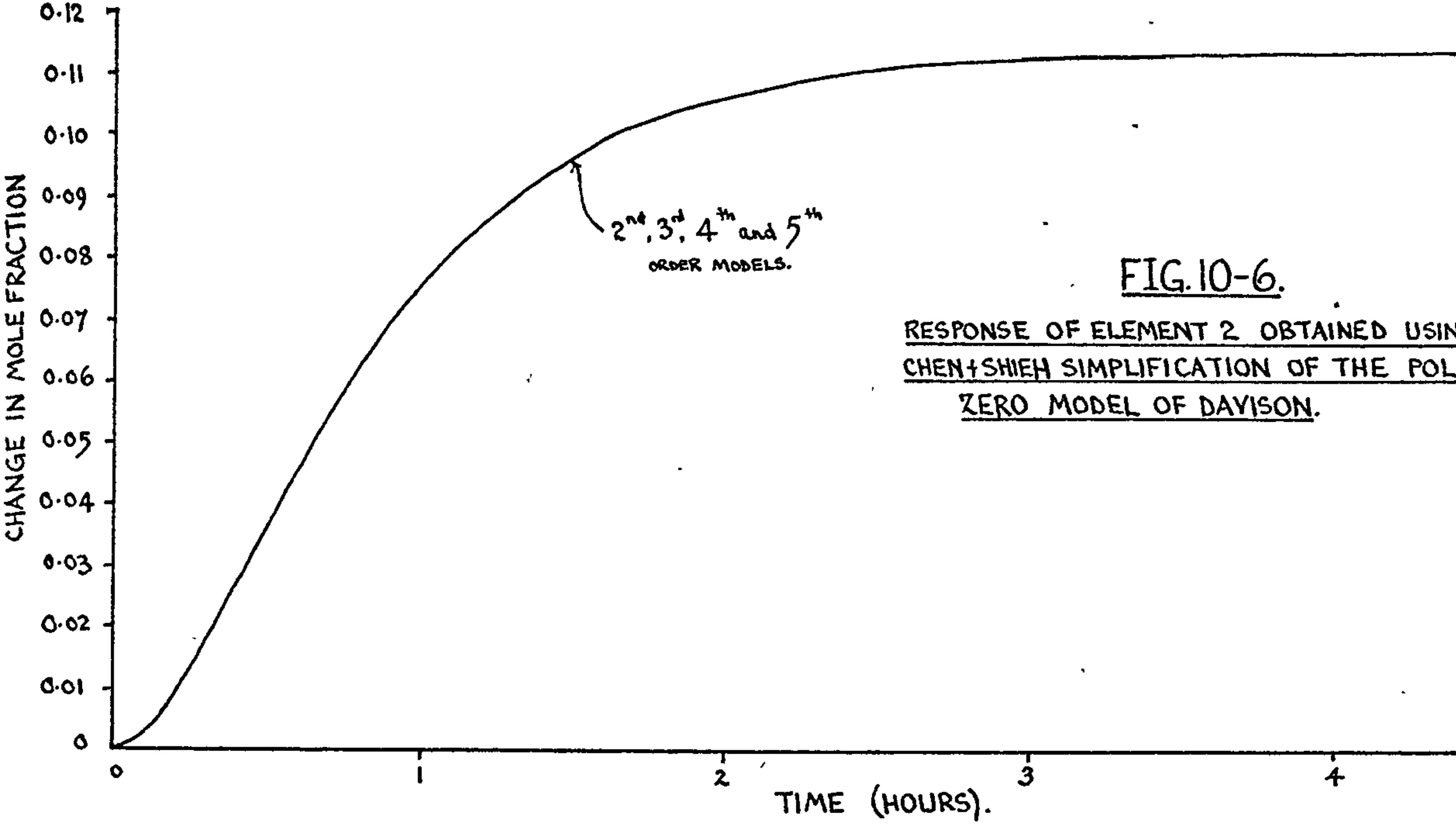


FIG. 10-6.

RESPONSE OF ELEMENT 2 OBTAINED USING CHEN + SHIEH SIMPLIFICATION OF THE POLE ZERO MODEL OF DAVISON.

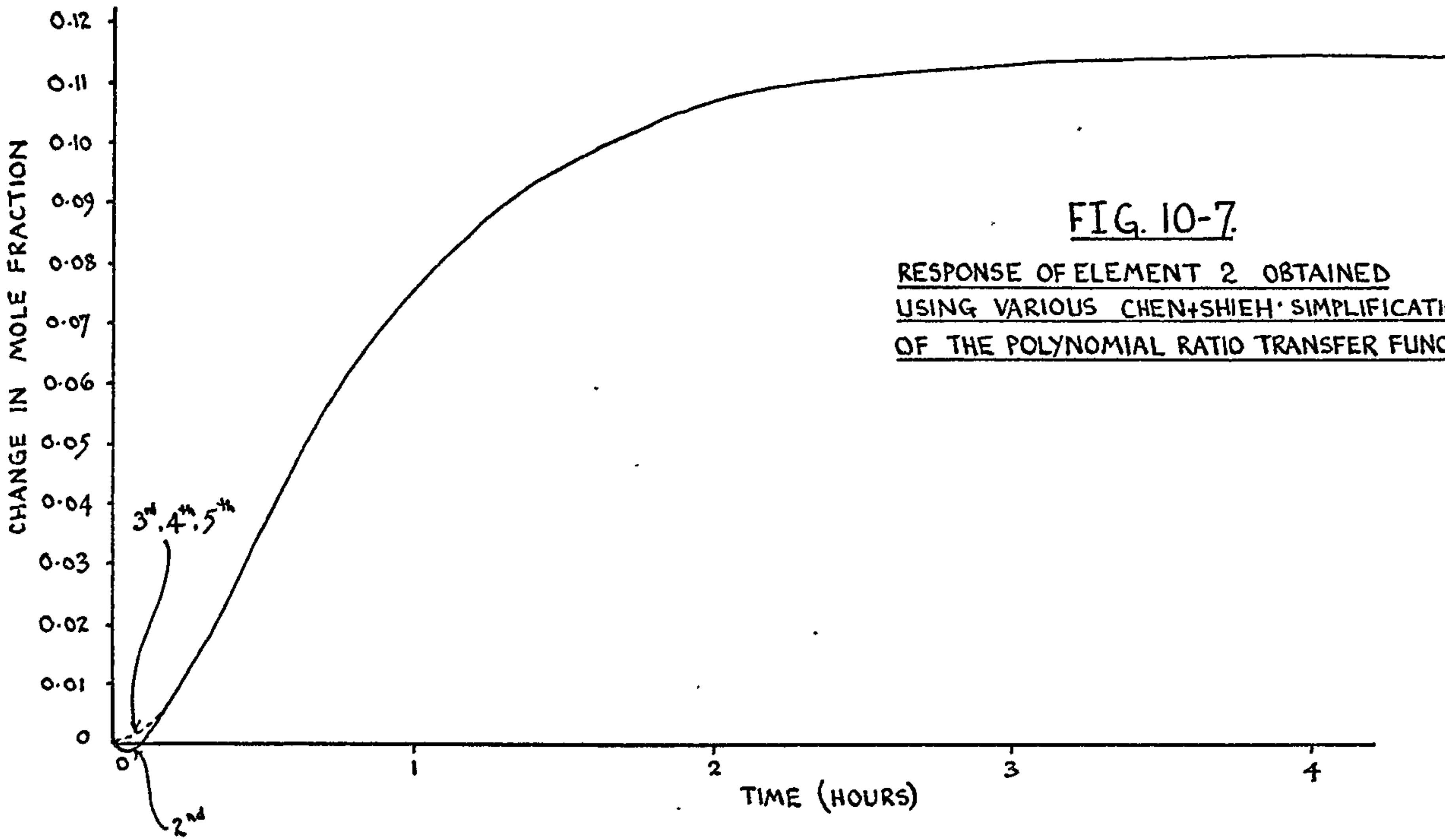


FIG. 10-7.

RESPONSE OF ELEMENT 2 OBTAINED USING VARIOUS CHEN+SHIEH SIMPLIFICATIONS OF THE POLYNOMIAL RATIO TRANSFER FUNCTION.

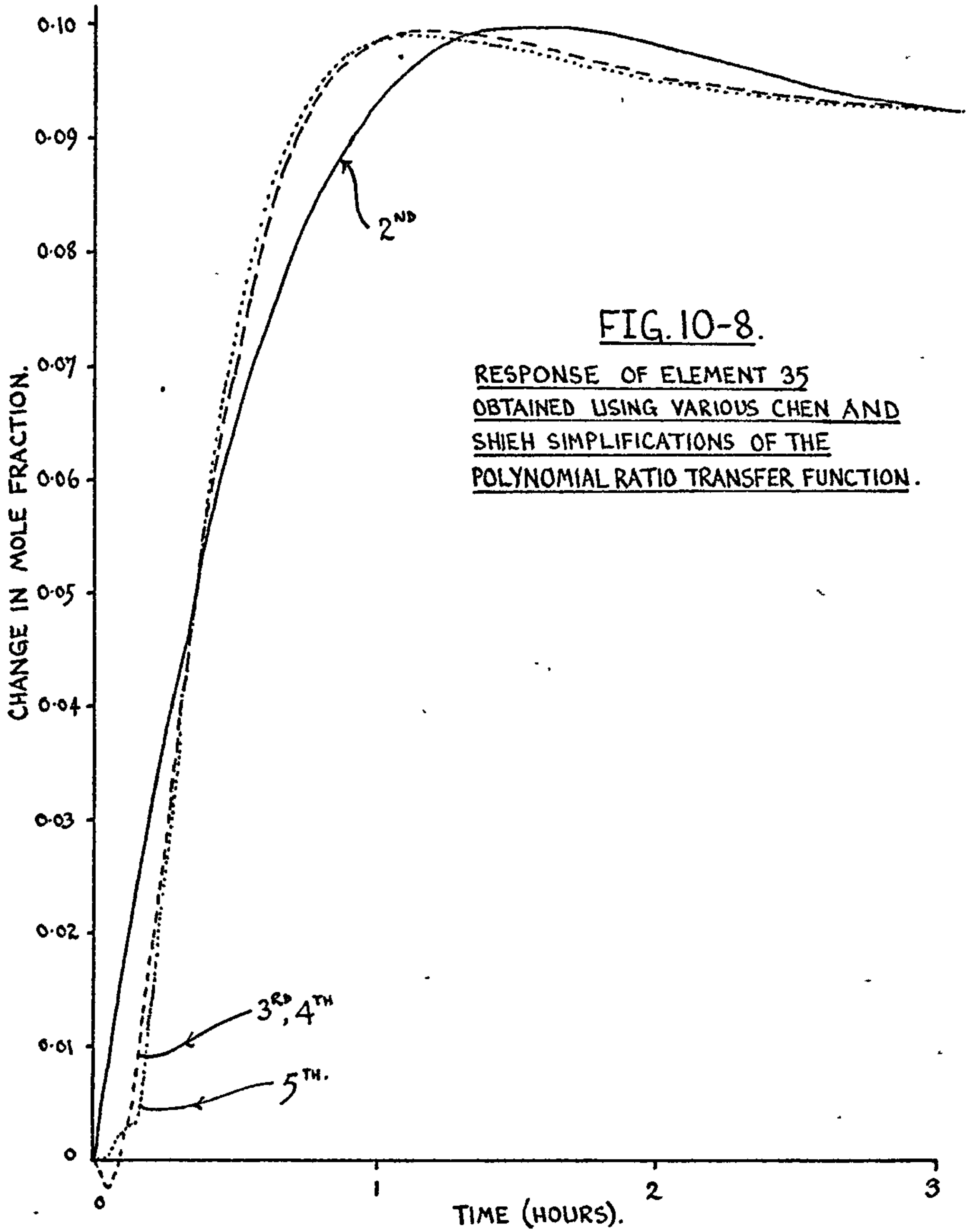


FIG. 10-8.

RESPONSE OF ELEMENT 35 OBTAINED USING VARIOUS CHEN AND SHIEH SIMPLIFICATIONS OF THE POLYNOMIAL RATIO TRANSFER FUNCTION.

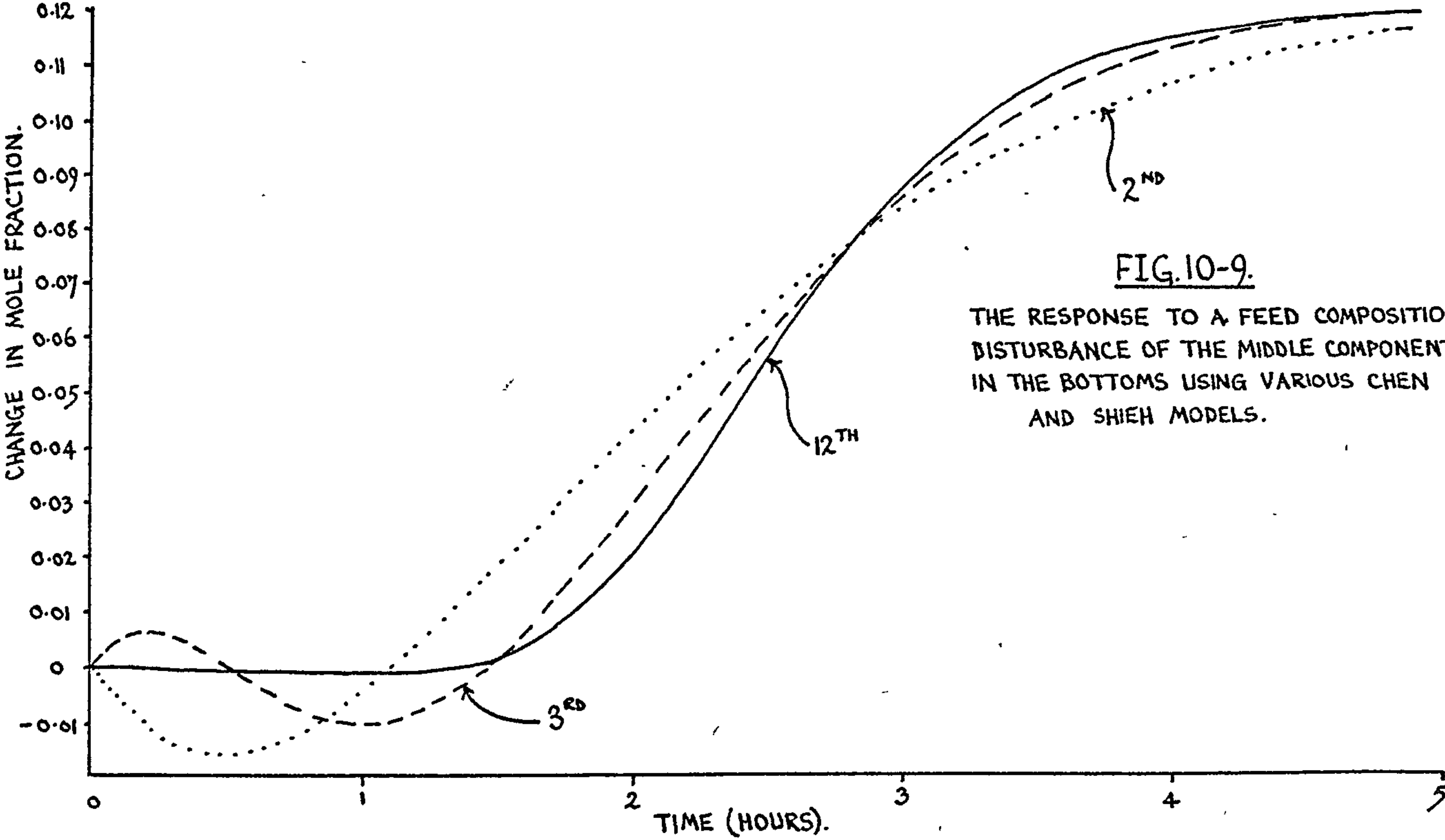


FIG. 10-9.

THE RESPONSE TO A FEED COMPOSITION DISTURBANCE OF THE MIDDLE COMPONENT IN THE BOTTOMS USING VARIOUS CHEN AND SHIEH MODELS.

10.4.3 Inverse response of low-order models.

Although this is not clearly demonstrated by the examples used in this chapter, low order Chen-Shieh models can exhibit undesirable qualities. The predicted response to a feed composition disturbance for the middle component in the bottoms of a ten plate unit distilling a three component mixture is given in Fig. 10-9. The system modelled is similar but not identical to that described in Chapter 8, and is outlined in Appendix 10.

An appreciable lag occurs at the start of this response and the low-order models exhibit appreciable oscillation over this part of the curve. This could lead to poor control action if for instance the second order model were used in a control system.

CHAPTER 11. ANALYTICAL AND NUMERICAL SOLUTIONS TO COMPLETE PROBLEMS.

11.1 The analytical solution to the state variable equation.

Lees(55) gives a good treatment of this and this section draws heavily on this reference.

Consider the basic equation:-

$$\dot{\underline{x}} = A\underline{x} + B\underline{u} \qquad \text{....(11-1)}$$

where $\underline{x}$ is the state vector, A the system matrix and $B\underline{u}$ is the forcing function. The time domain solution of equation (11-1) is:-

$$\underline{x} = \exp\left\{At\right\} \underline{x}(o) + \exp\left\{At\right\} \int_0^t e^{-A\tau} B\underline{u}(\tau)d\tau \qquad \text{....(11-2)}$$

If $\underline{x}(0) = \underline{0}$ then

$$\underline{x} = \exp\left\{At\right\} \int_0^t e^{-A\tau} B\underline{u}(\tau)\, d\tau \qquad \text{....(11-3)}$$

The time solution may be obtained via the eigenvalue and eigenvectors using the relation

$$\exp\left\{At\right\} = U \exp \left\{Jt\right\} U^{-1} \qquad \text{....(11-4)}$$

where J is the diagonal or tridiagonal matrix having the system eigenvalues for its non-zero elements. (This is given in more detail later.) U is the modal matrix or matrix of eigenvectors.

The impulse response follows from equation (11-3), since for $\tau > 0$, and $B\underline{u}\ (\tau) = o$:-

$$\underline{x}(t) = \exp\left\{At\right\} B\underline{u}(o) \qquad \text{....(11-5)}$$

Integrating this to give the step response yields:-

$$\underline{x}(t) = \int_0^t \exp\left\{At\right\} B\underline{u}(o)\, dt \qquad \text{....(11-6)}$$

For the case of distinct real roots or distinct complex roots in conjugate pairs - the case which includes distillation and similar systems - the matrix J is of the form:-

$$J = \begin{bmatrix} \lambda_1 & & & & \\ & \lambda_2 & -W_2 & & \\ & W_2 & \lambda_2 & & \\ & & & \ddots & \\ & & & & \lambda_n \end{bmatrix} \qquad \ldots.(11\text{-}7)$$

where λ = real part of root

w = imaginary part of root.

The column of U corresponding to equation (11-7) would then be:-

$\left[\text{Real} \quad \text{Real} \quad \text{Imaginary} \ldots\ldots\ldots \text{Real}\right]$

The impulse response obtained by substituting $\exp\left\{At\right\}$ from equation (11-4) into equation (11-5) is:-

$$\underline{x}(t) = U \exp\left\{Jt\right\} U^{-1} \; B\underline{u}(o) \qquad \ldots.(11\text{-}8)$$

Let $U \; B\underline{u}(0) = \underline{z}$ ....(11-9)

Then equation (11-8) may be written:-

$$\underline{x} = U \begin{bmatrix} \exp\lambda_1 t & & & & \\ & \exp\lambda_2 t \cos w_2 t & -\exp\lambda_2 t \sin w_2 t & & \\ & \exp\lambda_2 t \sin w_2 t & \exp\lambda_2 t \cos w_2 t & & \\ & & & \ddots & \\ & & & & \exp\lambda_n t \end{bmatrix} \qquad \ldots.(11\text{-}10)$$

By Kropholler's extension to Ogata (54) equation (11-10) may be written:-

$$\underline{x} = U \begin{bmatrix} Z_1 & & & & \\ & Z_2 & & & \\ & & \ddots & & \\ & & & & Z_n \end{bmatrix} \begin{bmatrix} \exp \lambda_1 t \\ \exp \lambda_2 t \cos w_2 t \\ \exp \lambda_2 t \sin w_2 t \\ \vdots \\ \exp \lambda_n t \end{bmatrix} \qquad \ldots.(11\text{-}11)$$

The step response may then be obtained by integration of the right hand vector, where

$$\int_0^t \exp \lambda t \cos wt \, dt = \frac{1}{\lambda^2 + w^2} \left\{ (w \sin wt + \lambda \cos wt) \exp \lambda t - \lambda \right\} \qquad \ldots.(11\text{-}12)$$

and

$$\int_0^t \exp \lambda t \sin wt \, dt = \frac{1}{\lambda^2 + w^2} \left\{ (\lambda \sin wt - w \cos wt) \exp \lambda t + w \right\} \qquad \ldots.(11\text{-}13)$$

The author utilised a tested computer program written by Hak(64) which calculated the matrix:-

$$U \begin{bmatrix} Z_1 & & & & \\ & Z_2 & & & \\ & & \ddots & & \\ & & & & Z_n \end{bmatrix}$$

This was extended to perform the full step response calculation using the relations in equations (11-12) and (11-13). In order to handle the 36th order distillation problem described in section 8.5 it was necessary to split this program into a suite of three programs, the card output of the first and second acting as data to the third.

11.2 Numerical integration of the state variable equation by the method of Gibilaro et al.

This method is described in a paper by Gibilaro et al(58) but a brief outline is relevant here. The equation considered is the initial value form of equation (3-28):-

$$d/dt(\underline{x}) = A\,\underline{x} \qquad \text{subject to } \underline{x} = \underline{x}(0) \text{ at } t = 0 \qquad \ldots.(11\text{-}14)$$

The analytical solution to this is:-

$$\underline{x}(t) = e^{At}\underline{x}(0) \qquad \ldots.(11\text{-}15)$$

For a small time increment   the approximation is made:-

$$\underline{x}(t+\tau) = e^{D\tau}\underline{x}(t) \qquad \ldots.(11\text{-}16)$$

where D is a diagonal matrix formed by neglecting all but the diagonal elements of matrix A. That is for small intervals of time the system may be assumed to behave as a set of independent first order systems.

Now for a small time interval Δt the analytical solution may be written:-

$$x(t+\Delta t)-x(t) = \int_0^{\Delta t} Ax(t+\tau)d\tau \qquad \ldots.(11\text{-}17)$$

Substituting from equation (11-16) into equation (11-17) for $\underline{x}(t+\tau)$:-

$$x(t+\Delta t)-x(t) = \int_0^{\Delta t} Ae^{D\tau}x(t)d\tau$$

whence:

$$x(t+\Delta t) = \left\{I + AD^{-1}\left[e^{D\Delta t} - I\right]\right\}x(t) \qquad \ldots.(11\text{-}18)$$

$$\text{i.e.} \quad x(t+\Delta t) = P\,x\,(t) \qquad \ldots.(11\text{-}19)$$

where the matrix P may be obtained at the start of the calculation. The value of $\underline{x}$ after any time step is then obtained by pre-multiplying the value of $\underline{x}$ at the end of the previous time step by P.

This alone is of limited value since the approximation of equation (11-6) requires small time steps to be adequate. However, note from the form of equation (11-9) that further acceleration of the solution is possible. Suppose that values of $\underline{x}$ at intervals of Δt are required, but that the largest time step commensurate with acceptable truncation error is δt where

$$\Delta t = n \delta t \qquad \ldots.(11\text{-}20)$$

Then it may be seen that equation (11-19) may be written:

$$x(t + \Delta t) = P^n x(t)$$

In practice δt is reduced to make n an integral power of 2 so that P^n is produced by repeated matrix squaring. This produces a very efficient but still accurate method of numerical solution.

11.3 A comparison of the solutions to a distillation model obtained by analytical and numerical methods.

Computer programs exist for the two methods described in section 11.1 and 11.2. These were tested using small (normally third order) systems for which the solution may be calculated by hand. The first additional check to be applied in running the 36-order distillation model was to verify that the steady state gains were correctly predicted. These are given in Fig. 8-6. Sample results for the two methods are given in Fig. 11-1. From this it may be seen that whereas both solutions give good match to the steady state gain at the top of the column, neither is correct at the bottom.

Program runs were repeated using the same data decks as for runs on the Davison and Bosley transfer function elucidation programs, (for which the correct steady state gains for all variables were obtained). The incorrect results again emerged, leading the author to suspect inherent weaknesses in the methods. Isol ation and elimination of these weaknesses

VARIABLE	THEORETICAL STEADY STATE GAIN	PREDICTION OF THE ANALYTICAL SOLUTION	PREDICTION OF THE NUMERICAL SOLUTION
Overheads:			
Light component	0.1155	0.1174	0.1055
Heavy component	-0.1151	-0.1172	-0.1052
Bottoms:			
Middle component	-0.006452	0.002673	0.001636
Heavy component	0.0001562	0.001060	0.001962

Change in mole fraction composition of products before and after feed perturbation.

FIG.11-1

is not really within the scope of this project but the results are reported here for information.

Fig.11-2 gives a comparison of the response of variable 2 (the middle component in the overheads) and it may be seen that fairly good agreement is obtained throughout the transient. It is noteworthy that the analytical solution yields a better approximation to the final steady state than the numerical solution.

<u>11-4 A comparison of the solutions to a distillation model obtained by simplification of various transfer functions.</u>

The Chen and Shieh simplified forms of transfer functions obtained by the methods of Davison, Bosley and the matrix root locus are given in Fig. 11-3. The curves are so close as to be coincident. The analytical solution is plotted for comparison. It will be noted that the agreement between the second order simplified models and the analytical solution is very close throughout the entire transient. In addition the simplified models' transient approximates more closely to the final steady state.

Comparable response curves for the middle component in the bottoms are given in Fig. 11-4. The points of interest here are the inverses at the start of each curve and the oscillatory nature of the response. A slight overshoot is obtained demonstrating the ability of distillation system to give response other than an exponential decay to a feed composition perturbation.

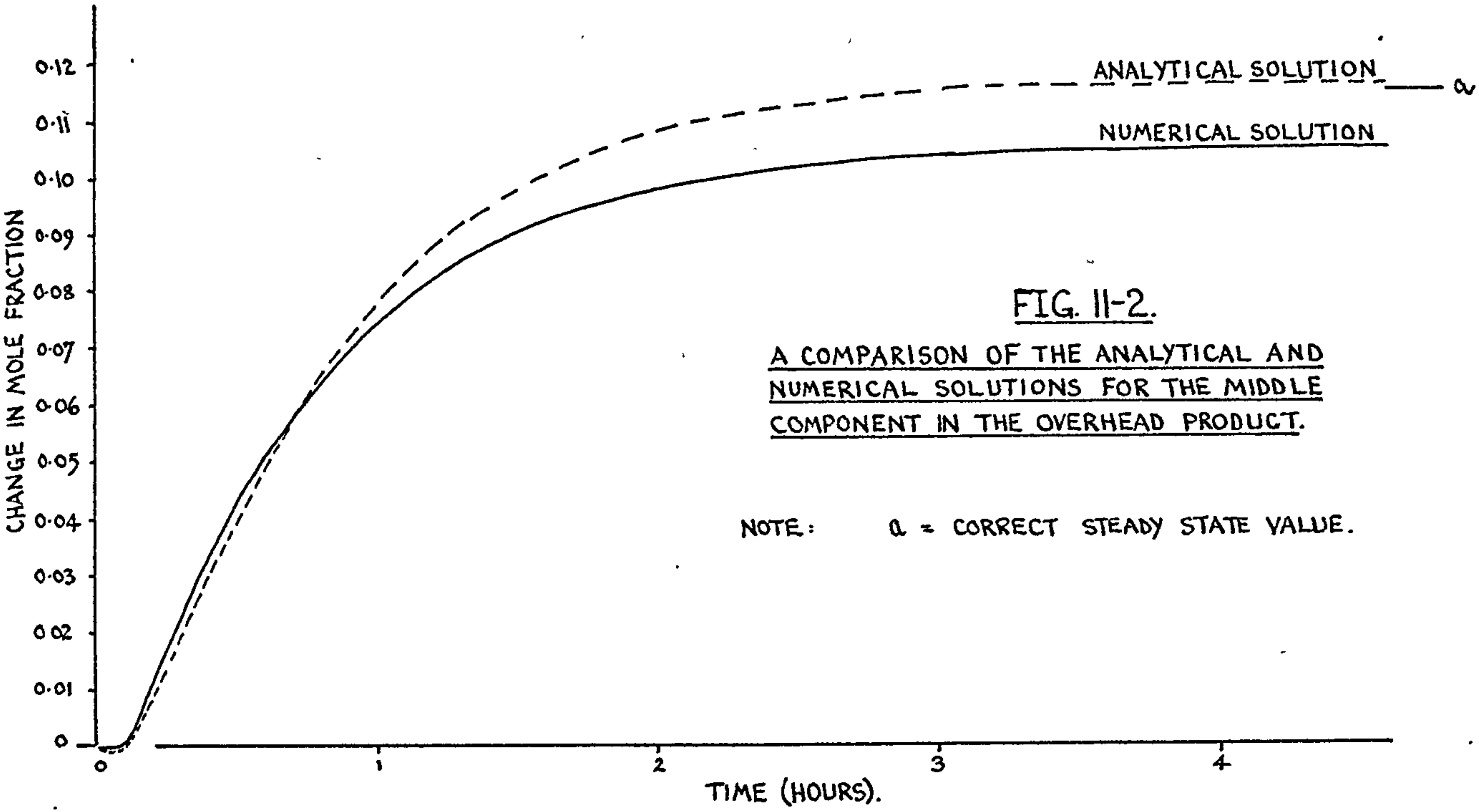


FIG. 11-2.

A COMPARISON OF THE ANALYTICAL AND NUMERICAL SOLUTIONS FOR THE MIDDLE COMPONENT IN THE OVERHEAD PRODUCT.

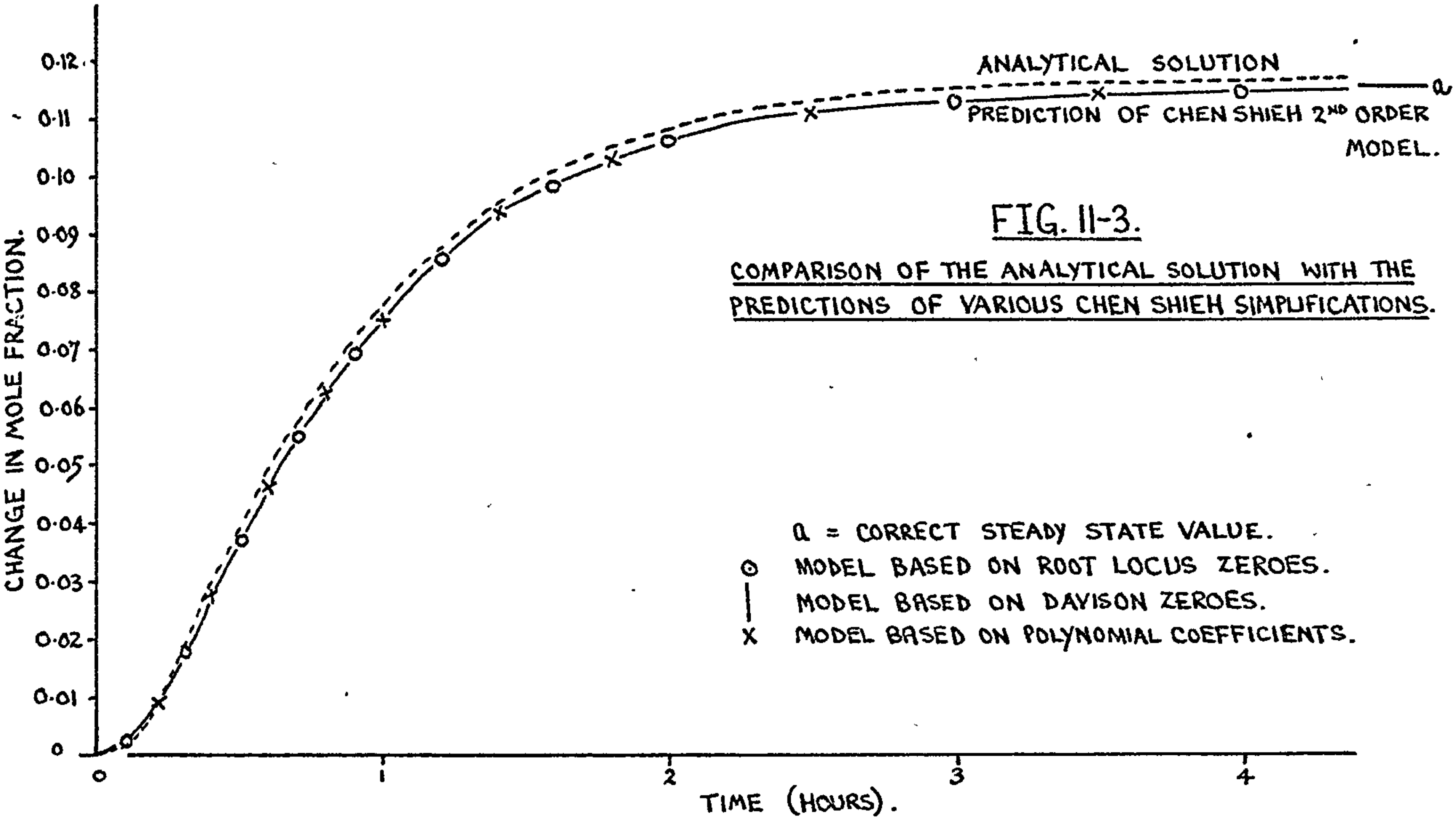


FIG. II-3.

COMPARISON OF THE ANALYTICAL SOLUTION WITH THE PREDICTIONS OF VARIOUS CHEN SHIEH SIMPLIFICATIONS.

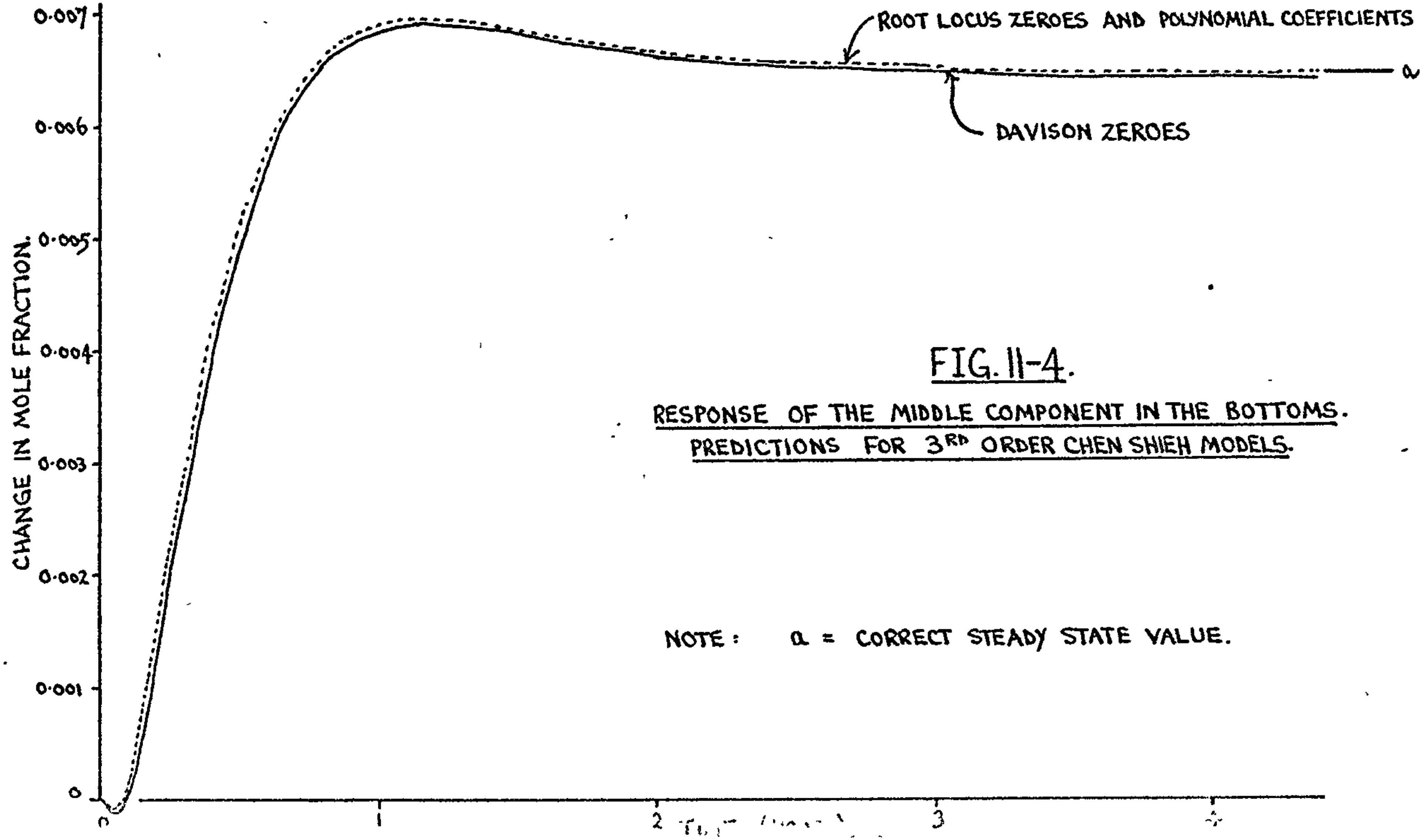


FIG. 11-4.

RESPONSE OF THE MIDDLE COMPONENT IN THE BOTTOMS.
PREDICTIONS FOR 3RD ORDER CHEN SHIEH MODELS.

NOTE: a = CORRECT STEADY STATE VALUE.

CHAPTER 12 CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER WORK.

12.1 Introduction

This chapter has been structured to correspond to Chapter 2 for ease of cross-reference.

During the period of the project some broadening has occurred from the original centre-line - the distillation of crude oil. This is because the initial work revealed that hydraulic disturbance alone did not account for an appreciable part of the response to perturbation of the particular distillation column studied. When attention was focussed on the modelling of the mass transfer characteristics of the unit it became apparent that much basic work was necessary before this could be tackled. The second half of this thesis is devoted to a study of these basic problems and their solution.

12.2 Practical and theoretical studies connected with the BP crude distillation unit.

12.2.1 The effect of the hydraulic and heat transfer transients on the column response.

A mathematical model was constructed and is described in Chapter 4. This considers the equations relating the hydraulics and heat transfer. In spite of simplifying assumptions the model yields a complex mathematical problem. A computer program for the ICL 1905 computer was written for the solution to the problem. This took appreciable computer time - of the order of sixty times real time for a 15-plate column example. The model yielded quite reasonable qualitative results but it was not possible to do a detailed check against experimental data.

It is noteworthy that the single oscillation on the model response curves is similar to the general experimental response curve. This suggests that the right sort of mechanism has been simulated. The time scale is out by a considerable factor, the model response being 20-30 times faster than the experimental response. Indeed the hydraulics and heat transfer response seems to act as an analogue for the full response which is then presumably due mainly to mass transfer.

Consideration of computer core store requirements led to the adoption of an iterative solution method for the model. The set of differential equations was solved by an implicit method described by Holland (33) on the basis of an assumed set of values for the vapour rates leaving each plate. On average about six iterations were needed to yield assumed and calculated values for the 15-element vapour rate vector agreeing to within 0.0001 lb/sec. This model might well prove to be more useful if tackled by Gear's method(70). This would need less core store and would obviate the need for iteration. This is suggested as a suitable basis for further work. The object of such a project would be to produce a model which could be used in conjunction with the mass transfer dynamics as a basis for a control system.

12.2.2 Determination of the open-loop response of the industrial column.

This is described in Chapter 5. The large effect on all the tray temperatures and product properties of changes in the reflux flow are well demonstrated by the experimental work. In particular the oscillatory nature of the response curves gives considerable insight into the origins of the long settling times required for the unit to settle after major flow changes are made. Three significant points emerge. The length of time required for the reflux drum hold-up to reaeh its new composition is about $1\frac{1}{2}$ hours. The length of time required for fractionation driving forces to reverse the effect of liquid dumping down the column is of the same order of magnitude. Perhaps of most interest is the oscillatory nature of the open loop response curves with a large overshoot and then swift damping for many variables.

12.2.3 Experimental work at Loughborough on the single sieve plate unit.

This is described in Chapter 6.

The experiments demonstrate that the equations used to describe the hydraulics in the large model described earlier are of the right form and give the correct type of response. Thus the set of equations used should be capable of simulating the responses of the hold up and liquid froth density to liquid flow changes. The results for vapour changes are not correct. This is not important in the present work but would be an interesting area to explore further. The control study of an absorber with fluctuating vapour feed would need a model that was valid in this area.

It is relevant at this point to re-iterate the need for a mechanistic model of the hydraulics of distillation plates to replace the rather crude and apparently not generally valid correlations currently available.

12.2.4 Application of the results to crude oil distillation.

This is discussed in Chapter 7. Two main points emerge. The first concerns control of the unit by using the tower top temperature to control the reflux flow. This appears to work well for 'steady state' operation. However, during major flow changes the beneficial effects of maintaining constant temperature near the top of the tower may be offset by the effects of varying liquid rates and compositions reaching trays lower in the tower. This would be particularly important in the case of the kerosine flash point which is extremely sensitive to small amounts of liquid material. The second point follows from the first and concerns the suggested way of achieving a major flow change by an initial step followed by a ramp. The improvements to be gained by this sort of approach to flow control during major changes seem to justify further work.

12.3 Multicomponent mass transfer models.

12.3.1 Selection of the unsimplified model.

This is described in Chapter 8. The formulation of Wood seems to justify the slight additional work involved in its construction. It is shown to be an intrinsically more sound model than that of Mah et al. It permits the description of right half plane zeroes and oscillatory response, displaying both real and complex eigenvalues. Moreover there is no necessity for the rather crude normalisation to constrain mole fractions to sum to unity. It has the disadvantage that component responses cannot be solved in isolation and even the quite small ten plate three component demonstration model used appreciable core store on an ICL 1905. With size also comes numerical difficulties. Chapter 9 demonstrates how these can be solved.

12.3.2 Conversion of models from state variable to transfer function form.

This is discussed in detail in Chapter 9. It is shown that the problem may be reduced to one of finding the numerator roots or the coefficients of the numerator polynomial. The method of Davison(46) by which the zeroes are located by solving an approximately equivalent eigenvalue problem is discussed. Certain modifications are suggested to aid in the solution of large order (say greater than 15th) problems on an ICL 1905 computer.

It is shown that the root locus may be obtained from a matrix formulation again by the construction of the approximately equivalent eigenvalue problem. Moreover under certain conditions Davison's method and the matrix formulation of the root locus become identical.

The claim is made in the paper by Davison that selection of the system zeroes from amongst the extraneous roots also obtained is straightforward. This has been found to be valid for the case of real zeroes. However, it is not easy to obtain the complex zeroes reliably. The same criticism is true of the matrix root locus method. Even when multiplying parameter is taken to the limits permited by numerical accuracy in the eigenvalue routine, the values of the complex zeroes are not constant. This poses two problems. The first is the decision as to whether a root is extraneous or a true zero. This is rarely serious, although the author found that practice was essential. Secondly, if the root is a true zero, what is the best value to choose for it? On the basis of the theory underlying Davison's method the results for the highest value of the multiplying factor were chosen.

However, it is at this point that numerical inaccuracy is increasing and it does not necessarily follow that the best estimate of a complex zero will be obtained. The complex roots in particular seem to be quite sensitive as the multiplying factor changes about this point. However, the responses obtained using simplified models based on zeroes obtained by these methods closely match those obtained using other methods, so this difficulty is not very serious.

As an interesting and useful off-shoot from the main theme a very simple way of obtaining the root locus for medium sized systems has been outlined. The value of this is not reduced by the numerical problems mentioned earlier since the root locus at very high gains is rarely required.

The method of Bosley et al also described in Chapter 9 is basically straightforward in its application and theoretically needs no user intervention for coefficient estimation. However, the application to 36 variable problem using an ICL 1905 computer reveals potential numerical problems, even though extensive use was made of double length (22 decimal digit) working. The modification of Kropholler(56) overcomes these although additional programming and computer time are required. Of the three methods that of Bosley et al with Kropholler's modification appears to be slightly superior.

The final stage of the work in this field will be the incorporation of the checks and ancillary calculations into robust computer programs for each method.

12.3.3 Simplification of a complicated transfer function.

This work is described in Chapter 10. The method of Chen and Shieh has been used to simplify pole/zero transfer functions generated by Davison's method and by the matrix root locus method and polynomial transfer functions generated by the method of Bosley et al.

The method appears to work quite satisfactorily for the 36 variable system studied. Second order models are quite good approximations - third and fourth order models give results very close to the actual system response curves. It is important to note one point on numerical accuracy and accumulation of round off error. H_1 to H_4 only are needed in second order models. If errors do accumulate they will only be apparent in the less important higher order coefficients.

One disadvantage of the method could be the oscillation near the origin obtained with some low order models. However as a general conclusion the Chen and Shieh method appears to offer an excellent simple and automatic approach to the final problem - that of extracting information for controller design from large state variable formulations which give rise to complicated transfer functions.

12.3.4 Analytical and numerical solutions to complete problems.

This work is described in Chapter 11. The comparison of simplified model responses based on the three methods indicates that close approximations to the true response are obtained using the predictions of Chen+Shieh models based on the pole/zero estimates of Davison and the Matrix root locus and the polynomial coefficient estimates of the method of Bosley.

The comparison of the prediction of the Chen and Shieh models with the complete analytical and numerical solutions is interesting. Results are given for the analytical solution described by Ogata(54) and for the numerical solution based on the work of Gibilaro et al (57). Good agreement is obtained for the middle component in the overheads. However, there is no real match for the middle component in the bottoms. Since it is responses of the simplified models which give the correct steady state gain it is assumed that these are nearer to being correct. The errors with the complete solutions are attributed to numerical problems in the programs. Solution of these does not fall within the scope of this thesis but improvements to the methods are certainly required.

12.4 Closing Remarks.

This project has considered the problem of the modelling of multistage systems. Experimental work on a crude oil distillation unit revealed interesting oscillatory response curves for column temperatures and product properties. Theoretical work with similar systems indicated that an analogous response could be obtained using only the hydraulic and heat transfer dynamics. This gives the right form of response but over a shorter time scale. The extension of the study into mass transfer dynamics revealed problems of formulation, simplification and solution. Methods of overcoming several numerical problems and producing simple transfer functions from complex state variable models are described and demonstrated. The author hopes that future workers will continue the study into the field of the modelling of larger and more complex systems such as crude oil distillation mass transfer dynamics.

However, it is fair to say that with little further work many of the principles described may be put into practice straight away. Chapter 11 indicates that simple 2nd and 3rd order models that can be readily derived are good approximations to 30th order systems. The problems that might arise with the application of these techniques to other systems are:

(i) an ill-conditioned system matrix could give rise to severe numerical problems, as could a matrix in which the elements were different by several powers of ten. In the example quoted the ratio of the largest to the smallest element is about 100.

(ii) as the size of the system is increased so the numerical problems associated with the simplification also become greater. Here the importance of the accuracy-checks described in detail in Chapter 9 is seen. With these it is possible to reject erroneous results instantly without the necessity for tedious back calculation.

Note, however, that the basic assumption of linearity may itself in many cases be a major source of error. Although the ability to describe a problem more fully may lead to significantly better models this is unlikely to remove problems associated with non-linearity.

The effectiveness of this rational reduction approach justifies the use of more complete formulations. The complexity associated with such models can be rapidly skirted using the techniques described, leading to simple models that have all the characteristics of the full mathematical description. These models are readily soluble and are also suitable for incorporation into a control system.

- - - - -

REFERENCES.

(1) BOLLES W.L. Petroleum Processing. Feb. 1956. p.65.

(2) PERRY J.H. Chemical Engineers Handbook 4th Edition. McGraw Hill.

(3) A.I.Ch.E. Research Committee "Final Report, University of Michigan" 1960 (New York: American Institute of Chemical Engineers).

(4) A.I.Ch.E. Research Committee "Final Report, University of Delaware" 1958 (New York: American Institute of Chemical Engineers).

(5) BERNARD J.D.T. and R.W.H. SARGENT. "Proceedings of the Symposium on Distillation". 1964 (London: Association of British Chemical Manufacturers/British Chemical Plant Manufacturers Association.)

(6) BERNARD J.D.T. and R.W.H. SARGENT. Transactions Instn. Chem. Engrs. (London) 44 (1966) p.314.

(7) Bubble Tray Design Manual 1958 (New York: American Institute of Chemical Engineers.)

(8) RODIONOV A.J. International Chemical Engineering 6 (1966) p.639.

(9) THOMAS W.J. and M. CAMPBELL. Transactions Instn. Chem. Engrs. (London) 45 (1967) p.53.

(10) GARDNER R.G. and A.Y. McLEAN. "Proceedings of the International Symposium on Distillation" 1969 (London: Institution of Chemical Engineers.

(11) WILKINSON W.L. and W.D. ARMSTRONG Proceedings of S.I.T. Conference 1956 in "Plant and Process Dynamic Characteristics" (Butterworths).

(12) VOETTER H. ibid.

(13) WESTCOTT J.H. ibid.

(14) ENDTZ J, J.M.L. JANSSEN and J.C. VERMEULEN ibid.

(15) ROSENBROCK H.H. Trans. Instn. of Chem. Engrs. (London) 35 (1957) p.347.

(16) CRANDALL S.H. Engineering Analysis. A survey of Numerical Procedures. Engineering Society Monographs McGraw Hill, New York, 1956.

(17) RIJNSDORP J.E. The Birmingham University Chemical Engineer 12 Supplement S14 (1961).

(18) WILKINSON W.L. and W.D. ARMSTRONG. Chem. Eng. Sci. 7 (1957) p.1.

(19) ARMSTRONG W.D. and R.M. WOOD. Trans. Instn. Chem. Engrs. 39 (1961) p.65.

(20) ibid, idem. p.80.

(21) BABER M.F. and J.A. GERSTER. Proceedings of Symposium on Process Dynamics and Control. A.I.Ch.E. New York (1961).

(22) LAMB D.E., R.L. PIGFORD and D.W.T. RIPPIN. Chem. Eng. Prog. Symposium Series 1961, 57, p.132.

(23) MAH R.S.H., S. MICHAELSON and R.W.H. SARGENT. Chem. Eng. Sci. 17 (1962) p.619.

(24) SARGENT R.W.H. Trans. Instn. Chem. Engrs. 41 (1963) p.51.

(25) WOOD R.M. Trans. Instn. Chem. Engrs. 45 (1967) p.190.

(26) PEISER A.M. and S.S. GROVER. Chem. Eng. Prog. 58 (1962) 9, p.65.

(27) WEEKLEY G.H. Hydr. Proc. and Pet. Ref. 43,(1964),3,p.115.

(28) ROBBINS T. Ph.D.Thesis. Swansea University 1966.

(29) CECCHETTI R., R.H. HOHNSTON, J.L. NIEDZWIECKI and C.D. HOLLAND. Hyd.Proc. and Pet.Ref. 42 (1963)9,p.159.

(30) GILBERT R.J.H., J.LEATHER and J.F.G. ELLIS. A.I.Ch.E.Jl. 12 (1966)3,p.432.

(31) EDMISTER W.C. A.I.Ch.E.Jl. 3 (1957)2, p.165.

(32) HOLLAND C.D. Multicomponent Distillation. Prentice Hall (1963).

(33) HOLLAND C.D. Unsteady State Processes with Applications in Multicomponent Distillation. Prentice-Hall (1966).

(34) CLARK C.R. M.Sc. Thesis, Loughborough University of Technology 1969.

(35) HOFFMAN E.J. Chem.Eng.Sci. 23 (1968) p.957.

(36) GILBERT R.J.H, G.J. WANLESS and R.D. WILSDON. Proceedings of International Symposium on Distillation 1969. London: Instn.Chem.Engrs.

(37) KUEHN D.R. and H. DAVIDSON. Chem. Eng. Prog. 57 (1961)6, p.44.

(38) ROBBINS T. Private communication.

(39) CLEMENTSON A.T. Br.Chem.Eng. 8 (1963) 8, p.564.

(40) SHELTON R.J. and A.W. HUTCHINSON. Trans. Instn. Chem. Engrs. 45 (1967) p.334.

(41) REES N.W. Proceedings I.F.A.C. Congress (1966).

(42) STAINTHORP F.P. and M.J. WARREN. Paper presented at Colloquium "Making Plant Models" 1966. (London: Instn. Elec. Engrs.)

(43) PIPES L.A. and S.A. HOVANESSIAN. Matrix Computer Methods in Engineering. Wiley (1969).

(44) CHEN C.F. and I.J. HAAS. Elements of Control Systems Analysis: Classical and Modern Approaches. 1968 (Prentice Hall).

(45) HENNION P.E. Communications of the A.C.M. 6 (1963)4, p.165.

(46) DAVISON E.J. Paper presented at 3rd I.F.A.C. Conference, London 1966.

(47) idem. A.I.Ch.E.Jl. 14 (1968)1, p.46.

(48) idem. Automatica 6 (1970) p.481.

(49) BOSLEY M.J., H.W. KROPHOLLER, F.P. LEES and R.M. NEALE. Paper submitted to Automatica for publication.

(50) HALL H.S. and S.R. KNIGHT. Higher Algebra. 4th Edn. (1950). (Macmillan.)

(51) CHEN C.F. and L.S. SHIEH. Int.J.Control 8 (1968),6,p.561.

(52) idem, ibid. 11 (1970),5,p.717.

(53) MAEHLY H.J. Journal of A.C.M. 7 (1960) p.150.

(54) OGATA K. State-space Analysis of Control Systems. Prentice-Hall (1967).

(55) LEES F.P. Ph.D.Thesis. Loughborough University of Technology. 1968.

(56) KROPHOLLER H.W. Private Communication.

(57) GIBILARO L., H.W. KROPHOLLER and D.J. SPIKINS. Chem.Eng.Sci. 22 (1967) p.517.

(58) idem. Inst.Chem.Engrs. Symposium Series No. 23. (1967). Inst.Chem.Engrs., London.

(59) KREYSZIG E., Advanced Engineering Mathematics, Ch.7. 2nd Edn. Wiley (1967).

(60) SHORE D. and G.G. HASELDEN. Paper presented at International Symposium on Distillation 1969. (London: Instn. Chem. Engrs.)

(62) ACRIVOS A. and N.R. AMUNDSEN. Ind.Eng.Chem. 47. (1955) p.1533.

(63) Fortran Scientific Subroutine Manual for 1900 Series Computers. International Computers Ltd., London.

(64) HAK S.K. Ph.D.Thesis to be submitted to Loughborough University of Technology.

(65) Closing remarks by Chairman, International Symposium on Distillation, 1969. (Instn. of Chem. Engrs., London).

(66) HO G.E., R.L. MULLER and R.G.H. PRINCE. Paper presented at International Symposium on Distillation, 1969 (Instn. of Chem. Engrs., London).

(67) ACRIVOS A. and N.R. AMUNDSEN. Matrix methods in Chemical Engineering. Prentice Hall 1964.

(68) GIBILARO L.G. and F.P. LEES, Ch.Eng.Sci. 24 (1969) p.85.

(69) KROPHOLLER H.W. et al. Ind. Eng. Chem. To be published.

(70) GEAR C.W. Proceedings of 1968 I.F.I.P.S. Congress, Edinburgh P.A81 (1967).

ACKNOWLEDGEMENTS.

This research project has been directed by Mr. H.W.Kropholler, to whom I am indebted for enthusiastic support and practical assistance as well as academic guidance. The work has been carried out mainly in the Department of Chemical Engineering at Loughborough University of Technology and I would like to thank the Head of Department, Professor D.C.Freshwater, for his continual encouragement.

Considerable support, detailed suggestions and advice have been received from the Industrial Supervisor of the project, Mr.J.N.Turnbull of BP Research Centre, to whom I am extremely grateful.

My thanks are due to The British Petroleum Company Ltd. For the generous provision of experimental facilities on a large production unit, technical literature and practical assistance from many members of staff. The refinery experimental work has been made possible chiefly through the energetic organisational efforts of Dr.T.Robbins at BP Refinery (Llandarcy) Ltd; considerable technical advice on all aspects of the project has also been received from the latter. H.C.Moore of Loughborough University of Technology provided considerable experimental assistance during Run TR3 at Llandarcy Refinery.

This thesis forms a part of a much larger programme of work which is still being pursued by the Process Dynamics and Control Section in the Department of Chemical Engineering. I am indebted to members of staff in the section, particularly Dr.F.P.Lees, and to fellow research students, particularly M.J.Bosley, for many helpful discussions and suggestions and the use of their computer programs.

Many of the ideas in the second half of this thesis rely extensively on computer calculations. The success of these is partly attributable to the fast and reliable service offered by Loughborough University Computer Centre.

This project has been financed by the Science Research Council with a supplementary grant by The British Petroleum Co. Ltd., both of which I acknowledge with thanks.

APPENDIX 1. A MATHEMATICAL MODEL OF A CRUDE OIL DISTILLATION UNIT - LINEARISATION AND MANIPULATION OF THE BASIC EQUATIONS.

The nomenclature used in this Appendix is given in Chapter 4.

A1.1 The hydraulic equations.

A1.1.1 The special case of the top tray.

The non-linearised equations are:-

$$d/dt\,(W_{Ln}) = V_2 + SV_2 + SR_1 - L_1 - V_1 \qquad \ldots.(A1\text{-}1)$$

$$W_{L1} = \varepsilon_1 \rho_{L1} A_{T1} \left(\psi_{W1} + \psi_1\right) \qquad \ldots.(A1\text{-}2)$$

$$L_1 = e_9\, \ell_1\, \varepsilon_1\, \rho_{L1}\, \psi_1^{3/2} \qquad \ldots.(A1\text{-}3)$$

$$\psi_1 = e_1(V_2 + SV_2) + e_2 SR_1 + e_3 \psi_{W1} + e_{10}(V_2 + SV_2)^2 + e_{11} \ldots.(A1\text{-}4)$$

Linearising:-

$$\Delta \dot{W}_{L1} = \Delta V_2 + \Delta SV_2 + \Delta SR_1 - \Delta L_1 - \Delta V_1 + g_1 \qquad \ldots.(A1\text{-}5)$$

where $g_1 = \left| V_2 + SV_2 + SR_1 - L_1 - V_1 \right|_{\text{reference state}}$

$$\Delta W_{L1} = \varepsilon_1 \rho_{L1} A_{T1} \Delta\psi_1 + \rho_{L1} A_{T1} (\psi_{W1} + \psi_1)\, \Delta\varepsilon_1 \qquad \ldots.(A1\text{-}6)$$

$$\Delta L_1 = 3/2\; e_9\, \ell_1\, \varepsilon_1\, \rho_{L1}\, \psi_1^{1/2} \Delta\psi_1 + e_9\, \ell_1\, \rho_{L1}\, \psi_1^{3/2} \Delta\varepsilon_1 \qquad \ldots.(A1\text{-}7)$$

$$\Delta\psi_1 = e_1(\Delta V_2 + \Delta SV_2) + e_2 \Delta SR_1 + 2e_{10}(V_2 + SV_2)(\Delta V_2 + \Delta SV_2) \qquad \ldots.(A1\text{-}8)$$

Write $\Delta\psi_1 = a_1 \Delta V_2 + a_2$

where $a_1 = e_1 + 2e_{10}(V_2 + SV_2)$

$$a_2 = [e_1 + 2e_{10}(V_2 + SV_2)]\Delta SV_2 + e_2\, \Delta SR_1$$

Hence substituting for $\Delta\psi_1$ from equation (A1-8) into equations (A1-5) to (A1-7) we obtain:-

$$\Delta W_{L1} = \varepsilon_1 \rho_{L1} A_{T1} [a_1 \Delta V_2 + a_2] + \rho_{L1} A_{T1} (\psi_{W1} + \psi_1)\, \Delta\varepsilon_1 \qquad \ldots.(A1\text{-}9)$$

$$\Delta L_1 = 3/2\, e_9\, \ell_1\, \varepsilon_1\, \rho_{L1}\, \psi_1^{1/2} [a_1 \Delta V_2 + a_2] + e_9\, \ell_1\, \rho_{L1}\, \psi_1^{3/2} \Delta\varepsilon_1 \ldots.(A1\text{-}10)$$

From equation (A1-10):-

$$\Delta\varepsilon_1 = \frac{\Delta L_1}{e_9\, \ell_1\, \rho_{L1}\, \psi_1^{3/2}} - \frac{3\varepsilon_1}{2\psi_1}\left(a_1 \Delta V_2 + a_2\right) \qquad \ldots.(A1\text{-}11)$$

Hence substituting for $\Delta\varepsilon_1$ from equation (A1-11) into equation (A1-9) yields:-

$$\Delta W_{L1} = \rho_{L1} A_{T1} (\psi_{W1} + \psi_1)\left[\Delta L_1/(e_9 \ell_1 \rho_{L1} \psi_1^{3/2}) - (3\varepsilon_1/2\psi_1)(a_1 \Delta V_2 + a_2)\right] + \varepsilon_1 \rho_{L1} A_{T1}\left[a_1 \Delta V_2 + a_2\right] \quad \ldots. \text{(A1-12)}$$

Differentiation of equation (A1-12) with respect to time gives:-

$$\Delta \dot{W}_{L1} = \frac{A_{T1}(\psi_{W1} + \psi_1)}{e_9 \ell_1 \psi_1^{3/2}} \Delta \dot{L}_1 \quad \ldots. \text{(A1-13)}$$

since the assumption of zero vapour hold-up implies $d/dt(\Delta V_n) = 0$.

Hence the equation for the top tray is:-

$$\frac{A_{T1}(\psi_{W1} + \psi_1)}{e_9 \ell_1 \psi_1^{3/2}} \Delta \dot{L}_1 = -\Delta L_1 + \left\{\Delta V_2 + \Delta SV_2 + \Delta SR_1 - \Delta V_1 + g_1\right\} \quad \ldots. \text{(A1-14)}$$

A1.1.2 <u>The equations for the general tray</u>

Start with the linearised equations (4-12) to (4-18). First write equation (4-18) in the form:-

$$\Delta \psi_n = a_1 \Delta V_{n+1} + e_2 \Delta L_{Dn} + a_2$$

where

$$a_1 = e_1 + 2e_{10}(V_{n+1} + SV_{n+1}) \qquad 1 < n < n_T$$

$$a_1 = e_1 + 2e_{10} SV_{n+1} \qquad n = n_T$$

$$a_2 = [e_1 + 2e_{10}(V_{n+1} + SV_{n+1})]\Delta SV_{n+1} + e_2 \Delta SR_n \qquad 1 < n < n_T$$

$$a_2 = [e_1 + 2e_{10} SV_{n+1}]\Delta SV_{n+1} + e_2 \Delta SR_n \qquad n = n_T$$

Substituting for $\Delta\psi_n$ in equations (4-14),(4-16) and (4-17) we obtain:-

$$\Delta W_{Ln} = \varepsilon_n \rho_{Ln} A_{Tn}[a_1 \Delta V_{n+1} + e_2 \Delta L_{Dn} + a_2] + \rho_{Ln} A_{Tn}(\psi_{Wn} + \psi_n)\Delta\varepsilon_n \quad \ldots. \text{(A1-15)}$$

$$\Delta \psi_{Dn} = \varepsilon_n[a_1 \Delta V_{n+1} + e_2 \Delta L_{Dn} + a_2] + (\psi_{Wn} + \psi_n)\Delta\varepsilon_n + 2C_{Ln} L_{Dn} \Delta L_{Dn} + 2C_{Vn-1}(V_n + SV_n)(\Delta V_n + \Delta SV_n) + \varepsilon_{n-1}[a_1^p \Delta V_n + e_2^p \Delta L_{Dn-1} + a_2^p] + (\psi_{Wn-1} + \psi_{n-1})\Delta\varepsilon_{n-1} \quad \ldots. \text{(A1-16)}$$

where superscript p denotes the value of the coefficient for the previous plate.

$$\Delta L_n = 3/2\, e_9 \ell_n \varepsilon_n \rho_{Ln} \psi_n^{1/2}(a_1 \Delta V_{n+1} + e_2 \Delta L_{Dn} + a_2) + e_9 \ell_n \rho_{Ln} \psi_n^{3/2} \Delta\varepsilon_n \quad \ldots. \text{(A1-17)}$$

Simplification of equation (A1-17) gives:-

$$\Delta L_n = a_3 a_1 \Delta V_{n+1} + a_3 e_2 \Delta L_{Dn} + a_3 a_2 + \frac{2 a_3 \psi_n}{3 \mathcal{E}_n} \Delta \mathcal{E}_n \quad \ldots .(A1\text{-}18)$$

where $a_3 = 3/2\ e_9\, \ell_n\, \mathcal{E}_n\, \rho_{Ln}\, \psi_n^{1/2}$

From equation (A1-18) it follows that:-

$$\Delta \mathcal{E}_n = \frac{3\mathcal{E}_n}{2a_3\psi_n}\left[\Delta L_n - a_3 a_1 \Delta V_{n+1} - a_3 e_2 \Delta L_{Dn} - a_3 a_2\right]$$

i.e. $$\Delta \mathcal{E}_n = \frac{3\mathcal{E}_n}{2\psi_n}\left[\frac{\Delta L_n}{a_3} - a_1 \Delta V_{n+1} - e_2 \Delta L_{Dn} - a_2\right] \ldots .(A1\text{-}19)$$

Equation (A1-19) may be used to remove $\Delta\mathcal{E}_n$ from equations (A1-15) and (A1-16) to yield:-

$$\Delta W_{Ln} = \mathcal{E}_n \rho_{Ln} A_{Tn}\left[a_1 \Delta V_{n+1} + e_2 \Delta L_{Dn} + a_2\right] + \rho_{Ln} A_{Tn}(\psi_{Wn}+\psi_n)\frac{3\mathcal{E}_n}{2\psi_n}\left[\frac{\Delta L_n}{a_3} - a_1\Delta V_{n+1} - e_2\Delta L_{Dn} - a_2\right] \ldots .(A1\text{-}20)$$

$$\begin{aligned}\Delta\psi_{Dn} = {} & \mathcal{E}_n\left[a_1\Delta V_{n+1} + e_2\Delta L_{Dn} + a_2\right] + (\psi_{Wn}+\psi_n)\frac{3\mathcal{E}_n}{2\psi_n}\left[\frac{\Delta L_n}{a_3} - a_1\Delta V_{n+1} - e_2\Delta L_{Dn} - a_2\right] \\ & + 2C_{Ln}L_{Dn}\Delta L_{Dn} + 2C_{Vn-1}(V_n + SV_n)(\Delta V_n + \Delta SV_n) + \mathcal{E}_{n-1}\left[a_1^P\Delta V_n + e_2^P\Delta L_{Dn-1} + a_2^P\right] \\ & + (\psi_{Wn-1}+\psi_{n-1})\frac{3\mathcal{E}_{n-1}}{2\psi_{n-1}}\left[\frac{\Delta L_{n-1}}{a_3^P} - a_1^P\Delta V_n - e_2^P\Delta L_{Dn-1} - a_2^P\right] \quad \ldots .(A1\text{-}21)\end{aligned}$$

Using equation (A1-21) to eliminate $\Delta\psi_{Dn}$ from equation (4-15) and differentiating equations (A1-20) and (4-15) we obtain:-

$$\begin{aligned} d/dt(\Delta W_{Ln}) = {} & \left\{\mathcal{E}_n\rho_{Ln}A_{Tn}e_2 - \rho_{Ln}A_{Tn}(\psi_{Wn}+\psi_n)\frac{3\mathcal{E}_n e_2}{2\psi_n}\right\}\Delta\dot{L}_{Dn} \\ & + \rho_{Ln}A_{Tn}(\psi_{Wn}+\psi_n)\frac{3\mathcal{E}_n}{2\psi_n a_3}\Delta\dot{L}_n \quad \ldots .(A1\text{-}22)\end{aligned}$$

$$\begin{aligned} d/dt(\Delta W_{Dn}) = {} & \rho_{LDn}A_{Dn}\left\{\mathcal{E}_{n-1}e_2^P - (\psi_{Wn-1}+\psi_{n-1})\frac{3\mathcal{E}_{n-1}}{2\psi_{n-1}}e_2^P\right\}\Delta\dot{L}_{Dn-1} + \left[(\psi_{Wn-1}+\psi_{n-1})\frac{3\mathcal{E}_{n-1}}{2\psi_{n-1}a_3^P}\right]\Delta\dot{L}_{n-1} \\ & + \left[\mathcal{E}_n e_2 - (\psi_{Wn}+\psi_n)\frac{3\mathcal{E}_n}{2\psi_n}e_2 + 2C_{Ln}L_{Dn}\right]\Delta\dot{L}_{Dn} \\ & + \left[(\psi_{Wn}+\psi_n)\frac{3\mathcal{E}_n}{2\psi_n a_3}\right]\Delta\dot{L}_n \quad \ldots .(A1\text{-}23)\end{aligned}$$

Equations (A1-22) and (A1-23) may thus be written:-

$$d/dt(\Delta W_{Ln}) = b_1\Delta\dot{L}_{Dn} + b_2\Delta\dot{L}_n \quad \ldots .(A1\text{-}24)$$

$$d/dt(\Delta W_{Dn}) = b_3\Delta\dot{L}_{Dn-1} + b_4\Delta\dot{L}_{n-1} + b_5\Delta\dot{L}_{Dn} + b_6\Delta\dot{L}_n \quad \ldots .(A1\text{-}25)$$

Substituting for $d/dt(\Delta W_{Ln})$ and $d/dt(\Delta W_{Dn})$ from equations (A1-24) and (A1-25) into equations (4-12) and (4-13) we finally obtain:-

$$b_1\Delta\dot{L}_{Dn} + b_2\Delta\dot{L}_n = \Delta L_{Dn} + \Delta V_{n+1} + \Delta SV_{n+1} + \Delta SR_n - \Delta L_n - \Delta V_n + g_1 \quad \ldots .(A1\text{-}26)$$

$$b_3\Delta\dot{L}_{Dn-1} + b_4\Delta\dot{L}_{n-1} + b_5\Delta\dot{L}_{Dn} + b_6\Delta\dot{L}_n = \Delta L_{n-1} - \Delta L_{Dn} - \Delta SL_{n-1} + g_2 \quad \ldots .(A1\text{-}27)$$

where b_1 - b_6 are defined by:-

$$b_1 = \varepsilon_n \rho_{Ln} A_{Tn} e_2 \{1 - 3(\psi_{Wn} + \psi_n)/(2\psi_n)\}$$
$$b_2 = \rho_{Ln} A_{Tn} (\psi_{Wn} + \psi_n)(3\varepsilon_n)/(2\psi_n a_3)$$
$$b_3 = \rho_{LDn} A_{Dn} \varepsilon_{n-1} e_2^p \{1 - 3(\psi_{Wn-1} + \psi_{n-1})/(2\psi_{n-1})\} \quad *$$
$$b_4 = \rho_{LDn} A_{Dn} (\psi_{Wn-1} + \psi_{n-1})(3\varepsilon_{n-1})/(2\psi_{n-1} a_3^p)$$
$$b_5 = \rho_{LDn} A_{Dn} \{\varepsilon_n e_2[1 - 3(\psi_{Wn} + \psi_n)/(2\psi_n)] + 2C_{Ln} L_{Dn}\}$$
$$b_6 = \rho_{LDn} A_{Dn} [(\psi_{Wn} + \psi_n)(3\varepsilon_n)/(2\psi_n a_3)]$$

* This term is zero for tray 2. Otherwise the equations are valid for tray 2.

All coefficients are valid for the bottom tray.

A1.2 The heat balance equations.

A1.2.1 The heat balance equations for the top tray.

Equation (4-8) for the general tray may be manipulated as in section A1.2.2 with the omission of the terms in ΔL_{Dn}:-

$$\begin{aligned} W_{Ln} \tau\, d/dt(\Delta\theta_n) = {} & H_{n+1}\Delta V_{n+1} + pV_{n+1}\Delta\theta_{n+1} + H_{SVn+1}\Delta SV_{n+1} + h_{SRn}\Delta SR_n \\ & - h_n \Delta L_n - \tau L_n \Delta\theta_n - H_n\Delta V_n - pV_n\Delta\theta_n + g_3 \\ & - [\tau\theta_n + \tau\Delta\theta_n + s][\Delta V_{n+1} + \Delta SV_{n+1} + \Delta SR_n - \Delta L_n - \Delta V_n + g_1] \end{aligned}$$

where $g_3 = \left| H_{n+1}V_{n+1} - H_{SVn+1}SV_{n+1} + h_{SRn}SR_n - h_nL_n - H_nV_n \right|_{\text{reference state}}$

Hence

$$\begin{aligned} W_{Ln} \tau\, d/dt(\Delta\theta_n) = {} & (H_{n+1} - h_n)\Delta V_{n+1} + pV_{n+1}\Delta\theta_{n+1} + (H_{SVn+1} - h_n)\Delta SV_{n+1} \\ & + (h_{SRn} - h_n)\Delta SR_n - [\tau(L_n + g_1) + pV_n]\Delta\theta_n \\ & + (h_n - H_n)\Delta V_n + (g_3 - h_n g_1) \qquad \ldots (4\text{-}19) \end{aligned}$$

A1.2.2 The heat balance equations for the general tray

For the general plate we have the basic equation:-

$$d/dt\,(h_n W_{Ln}) = h_{LDn}L_{Dn} + H_{n+1}V_{n+1} + H_{SVn+1}SV_{n+1} + h_{SRn}SR_n - h_n L_n - H_n V_n \quad \ldots.\ (4\text{-}8)$$

Using the superscript ' to denote reference state and linearising in the normal way (making use of $h = r\theta + s$; $H = p\theta + q$):-

$$d/dt\,(h_n W_{Ln}) = d/dt\left\{(r\theta_n' + r\Delta\theta_n + s)(W_{Ln}' + \Delta W_{Ln})\right\}$$
$$= W_{Ln}'\, r\, d/dt\,(\Delta\theta_n) + (r\theta_n' + r\Delta\theta_n + s)\, d/dt\,(\Delta W_{Ln})$$

and substituting for $d/dt(\Delta W_{Ln})$ from equation (4-12) we obtain:-

$$d/dt(h_n W_{Ln}) = W_{Ln}'\, r\, d/dt\,(\Delta\theta_n)$$
$$+ (r\theta_n' + r\Delta\theta_n + s)(\Delta L_{Dn} + \Delta V_{n+1} + \Delta SV_{n+1} + \Delta SR_n - \Delta L_n - \Delta V_n + g_1)$$

Hence the complete linearised form of equation (4-8) becomes:-

$$W_{Ln}'\, r\, d/dt\,(\Delta\theta_n) = h_{LDn}\Delta L_{Dn} + rL_{Dn}\Delta\theta_{Dn} + H_{n+1}\Delta V_{n+1} + pV_{n+1}\Delta\theta_{n+1} + H_{SVn+1}\Delta SV_{n+1}$$
$$+ h_{SRn}\Delta SR_n - h_n\Delta L_n - rL_n\Delta\theta_n - H_n\Delta V_n - pV_n\Delta\theta_n + g_3$$
$$- (r\theta_n' + r\Delta\theta_n + s)(\Delta L_{Dn} + \Delta V_{n+1} + \Delta SV_{n+1} + \Delta SR_n - \Delta L_n - \Delta V_n + g_1)$$

where

$$g_3 = \left| h_{LDn}L_{Dn} + H_{n+1}V_{n+1} + H_{SVn+1}SV_{n+1} + h_{SRn}SR_n - h_n L_n - H_n V_n \right|_{\text{reference state.}}$$

Hence we obtain:-

$$W_{Ln}'\, r\, d/dt\,(\Delta\theta_n) = \left\{(r\theta_{Dn} + s) - (r\theta_n + s)\right\}\Delta L_{Dn} + \left\{rL_{Dn}\right\}\Delta\theta_{Dn} + \left\{H_{n+1} - h_n\right\}\Delta V_{n+1}$$
$$+ pV_{n+1}\Delta\theta_{n+1} + \left\{H_{SVn+1} - h_n\right\}\Delta SV_{n+1} + \left\{h_{SRn} - h_n\right\}\Delta SR_n$$
$$- \left\{rL_n + rg_1 + pV_n\right\}\Delta\theta_n - \left\{H_n - h_n\right\}\Delta V_n + \left\{g_3 - h_n g_1\right\}$$

Simplifying

$$W_{Ln}\, r\, d/dt\,(\Delta\theta_n) = r(\theta_{Dn} - \theta_n)\Delta L_{Dn} + rL_{Dn}\Delta\theta_{Dn} + (H_{n+1} - h_n)\Delta V_{n+1} + pV_{n+1}\Delta\theta_{n+1}$$
$$+ (H_{SVn+1} - h_n)\Delta SV_{n+1} + (h_{SRn} - h_n)\Delta SR_n - [r(L_n + g_1) + pV_n]\Delta\theta_n$$
$$- (H_n - h_n)\Delta V_n + (g_3 - h_n g_1) \quad \ldots.\ (4\text{-}19)$$

For the downcomer the basic equation is:-

$$d/dt\,(h_{Dn}W_{Dn}) = h_{n-1}L_{n-1} - h_{Dn}L_{Dn} - h_{n-1}SL_{n-1} \quad \ldots.\ (4\text{-}9)$$

Proceeding as before:-

$$d/dt\,(h_{Dn}W_{Dn}) = d/dt\left([r\theta_{Dn}' + r\Delta\theta_{Dn} + s][W_{Dn}' + \Delta W_{Dn}]\right)$$
$$= (r\theta_{Dn}' + r\Delta\theta_{Dn} + s)\, d/dt\,(\Delta W_{Dn}) + W_{Dn}'\, r\, d/dt\,(\Delta\theta_{Dn})$$

Hence:-

$$W'_{Dn}\,\gamma\, d/dt\,(\Delta\theta_{Dn}) = h_{n-1}\Delta L_{n-1} + \gamma L_{n-1}\Delta\theta_{n-1} - h_{Dn}\Delta L_{Dn} - \gamma L_{Dn}\Delta\theta_{Dn}$$
$$- h_{n-1}\Delta SL_{n-1} - \gamma\, SL_{n-1}\Delta\theta_{n-1}$$
$$- (\gamma\theta'_{Dn} + \gamma\Delta\theta_{Dn} + s)(\Delta L_{n-1} - \Delta L_{Dn} - \Delta SL_{n-1} + g_2)$$

Simplifying this gives:-

$$W'_{Dn}\,\gamma\, d/dt\,(\Delta\theta_{Dn}) = (h_{n-1} - h_{Dn})\Delta L_{n-1} + (\gamma L_{n-1} - \gamma SL_{n-1})\Delta\theta_{n-1}$$
$$- \gamma L_{Dn}\Delta\theta_{Dn} + (h_{Dn} - h_{n-1})\Delta SL_{n-1}$$
$$- (h_{Dn} + \gamma\Delta\theta_{Dn})\, g_2 \qquad \ldots (4\text{-}20)$$

The heat transfer equation is:-

$$H_{n+1}V_{n+1} + H_{SVn+1}SV_{n+1} - H_nV_n = m_nV_{n+1}(\theta_{n+1} - \theta_n) + m_nSV_{n+1}(\theta_{SVn+1} - \theta_n) \quad \ldots (4\text{-}10)$$

From which we obtain:-

$$H_{n+1}\Delta V_{n+1} + pV_{n+1}\Delta\theta_{n+1} + H_{SVn+1}\Delta SV_{n+1} - H_n\Delta V_n - pV_n\Delta\theta_n$$
$$= m_nV_{n+1}(\Delta\theta_{n+1} - \Delta\theta_n) + m_n(\theta_{n+1} - \theta_n)\Delta V_{n+1}$$
$$+ m_n(\theta_{SVn+1} - \theta_n)\Delta SV_{n+1} - m_n SV_{n+1}\Delta\theta_n$$

Simplifying this gives:-

$$\{H_{n+1} - m_n(\theta_{n+1} - \theta_n)\}\Delta V_{n+1} - H_n\Delta V_n$$
$$= \{pV_n - m_nV_{n+1} - m_nSV_{n+1}\}\Delta\theta_n + \{m_nV_{n+1} - pV_{n+1}\}\Delta\theta_{n+1}$$
$$+ \{m_n(\theta_{SVn+1} - \theta_n)\Delta SV_{n+1} - H_{SVn+1}\Delta SV_{n+1}\} \qquad \ldots (4\text{-}21)$$

\- - - - - - -

APPENDIX 2. A MATHEMATICAL MODEL OF A CRUDE OIL DISTILLATION UNIT - THE COMPUTER PROGRAM.

A2.1 Function of the program.

The program predicts the response of the internal flowrates and temperatures of a crude oil distillation unit to certain forcing functions. The forcing functions are changes in the flow and enthalpy of feeds to the unit and changes of withdrawal rates from the unit.

A2.2 Language and machine.

The program is written in Fortran IV for a standard ICL 1905 computer with 32 000 words of central core. Disc and tape files are not used.

A2.3 Limitations.

The maximum size of distillation unit which can be simulated contains 44 plates. No limit is placed on the number and location of feeds or withdrawals. Computation time is a serious limiting factor and current calculations require approximately sixty times real time. Convergence of the ΔV vector is not assured, and after 30 iterations the program proceeds regardless using the most recently calculated value of the ΔV vector. Hence for a given problem the user must experiment a little with the value of μ, the implicit parameter, and with the time increment and relinearisation frequency to find the combination of these that will produce the correct response most rapidly.

A2.4 Method.

A2.4.1 Data input.

The operations in this section are carried out in subroutine INFORM, the subroutines being arranged in alphabetical order after the Master segment of the program (see listing given later in this appendix.) The arrays used to store perturbations and feed and withdrawal data are first set to zero. Then a title and geometric details of the column itself are entered. Then follow the operational data and the constants for use in the correlations and mathematical method. No further data is required during execution. Precise information on data presentation is given in section A2.5.

A2.4.2 Initial auxiliary calculations.

Subroutine STEADY is used to calculate the values of the tray heat transfer coefficients and the values of the liquid and vapour enthalpies using the correlation coefficients and the tray temperatures, both of which are presented in the data. Subroutine STEADY then calls subroutine PARAM. This calculates the initial values of the hydraulic parameters such as the downcomer head and the froth density using the steady state versions of the model equations presented in the main body of the thesis (section 4.2.3). The initial steady state values of all the column variables are then printed out using subroutine PRINT2. Subroutine INFORM is then called again to input the particular perturbation to which the column response is required. Control is transferred back to the Master segment of the program where counters are set up and accumulators cleared prior to the calculation of the transient.

A2.4.3 Formulation of the dynamic problem.

As a first estimate $\Delta\underline{V}$ is set to zero. $\Delta\underline{X}(0)$ is also set to zero. The current values of $\Delta\underline{X}$ and $\Delta\underline{V}$ are transferred to subroutine matrix via the argument list in the CALL statement. Subroutine matrix is then used to calculate the values of the non-zero elements in the band matrix E and the vector $\underline{F}$. This routine repeatedly calls another routine, subroutine COEFFS, to calculate the coefficients of the A and B matrices on a tray by tray basis. (For details of A,B,E and F see the main part of this thesis, section 4.3)

A2.4.4 <u>Solution of the problem - the inner iterative loop.</u>

The problem set up by subroutine MATRIX is to solve:-

$$\Delta X_{n+1} = E^{-1} F$$

This is solved for $\Delta \underline{X}_{n+1}$ using subroutine BAND. This routine inverts the band matrix E by a series of matrix operations. These operations correspond to Jordan's method of matrix inversion because each operation converts one column of the band matrix to the corresponding column of the unit matrix. The same operations are carried out on the $\underline{F}$ vector so that on leaving the routine $\underline{F}$ contains $\Delta \underline{X}_{n+1}$.

The operation of the routine will be demonstrated using a band matrix of five element width:-

$$E = \left[\begin{array}{ccccc|cccc}
a_{11} & a_{12} & a_{13} & 0 & 0 & 0 & 0 & . & . \\
a_{21} & a_{22} & a_{23} & a_{24} & 0 & 0 & 0 & . & . \\
a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & 0 & 0 & . & . \\
\hline
0 & a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & 0 & . & . \\
0 & 0 & a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & . & . \\
. & . & . & . & . & . & . & & \\
. & . & . & . & . & . & . & &
\end{array}\right.$$

Consider only the partitioned region. This is of size 5 x 3. Pivoting is achieved by row swapping in this region. The pivotal element is selected from the first column as the largest value of a_{i1}/ε_i where ε_i is the Euclidean norm (the root mean square) of row i.

The matrix R_1 is then formed:-

$$R_1 = \left[\begin{array}{llll} 1/a_{11} & 0 & 0 & \cdots \\ -a_{21}/a_{11} & 1 & 0 & \cdots \\ -a_{31}/a_{11} & 0 & 1 & \\ \cdot & \cdot & \cdot & \cdot \end{array}\right.$$

and the product R E is calculated:-

$$R_1E = \left[\begin{array}{lllllllll} 1 & b_{11} & b_{12} & b_{13} & b_{14} & 0 & 0 & 0 & 0 \\ 0 & b_{21} & b_{22} & b_{23} & b_{24} & 0 & 0 & 0 & 0 \\ 0 & b_{31} & b_{32} & b_{33} & b_{34} & b_{35} & 0 & 0 & 0 \\ 0 & b_{41} & b_{42} & b_{43} & b_{44} & b_{45} & 0 & 0 & 0 \\ 0 & 0 & a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{array}\right.$$

The operation is repeated on the whole of the partitioned region, the pivot being selected from the bottom three rows in this region. Hence

$$R_2 = \left[\begin{array}{lllll} 1 & -b_{11}/b_{21} & 0 & & \\ 0 & 1/b_{21} & 0 & & \\ 0 & -b_{31}/b_{21} & 1 & & \\ 0 & -b_{41}/b_{21} & 0 & 1 & \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & & \end{array}\right.$$

and

$$R_2R_1E = \left[\begin{array}{lllllllll} 1 & 0 & c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 & 0 \\ 0 & 1 & c_{21} & c_{22} & c_{23} & c_{24} & 0 & 0 & 0 \\ 0 & 0 & c_{31} & c_{32} & c_{33} & c_{34} & 0 & 0 & 0 \\ & & c_{41} & c_{42} & c_{43} & c_{44} & 0 & 0 & 0 \\ & & c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & 0 & 0 \\ & & & a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & 0 \end{array}\right.$$

and so on.

The solution is obtained by operating concurrently on the $\underline{F}$ vector to form $R_1\underline{F}$, $R_2R_1\underline{F}$ etc.

With the nine element band width used in the computer program being considered it may be seen that pivoting over five rows is possible. It will also be seen that at no time does the size of the transformed matrix exceed that of the original band matrix.

A2.4.5 Solution of the problem - convergence of the V vector.

Subroutine BAND has been used to produce an estimate of the new value for the state vector $\Delta\underline{X}_{n+1}$. This estimate has been based on an assumed value of $\Delta\underline{V}$. $\Delta\underline{X}_{n+1}$ is now substituted back into the linearised equations to obtain a new value for $\Delta\underline{V}$. Experience with the program showed that direct iteration produced the most consistently rapid convergent solution. Hence the newly calculated value of $\Delta\underline{V}$ is used directly in the new formulation of the problem using subroutine MATRIX as before. The problem is deemed to have converged when all elements of $\Delta\underline{V}$ are within 0.0001 lb/sec of their values at the previous iteration. Current experience with the program using a fifteen plate unit indicates that convergence is achieved in 3-16 iterations with no relinearisation of the system matrix and in 3-6 iterations with frequent relinearisation.

A2.4.6 Printout and relinearisation.

When convergence of the $\Delta\underline{V}$ vector has been achieved the printout and relinearisation counters are incremented. A check is made with the parameters in the data. If it is time to reset the problem the hydraulic parameters and then the system matrix are recalculated. The subroutine PRINT2 is then used to print out the current state of the unit. It may be that only a printout is required. In this case the hydraulic variables except for $\Delta \underline{V}$ and those in the state vector, remain at their previous values.

The program finally halts when a check shows that the maximum transient time requested in the data has been reached.

A2.5 <u>Data for the program.</u>

The program requires considerable detailed data as is apparent from the generality built into it. The information on the data cards is output at the beginning of the results in a readily comprehendable form to facilitate data checking. In addition the first 24 columns of many of the data cards are reserved for data labels. These labels are output with the data check.

A2.5.1 <u>Title.</u>

The first two data cards are stored as a title and output at the head of the results.

A2.5.2 <u>Column geometry and operational details.</u>

Each of the items numbered below must start on a new card. Apart from this numbers may be presented in any convenient form provided they are terminated by two or more spaces or the end of a card. Very large or very small numbers may be abbreviated. e.g. 37000.0 may be written 3.7E4 (meaning 3.7×10^4) and 0.00037 may be written 3.7E-4 (meaning 3.7×10^{-4}). Integer numbers are marked with an asterisk in the list below and must not contain a decimal point. Other numbers may, but need not, have a decimal point.

* 1) Number of trays - NT.

* 2) Types of trays. NT integer numbers. Number 10 represents a bubble cap plate. Number 20 represents a sieve plate.

3) Liquid densities. NT values representing the estimated liquid density at the column conditions for each plate. (lb/ft^3).

4) Vapour densities. As for the liquid densities. (lb/ft^3).

5) Tray areas. NT numbers representing the bubbling area of each tray. This is effectively the cross-sectional area of the tower less the area of the downcomers. (ft^2).

6) Areas under the downcomer weirs. NT numbers representing the areas available for liquid flow under each of the downcomer weirs. (These areas are measured in the vertical plane.) (ft^2).

7) Hole area. NT numbers representing the total area available for vapour flow through each tray. (ft^2).

8) Downcomer area. NT numbers representing the mean cross-sectional area of each downcomer. (ft^2).

9) Weir heights. NT numbers representing the height of the outlet weir for each plate. (ft^2).

10) The average liquid flowpath width. NT numbers representing the average width of the liquid flowpath across each plate. (ft).

11) The initial tray liquid temperatures. NT numbers representing the measured or estimated temperatures of the liquid on each tray. (°F).

* 12) The number of plates having vapour or liquid feeds or withdrawals (including pumparound offtake or return). A single integer. Note that the vapour from the top plate and the liquid from the bottom plate need not be specified at this stage.

13) This item consists of K cards where K is the number of plates having a feed or withdrawal as specified in the last item. Each card contains the following data in order:-

a) a 24 character label.

* b) the number of the plate, an integer.

c) the withdrawal rate of liquid from the plate. (lb/sec.)

d) the feed rate of liquid to the plate. (lb/sec.)

e) the enthalpy of the liquid feed. (BTU/lb.)

f) the feed rate of vapour to the plate. (lb/sec.)

g) the enthalpy of the vapour feed. (BTU/lb.)

h) the temperature of the vapour return. (°F).

14) Data on the bottoms stripping steam. This consists of one card containing the following information:-

a) a 24 character label.

b) the steam rate. (lb/sec.)

c) the steam enthalpy. (BTU/lb.)

d) the steam temperature. (°F).

* 15) The number of constants to be supplied. This card contains a 24 character label followed by an integer.

16) The constants. This item contains K cards where K is specified in the previous item. Each card contains a 24-character title followed by an integer then the value of the constant. The integer specifies the location in the constant vector $\underline{c}$ in the program store into which the value is to be loaded.

* 17) The number of step changes to be made at time zero. This is to facilitate the calculation of the transient response to complex forcing functions made up of changes in several variables.

18) The step changes. This item consists of K cards where K is given in the previous item. Each card contains the following information in order:-

a) a 24-character title.

b) the number of the tray at which the change is made.

c) the change in the liquid withdrawal rate (lb/sec.)

d) the change in the liquid feed rate (lb/sec.)

e) the new enthalpy of the liquid feed (BTU/lb.)

f) the change in the vapour feed rate (lb/sec.)

g) the new enthalpy of the vapour feed (BTU/lb).

19) The initial liquid and vapour rate profile for the unit. (lb/sec.) This consists of a series of numbers representing L_1, V_1, L_2, V_2, etc. in that order upt L_{NT}, V_{NT}, where NT is the total number of plates in the column. No provision for a label is made with this data item.

A2.6 The Fortran mnemonics for the program.

```
      LIST
      SEND TO (ED,ICLA-DEFAULT.AXXX)
      PROGRAM(G472)
      INPUT 1=CR7
      OUTPUT 2=LP7
      COMPRESS INTEGER AND LOGICAL
      TRACE 0
      END
      MASTER CDU3
      REAL L,ID
      DIMENSION D(174,9),E(174),A(174),B(174),DELTA1(174),DV(44)
      DIMENSION DV1(44),DV2(44),RESULT(44)
      COMMON I(44),V(44),LD(44),T(44),TD(44),WL(44),WD(44),PSI(44),
     1PSID(44),PSIU(44),EPS(44),RHOL(44),RHOLD(44),RHOV(44),AVL(44),
     2AD(44),AT(44),AP(44),AUD(44),HL(44),HV(44),HLD(44),HSR(44),
     3HSV(45),SL(44),SV(45),SR(44),DELV(44),DELSL(44),DELSV(45),
     4DELSR(44),ITYPE(44),INDEX(44),C(50),NT,TSV(45),HTC(44)
C
      C(50)=+1.0
      C(49) = -1.0
      C(48) = -1.0
      CALL INFORM(1)
      CALL STEADY
      CALL PRINT2(0,0,0)
      CALL INFORM(2)
  100 A1=C(38)+0.1
      J3=IFIX(A1)
      A2=C(39)+0.1
      J4=IFIX(A2)
      J5=0
C
      J=4*NT-2
      J1=0
      CUMTIM=0.0
      CUM=0.0
      CUM1=0.0
C
   30 DO 10 I=1,J
   10 DELTA1(I)=0.0
   36 CONTINUE
C
      DO 91 I=1,NT
      DV(I) = 0.0
   91 DV1(I) = 0.0
      IFLAG = 1
      GO TO 70
C
   35 CONTINUE
      IF(C(48).GT.0.0) GO TO 36
   70 DO 90 J2=1,J3
```

```
      DO 96 I=1,NT
   96 DV2(I) = DELV(I)
      CALL TEST(58,DELTA1,1)
      CALL MATRIX(D,E,DELTA1,J,174)
      CALL TEST(58,E,2)
      CALL BAND(D,E,A,B,J,9,174)
      CALL TEST(58,F,3)
      CALL CORECT(E)
      CALL TEST(15,DELV,4)
      DO 92 I=1,NT
   92 IF(ABS(DV2(I)-DELV(I)).GT.0.0001) GO TO 95
      WRITE(2,93) I2
   93 FORMAT(28H0DELV VECTOR CONVERGED AFTER,I3,12H ITERATIONS.)
      GO TO 94
C
   95 DO 102 I=1,NT
  102 RESULT(I) = DELV(I)
C
      IF(IFLAG) 97,97,99
   97 DO 98 I=1,NT
      DELV(I) = (DELV(I)*DV1(I)-DV(I)*DV2(I))/
     1          (DV1(I)-DV2(I)-DV(I)+DELV(I))
      GO TO 1
    2 DELV(I) = DELV(I)/10.0
    1 CONTINUE
      IF(ABS(DELV(I)).GT.1.0) GO TO 2
   98 CONTINUE
C
   99 IFLAG = -1
C
      DO 101 I=1,NT
      DV1(I) = DV2(I)
  101 DV(I) = RESULT(I)
C
   90 CONTINUE
C
   94 CONTINUE
      DO 20 I=1,J
   20 DELTA1(I)=F(I)
C
      CUMTIM=CUMTIM+C(5)
      CUM=CUM+C(5)
      CUM1=CUM1+C(5)
C
      IF((CUM1+0.001).LT.C(37)) GO TO 110
      WRITE(2,120) CUMTIM
  120 FORMAT(26H0SYSTEM MATRIX RESET AFTER,G8.5,9H SECONDS.)
      CALL UPDATE(1,DELTA1)
      CALL PARAM(2)
      CALL UPDATE(0,DELTA1)
```

```
      CUM1=0.0
C
  110 IF((CUM+0.001).LT.C(7)) GO TO 50
      CALL UPDATE(1,DELTA1)
      CALL PRINT2(J1,CUMTIM)
      J1=J1+1
      CALL UPDATE(-1,DELTA1)
      CUM=0.0
C
   50 IF((CUMTIM+0.001).GT.C(8)) GO TO 60
      J5=J5+1
      IF(CUMTIM.LT.61.0) GO TO 35
      IF(C(49).GT.0.0) GO TO 35
      READ(1,3) C(5), C(6), C(7), C(37), C(48), C(49)
    3 FORMAT(100F0.0)
      GO TO 35
   60 STOP
      END
      SUBROUTINE BAND (E,F,R,STORE,NM,NB,NROWS)
       DIMENSION  E(NROWS,NB),F(NM),R(NM),STORE(NM)
C  THIS ROUTINE SOLVES THE EQUATION EX = F WHERE E IS SQUARE BAND
C  MATRIX WITH BAND WIDTH NB AND MATRIX SIZE NM, AND F IS A COLUMN
C  VECTOR OF LENGTH NM.   ONLY THE BAND ELEMENTS OF THE MATRIX E ARE
C  PRESENTED TO REDUCE STORE SPACE CONSIDERABLY.   R AND STORE ARE
C  COLUMN VECTORS OF LENGTH NM USED AS WORKING SPACE.
C
C
      N6 = 0
      N1 = (NB+1)/2
      N2 = N1-1
      N5 = N2
      N4 = 1
C
C  THE FIRST N2 ROWS OF THE MATRIX ARE SHIFTED TO FORM A RECTANGULAR
C  STORAGE UNIT
C
    1 N3 = 1
    3 E(N4,N3) = E(N4,N3+N2)
      IF((N3+N2).EQ.NB) GO TO 2
      N3 = N3+1
      GO TO 3
    2 N3 = N3+1
      E(N4,N3) = 0.0
      IF(N3.EQ.NB) GO TO 5
      GO TO 2
    5 IF(N4.EQ.N5) GO TO 6
      N4 = N4+1
      N2 = N2-1
      GO TO 1
C
```

```
C   SET UP THE VALUES OF IRLEN, THE LENGTH OF THE R-VECTOR, AND IWIDTH
C   THE LENGTH OF THE ROWS TO BE MANIPULATED.
C
     6 N6 = N6+1
       IRLEN = (NB+1)/2 + N6-1
       IF(IRLEN.GT.NM) IRLEN = NM
       IF(N6.GT.(NM-N1-2)) GO TO 7
       IWIDTH = NB
       GO TO 8
     7 IWIDTH = NM-N6+1
C
C   LOCATION OF THE PIVOTAL ELEMENT.
C
     8 N7 = N6-1
       IF(N6.EQ.NM) GO TO 10
       RNORM1 = 0.0
     9 N7 = N7+1
       N8 = 0
       RNORM = 0.0
    11 N8 = N8+1
       RNORM = E(N7,N8)**2 + RNORM
       IF(N8.LT.IWIDTH) GO TO 11
       RNORM = RNORM + F(N7)**2
       RNORM = SQRT(RNORM/FLOAT(IWIDTH+1))
       IF(ABS(RNORM).GT.1.0E-30) GO TO 12
       WRITE(2,500) RNORM
   500 FORMAT(88H0THE MATRIX E PROVED TO BE SINGULAR. PROGRAM HALTED IN S
      1UBROUTINE BMM3. VALUE OF RNORM =,G13.4)
       STOP
    12 RNORM = E(N7,1)/RNORM
       IF((ABS(RNORM)).GT.(ABS(RNORM1))) MAXIM = N7
       IF((ABS(RNORM)).GT.(ABS(RNORM1))) RNORM1 = RNORM
       IF(N7.LT.IRLEN) GO TO 9
C
C   INTERCHANGE ROWS IF NECESSARY SO THAT PIVOTAL ELEMENT IS
C   ON THE DIAGONAL OF E.
C
       IF(MAXIM.EQ.N6) GO TO 10
       STORE(1) = F(N6)
       F(N6) = F(MAXIM)
       F(MAXIM) = STORE(1)
       DO 13 I = 1,IWIDTH
       STORE(I) = E(N6,I)
       E(N6,I) = E(MAXIM,I)
    13 E(MAXIM,I) = STORE(I)
C
C   FORM THE R-VECTOR
C
    10 DO 14 N7 = 1,IRLEN
       R(N7) = -E(N7,1)/E(N6,1)
```

```
      IF(N7.EQ.N6) R(N7) = 1.0/F(N6,1)
   14 CONTINUE
C
C  CALCULATE RE AND RF AND SHIFT STORAGE.
C
      DO 19 I = 1,IRLEN
      IF(I.EQ N6) GO TO 19
      F(I) = F(I) + F(N6)*R(I)
   19 CONTINUE
      F(N6) = F(N6)/E(N6,1)
C
      IF(N6.EQ.NM) RETURN
C
      DO 22 J = 1,IRLEN
      IF(J.EQ N6) GO TO 22
      DO 20 I = 1,IWIDTH
   20 STORE(I) = E(J,I)
C
      DO 21 I = 1,IWIDTH-1
   21 E(J,I) = STORE(I+1) + R(J)*E(N6,I+1)
      E(J,IWIDTH) = 0.0
   22 CONTINUE
C
      DO 29 I = 1,IWIDTH
   29 STORE(I) = E(N6,I)
   23 DO 24 I = 1,IWIDTH-1
   24 E(N6,I) = STORE(I+1)/STORE(1)
      E(N6,IWIDTH) = 0.0
C
   17 IF(N6.EQ.NM) RETURN
      GO TO 6
      END
      SUBROUTINE COEFFS(I,A,B,D)
C
C     THIS ROUTINE SUPPLIES THE COEFFICIENTS FOR THE COMBINED HYDRO-
C     DYNAMIC AND HEAT BALANCE MATRIX EQUATION AX.=BX+D WHERE THE VECTOR
C     D IS BASED ON THE CURRENT BEST ESTIMATE OF THE VAPOUR RATES. THE
C     ROUTINE MUST BE CALLED ONCE FOR EACH TRAY. I=TRAY NUMBER.
C
      REAL L,LD
      DIMENSION A(4,9),B(4,9),D(4),G1F(44),G3F(44),G2F(44),G4F(44)
      COMMON L(44),V(44),LD(44),T(44),TD(44),WL(44),WD(44),PSI(44),
     1PSID(44),PSW(44),FPS(44),RHOL(44),RHOLD(44),RHOV(44),AVL(44),
     2AD(44),AT(44),AP(44),AWD(44),HL(44),HV(44),HLD(44),HSR(44),
     3HSV(45),SL(44),SV(45),SR(44),DELV(44),DELSL(44),DELSV(45),
     4DELSR(44),ITYPE(44),INDEX(44),C(50),NT,TSV(45),HTC(44)
C
      DO 17 J=1,4
      D(J) = 0.0
      DO 17 K=1,9
```

```
      A(J,K) = 0.0
   17 B(J,K) = 0.0
C
C  CALCULATION OF CURRENT VALUES OF ENTHALPIES.
C
      DO 30 J=2,NT
      HL(J) = 0.582*T(J) + 27.2
      HLD(J) = 0.582*TD(J) + 27.2
      HV(J) = C(10)*T(J)**2 + C(11)*T(J) + C(12)
   30 CONTINUE
      HL(1) = 0.582*T(1) + 27.2
      HV(1) = C(10)*T(1)**2 + C(11)*T(1) + C(12)
C
      IF(ITYPE(I).EQ.20) GO TO 15
      E2=C(14)/(RHOL(I)*AVL(I)*0.5)
      E9 = C(16)
      GO TO 20
   15 E2 = C(26)/(RHOL(I)*AVL(I))
      E9 = C(28)
C
   20 IF(I.GT.1) GO TO 10
C
C  TOP TRAY COEFFICIENTS.
C
      G1=V(2)+SV(2)+SR(1)-L(1)-V(1)
      IF(C(50).GT.0.0)G1F(1)=G1
      G1=G1-G1F(1)
      A(1,5) = AT(1)*(PSIW(1)+PSI(1))/(E9*AVL(1)*PSI(1)**1.5)
      B(1,5) = -1.0
      D(1) = DELV(2)+DELSV(2)+DELSR(1)-DELV(1)+G1
      A3P = 1.5*E9*AVL(1)*EPS(1)*RHOL(1)*SQRT(PSI(1))
      E2P = E2
      G3=HV(2)*V(2)+HSV(2)*SV(2)+HSR(1)*SR(1)-HL(1)*L(1)-HV(1)*V(1)
      IF(C(50).GT.0.0)G3F(1)=G3
      G3=G3-G3F(1)
      A(2,5) = C(3)*UL(1)
      B(2,9) = C(1)*V(2)
      B(2,5) = -(C(3)*L(1)+C(1)*V(1)+C(3)*G1)
      D(2) = (HV(2)-HL(1))*DELV(2)+(HL(1)-HV(1))*DELV(1)
     1        +(HSV(2)-HL(1))*DELSV(2)+(HSR(1)-HL(1))*DELSR(1)
     2        +G3-HL(1)*G1
      RETURN
   10 CONTINUE
C
C  THE GENERAL TRAY COEFFICIENTS
C
      G2=L(I-1)-LD(I)-SL(I-1)
      IF(C(50).GT.0.0)G2F(I)=G2
      G2=G2-G2F(I)
      G4=HL(I-1)*L(I-1)-(LD(I)+SL(I-1))*HLD(I)
```

```
      IF(C(50).GT.0.0)G4F(I)=G4
      G4=G4-G4F(I)
      IF(I.EQ.NT) GO TO 11
      G1=LD(I)+V(I+1)+SV(I+1)+SR(I)-L(I)-V(I)
      IF(C(50).GT.0.0) G1F(I)=G1
      G1=G1-G1F(I)
      G3=HLD(I)*LD(I)+HV(I+1)*V(I+1)+HSV(I+1)*SV(I+1)
     1   +HSR(I)*SR(I)-HL(I)*L(I)-HV(I)*V(I)
      IF(C(50).GT.0.0)G3F(I)=G3
      G3=G3-G3F(I)
      GO TO 12
   11 CONTINUE
      G1=LD(I)+SV(I+1)+SR(I)-L(I)-V(I)
      IF(C(50).GT.0.0)G1F(I)=G1
      G1=G1-G1F(I)
      G3=HLD(I)*LD(I)+HSV(I+1)*SV(I+1)+HSR(I)*SR(I)
     1   -HL(I)*L(I)-HV(I)*V(I)
      IF(C(50).GT.0.0)G3F(I)=G3
      G3=G3-G3F(I)
   12 CONTINUE
C
      A3 = 1.5*E9*AVL(I)*EPS(I)*RHOL(I)*SQRT(PSI(I))
      A(3,3) = EPS(I)*RHOL(I)*AT(I)*E2*(1.0-1.5*(PSIW(I)+PSI(I))/PSI(I)
      A(3,5) = EPS(I)*RHOL(I)*AT(I)*(PSIW(I)+PSI(I))*1.5/(PSI(I)*A3)
      IF(I.EQ.2) GO TO 13
      A(1,1) = RHOLD(I)*AD(I)*EPS(I-1)*E2P*(1.0-1.5*(PSIW(I-1)+PSI(I-1)
     1   /PSI(I-1))
   13 CONTINUE
C
      A(1,3) = EPS(I-1)*RHOLD(I)*AD(I)*(PSIW(I-1)+PSI(I-1))*1.5/
     1         (PSI(I-1)*A3P)
      CL = 1.5/(0.36*2.0*32.2*(RHOL(I-1)*AUD(I))**2)
      A(1,5) = RHOLD(I)*AD(I)*(EPS(I)*E2*(1.0-1.5*(PSIW(I)+PSI(I))/
     1         PSI(I))+2.0*CL*LD(I))
      A(1,7) = EPS(I) *RHOLD(I)*AD(I)*(PSIW(I)+PSI(I))*1.5/(PSI(I)*A3P)
      B(3,3) = +1.0
      B(3,5) = -1.0
      B(1,3) = +1.0
      B(1,5) = -1.0
      D(1) = -DELSL(I-1)+G2
      D(3) = DELSV(I+1)+DELSR(I)+G1-DELV(I)
      IF(I.EQ.NT) GO TO 14
      D(3) = D(3)+DELV(I+1)
   14 CONTINUE
C
      A(4,5) = C(3)*UL(I)
      B(4,2) = C(3)*(TD(I)-T(I))
      B(4,3) = C(3)*LD(I)
      B(4,5) = -C(3)*(L(I)+G1)+C(1)*V(I)
      A(2,5) = C(3)*UD(I)
```

```
      B(2,2) = C(3)*(T(I-1)-TD(I))
      B(2,3) = C(3)*(L(I-1)-SL(I-1))
      B(2,5) = -C(3)*(LD(I)+G2)
      D(2) = G4+(HLD(I)-HL(I-1))*DELSL(I-1)-HLD(I)*G2
      IF(I.EQ.NT) GO TO 16
      B(4,9) = C(1)*V(I+1)
C
   16 D(4) = -(HV(I)-HL(I))*DELV(I)+HSV(I+1)*DELSV(I+1)
     1          +HSR(I)*DELSR(I)+G3-HL(I)*(DELSV(I+1)+DELSR(I)+G1)
      IF(I.LT.NT) D(4)=D(4)+(HV(I+1)-HL(I))*DELV(I+1)
      A3P=A3
      E2P=E2
C
      RETURN
      END
      SUBROUTINE CORECT(DELTA2)
      REAL L,LD
      DIMENSION DELTA2(174)
      COMMON L(44),V(44),LD(44),T(44),TD(44),WL(44),WD(44),PSI(44),
     1PSID(44),PSIU(44),EPS(44),RHOL(44),RHOLD(44),RHOV(44),AVL(44),
     2AD(44),AT(44),AP(44),AUD(44),HL(44),HV(44),HLD(44),HSR(44),
     3HSV(45),SL(44),SV(45),SR(44),DELV(44),DELSL(44),DELSV(45),
     4DELSR(44),ITYPE(44),INDEX(44),C(50),NT,TSV(45),HTC(44)
C
C   THIS ROUTINE IMPROVES THE CURRENT ESTIMATE OF THE CHANGE IN INTERNAL
C   VAPOUR FLOWRATES OVER THE TIME INCREMENT.
C
      J=4*NT-2
      I=0
      DELV(NT)=-(C(1)*V(NT)-HTC(NT)*SV(NT+1))*DELTA2(J)
     1          -(HTC(NT)*(TSV(NT+1)-T(NT))-HSV(NT+1))*DELSV(NT+1)
      DELV(NT)=DELV(NT)/HV(NT)
    1 CONTINUE
      I=I+1
      J=J-4
      K=NT-I
      K1=K+1
      DELV(K)=(HV(K1)-HTC(K)*(T(K1)-T(K)))*DELV(K1)
     1          -(HTC(K)*V(K1)-C(1)*V(K1))*DELTA2(J+4)
     2          -(C(1)*V(K)-HTC(K)*V(K1)-HTC(K)*SV(K1))*DELTA2(J)
     3          -(HTC(K)*(TSV(K1)-T(K))-HSV(K1))*DELSV(K1)
      DELV(K)=DELV(K)/HV(K)
      IF(I.LT.NT-1) GO TO 1
      RETURN
      END
      SUBROUTINE INFORM(MODE)
C
C   THIS IS THE DATA INPUT ROUTINE. MODE 1 SETS UP THE INITIAL COLUMN
C   CONDITIONS. MODE 2 INPUTS A STEP CHANGE. MODE 3 RESETS THE PARAMETERS
C   OR CAUSES TERMINATION.
```

```
C
      REAL L,LD
      DIMENSION TITLE(20),A(3)
      COMMON L(44),V(44),LD(44),T(44),TD(44),WL(44),WD(44),PSI(44),
     1PSID(44),PSTU(44),EPS(44),RHOL(44),RHOLD(44),RHOV(44),AVL(44),
     2AD(44),AT(44),AP(44),AUD(44),HL(44),HV(44),HLD(44),HSR(44),
     3HSV(45),SL(44),SV(45),SR(44),DELV(44),DELSL(44),DELSV(45),
     4DELSR(44),ITYPE(44),INDEX(44),C(50),NT,TSV(45),HTC(44)
      IF(MODE.EQ.2) GO TO 2
C
    1 CONTINUE
      DO 35 I=1,44
   35 INDEX(I) = I
      DO 40 I=1,45
      SV(I) = 0.0
      TSV(I) = 0.0
      HSV(I) = 0.0
      IF(I.EQ.45) GO TO 40
      DELV(I) = 0.0
      DELSL(I) = 0.0
      DELSV(I) = 0.0
      DELSR(I) = 0.0
      HSR(I) = 0.0
      SR(I) = 0.0
      SL(I) = 0.0
   40 CONTINUE
      READ(1,13)TITLE
      WRITE(2,14)TITLE
      READ(1,19) A,NT
      WRITE(2,12)A,NT
      WRITE(2,17) (INDEX(I),I=1,NT)
      READ(1,11) A,(ITYPE(I),I=1,NT)
      WRITE(2,12)A,(ITYPE(I),I=1,NT)
      READ(1,16) A,(RHOL(I),I=1,NT)
      WRITE(2,18)A,(RHOL(I),I=1,NT)
      READ(1,16) A,(RHOV(I),I=1,NT)
      WRITE(2,18)A,(RHOV(I),I=1,NT)
      READ(1,16) A,(AT(I),I=1,NT)
      WRITE(2,18)A,(AT(I),I=1,NT)
      READ(1,16) A,(AUD(I),I=1,NT)
      WRITE(2,18)A,(AUD(I),I=1,NT)
      READ(1,16) A,(AP(I),I=1,NT)
      WRITE(2,18)A,(AP(I),I=1,NT)
      READ(1,16) A,(AD(I),I=1,NT)
      WRITE(2,13)A,(AD(I),I=1,NT)
      READ(1,16) A,(PSTU(I),I=1,NT)
      WRITE(2,18)A,(PSTU(I),I=1,NT)
      READ(1,16) A,(AVL(I),I=1,NT)
      WRITE(2,18)A,(AVL(I),I=1,NT)
      READ(1,16) A,(T(I),I=1,NT)
```

```
      WRITE(2,18)A,(T(I),I=1,NT)
C
      DO 30 I=2,NT
      RHOLD(I)=RHOL(I)
   30 TD(I) = T(I-1)
      WRITE(2,15)
C
C  K=NO. OF PLATES HAVING SIDESTREAMS.
C
      READ(1,19) A,K
      DO 5 I=1,K
      READ(1,19) A,N,SL(N),SR(N),HSR(N),SV(N),HSV(N),TSV(N)
      WRITE(2,20)A,N,SL(N),SR(N),SV(N),TSV(N)
      DUM = 0.0
      IF(SL(N).GT 0.1) DUM = 0.582*T(N) + 27.2
      WRITE(2,21) DUM, HSR(N), HSV(N)
    5 CONTINUE
      READ(1,16) A,SV(NT+1),HSV(NT+1),TSV(NT+1)
      WRITE(2,13) A,SV(NT+1),HSV(NT+1),TSV(NT+1)
C
C  K=NO. OF CONSTANTS TO BE ENTERED.
C
      READ(1,19) A,K
      WRITE(2,22)
      DO 6 I=1,K
      READ(1,19) A,N,C(N)
      WRITE(2,20)A,N,C(N)
    6 CONTINUE
      RETURN
C
    2 CONTINUE
C  K=NO. OF STEPS TO BE INPUT.
      READ(1,19) A,K
      DO 7 I=1,K
      READ(1,19) A,N,DELSL(N),DELSR(N),HSR(N),DELSV(N),HSV(N)
    7 WRITE(2,20)A,N,DELSL(N),DELSR(N),HSR(N),DELSV(N),HSV(N)
      RETURN
C
   11 FORMAT(3A8,5I10)
   12 FORMAT(1H ,3A8,I7,6I13/(19X,7I13))
   13 FORMAT(10A8)
   14 FORMAT(1H1,20X,10A8/21X,40(2H- )/21X,10A8/21X,40(2H- ))
   15 FORMAT(1H0,25X,5HPLATE,4X,16HLIQUID WITHDRAWN,4X,15HLIQUID RETURNE
     1D,4X,15HVAPOUR RETURNED,4X,17HRETURN VAP. TEMP./26X,5(1H-),4X,16(
     2H-),4X,15(1H-),4X,15(1H-),4X,17(1H-))
   16 FORMAT(3A8,100F0.0)
   17 FORMAT(1H0,52X,12HPLATE NUMBER/1H ,52X,12(1H-)/9H VARIABLE,10X,7I
     13/1H ,8(1H-),10X,7I13/(22X,7I13))
   18 FORMAT(1H ,3A8,7G13.5/(25X,7G13.5))
   19 FORMAT(3A8,I0,15F0.0)
```

```
   20 FORMAT(1H ,3A8,I5,F16.4,F20.3,F19.3,2F18.3)
   21 FORMAT(1H ,5X,12H(ENTHALPIES),12X,F16.3,F20.3,F19.3)
   22 FORMAT(1H0,14HCONSTANTS ETC./1X,14(1H-))
    51 RETURN
      END
      SUBROUTINE MATRIX(D,E,DELTA1,NM,NROWS)
C
C  THIS ROUTINE SETS UP THE MATRIX FORMULATION OF THE DYNAMIC PROBLEM
C  FOR SOLUTION BY THE IMPLICIT METHOD.
C
      REAL L,LD
      DIMENSION D(NROWS,9),E(NM),A(4,9),B(4,9),F(4),DELTA1(NM)
      COMMON L(44),V(44),LD(44),T(44),TD(44),WL(44),WD(44),PSI(44),
     1PSID(44),PSIW(44),EPS(44),RHOL(44),RHOLD(44),RHOV(44),AVL(44),
     2AD(44),AT(44),AP(44),AUD(44),HL(44),HV(44),HLD(44),HSR(44),
     3HSV(45),SL(44),SV(45),SR(44),DELV(44),DELSL(44),DELSV(45),
     4DELSR(44),ITYPE(44),INDEX(44),C(50),NT,TSV(45),HTC(44)
C
      XMU = C(6)
      XMU1 = 1.0-C(6)
      DO 10 I=1,NT
      N1=4*I-5
      IF(I.EQ 1)N1=1
      N2=N1+3
      IF(I.EQ 1)N2=2
      CALL COEFFS(I,A,B,F)
      J1=0
      DO 5 J=N1,N2
      J1=J1+1
      STO=0.0
      MOD = J-5
      NZ1=6-J
      NZ2=4*NT-J+3
      IF(J.GT 4)NZ1=1
      K=4*NT-6
      IF(J.LT K)NZ2=9
C
      DO 3 K=NZ1,NZ2
    3 A(J1,K)=A(J1,K)/C(5)
      DO 4 K=NZ1,NZ2
      STO=STO+(A(J1,K)+XMU1*B(J1,K))*DELTA1(K+MOD)
    4 D(J,K)=A(J1,K)-XMU*B(J1,K)
C
      E(J)=STO + F(J1)
    5 CONTINUE
   10 CONTINUE
      C(50) = -1.0
      RETURN
      END
      SUBROUTINE PARAM(MODE)
```

```
C
C     THIS USES THE PRESENT VALUES OF L,LD,V TO OBTAIN THE HYDRAULIC
C     PARAMETERS AT STEADY OR UNSTEADY STATE.
C
      REAL L,LD
      DIMENSION G1(44),G2(44)
      COMMON L(44),V(44),LD(44),T(44),TD(44),WL(44),WD(44),PSI(44),
     1PSID(44),PSIW(44),EPS(44),RHOL(44),RHOLD(44),RHOV(44),AVL(44),
     2AD(44),AT(44),AP(44),AUD(44),HL(44),HV(44),HLD(44),HSR(44),
     3HSV(45),SL(44),SV(45),SR(44),DELV(44),DELSL(44),DELSV(45),
     4DELSR(44),ITYPE(44),INDEX(44),C(50),NT,TSV(45),HTC(44)
C
      Z=C(6)
      Z1=1.0-Z
      DO 10 I=1,NT
    1 RHOVAP=RHOV(I)
      IF(I.LT.NT)RHOVAP=RHOV(I+1)
      IF(ITYPE(I).EQ.20)GO TO 2
      E1=C(13)
      E2=C(14)
      E3=C(15)
      E9 = C(16)
      E10=C(17)/(RHOVAP**3*AT(I)**2)
      E11=C(18)
      GO TO 3
    2 E1=C(25)/(RHOVAP**1.5*AT(I))
      E2 = C(26)/(RHOL(I)*AVL(I))
      E3 = C(27)
      E9 = C(28)
      E10=C(29)
      E11 = C(30)
    3 IF(MODE.EQ.2) GO TO 11
      IF(I.EQ.1) GO TO 4
      IF(I.EQ.NT)GO TO 5
      G1(I)=LD(I)+V(I+1)+SV(I+1)+SR(I)-L(I)-V(I)
      G2(I)=L(I-1)-SL(I-1)-LD(I)
      PSI(I)=E1*(V(I+1)+SV(I+1))+E2*(LD(I)+SR(I))+E3*PSIW(I)
     1       +E10*(V(I+1)+SV(I+1))**2+E11
      IF(PSI(I).LT.0.01)PSI(I)=0.1
    7 EPS(I)=L(I)/(E9*AVL(I)*RHOL(I)*PSI(I)**1.5)
      CL=1.5/(0.36*2.0*32.2*(RHOL(I-1)*AUD(I))**2)
      CV=2.0/(322.0*EPS(I-1)*RHOL(I-1)*RHOV(I)*(0.6*AP(I-1))**2)
      PSID(I)=EPS(I)*(PSIW(I)+PSI(I))+CL*LD(I)**2
     1       +CV*(V(I)+SV(I))**2+EPS(I-1)*(PSIW(I-1)+PSI(I-1))
      WD(I)=RHOLD(I)*AD(I)*PSID(I)
      GO TO 6
    4 PSI(1)=E1*(V(2)+SV(2))+E2*SR(1)+E3*PSIW(1)
     1       +E10*(V(2)+SV(2))**2 + E11
      EPS(1) = L(1)/(E9*AVL(1)*RHOL(1)*PSI(1)**1.5)
      G1(1)=V(2)+SV(2)+SR(1)-L(1)-V(1)
```

```
      GO TO 6
    5 PSI(NT)=F1*SV(NT+1)+F2*(LD(NT)+SR(NT))
     1         +F3*PSIW(NT)+F10*SV(NT+1)**2+F11
      IF(PSI(NT).LT.0.01) PSI(NT)=0.4
      G1(NT)=LD(NT)+SV(NT+1)+SR(NT)-L(NT)-V(NT)
      G2(NT)=L(NT-1)-SL(NT-1)-LD(NT)
      GO TO 7
    6 WL(I)=EPS(I)*RHOL(I)*AT(I)*(PSIW(I)+PSI(I))
      GO TO 10
C
   11 IF(I.GT 1) GO TO 12
      WL(1)=WL(1)+(Z1*G1(1)+Z*(V(2)-L(1)-V(1)+SV(2)+SR(1))
     1         +DELSV(2)+DELSR(1))*C(37)
      G1(1)=V(2)+SV(2)+DELSV(2)+SR(1)+DELSR(1)-L(1)-V(1)
      GO TO 18
   12 IF(I.EQ NT) GO TO 13
      WL(I)=WL(I)+(Z1*G1(I)+Z*(LD(I)+V(I+1)+SV(I+1)+SR(I)
     1         -L(I)-V(I))+DELSV(I+1)+DELSR(I))*C(37)
      WD(I)=WD(I)+(Z1*G2(I)+Z*(L(I-1)-SL(I-1)-LD(I))-DELSL(I-1))*
     1         C(37)
      G1(I)=LD(I)+V(I+1)+SV(I+1)+SR(I)-L(I)-V(I)
     1         +DELSV(I+1)+DELSR(I)
      G2(I)=L(I-1)-SL(I-1)-DELSL(I-1)-LD(I)
      GO TO 19
   13 WL(NT)=WL(NT)+(Z1*G1(NT)+Z*(LD(NT)+SV(NT+1)+SR(NT)-L(NT)-V(NT))
     1         +DELSV(NT+1)+DELSR(NT))*C(37)
      WD(NT)=WD(NT)+(Z1*G2(NT)+Z*(L(NT-1)-SL(NT-1)-LD(NT))
     1         -DELSL(NT-1))*C(37)
      G1(NT)=LD(NT)+SV(NT+1)+SR(NT)-L(NT)-V(NT)+DELSV(NT+1)+DELSR(NT)
      G2(NT)=L(NT-1)-SL(NT-1)-DELSL(NT-1)-LD(NT)
   19 PSID(I)=WD(I)/(AD(I)*RHOLD(I))
   18 PSIG=0.3
      A1=WL(I)*F9*AVL(I)/(L(I)*AT(I))
      DO 14 J=1,12
      IF(PSIG LT.0.0) PSIG=0.01
      PSI(I)=PSIG-(PSIW(I)+PSIG-A1*PSIG**1.5)/(1.0-1.5*A1*SQRT(PSIG))
   16 IF(ABS(PSI(I)-PSIG).LT.0.001) GO TO 17
   14 PSIG=PSI(I)
      WRITE(2,100) I, PSI(I)
  100 FORMAT(44H0PSI CALCULATION FAILED TO CONVERGE FOR TRAY,I3,F20.7)
   17 IF(PSI(I).LT 0.005.OR.PSI(I).GT.1.2) PSI(I) = 0.1
      EPS(I)=WL(I)/(RHOL(I)*AT(I)*(PSIW(I)+PSI(I)))
   10 CONTINUE
      RETURN
      END
      SUBROUTINE PRINT2(I,CUMTIM)
      REAL L,LD
      COMMON L(44),V(44),LD(44),T(44),TD(44),WL(44),WD(44),PSI(44),
     1PSID(44),PSIW(44),EPS(44),RHOL(44),RHOLD(44),RHOV(44),AVL(44),
     2AD(44),AT(44),AP(44),AUD(44),HL(44),HV(44),HLD(44),HSR(44),
```

```
      3HSV(45).SL(44),SV(45),SR(44),DELV(44),DELSL(44),DELSV(45),
      4DELSR(44),ITYPE(44),INDEX(44),C(50),NT,TSV(45),HTC(44)
    1 WRITE(2,11)I,CUMTIM
      DO 2 J=1,NT
      WRITE(2,12)I,LD(J),L(J),V(J),SL(J),SV(J),SR(J),WL(J),WD(J),PSI(J)
     1EPS(J),PSID(J),T(J),TD(J)
    2 CONTINUE
      WRITE(2,13) SV(NT+1),HSV(NT+1),TSV(NT+1)
C
   11 FORMAT(13H0PRINTOUT NO.,I3,60X,17HCUMULATIVE TIME =,F7.2,9H SECON
     1S./4H0NO.,5X,2HLD,7X,1HL,8X,1HV,8X,2HSL,7X,2HSV,7X,2HSR,7X,2HWL,
     27X,2HWD,5X,3HPSI,5X,3HEPS,5X,4HPSID,6X,1HT,8X,2HTD)
   12 FORMAT(1H ,I3,8F9.3,3F8.4,2F9.3)
   13 FORMAT(10H SV(NT+1)=,F9.3,11H HSV(NT+1)=,F9.3,11H TSV(NT+1)=,F9.3
      RETURN
      END
      SUBROUTINE STEADY
C
C
      REAL L,LD
      DIMENSION A(88,7),B(88),D(88),E(88)
      COMMON L(44),V(44),LD(44),T(44),TD(44),WL(44),WD(44),PSI(44),
     1PSID(44),PSIU(44),EPS(44),PHOL(44),RHOLD(44),RHOV(44),AVL(44),
     2AD(44),AT(44),AP(44),AUD(44),HL(44),HV(44),HLD(44),HSR(44),
     3HSV(45),SL(44),SV(45),SR(44),DELV(44),DELSL(44),DELSV(45),
     4DELSR(44),ITYPE(44),INDEX(44),C(50),NT,TSV(45),HTC(44)
C
C
   11 DO 10 I=1,NT
      HL(I) = 0.582*T(I) + 27.2
   10 HV(I) = C(10)*T(I)**2 + C(11)*T(I) + C(12)
C
      READ(1,91)(L(I),V(I),I=1,NT)
   91 FORMAT(1000F0.0)
   41 DO 45 I=2,NT
      HLD(I) = HL(I-1)
   45 LD(I) = L(I-1)-SL(I-1)
      LD(1) = 0.0
      DO 80 I=1,NT-1
      HTC(I)=HV(I+1)*V(I+1)+HSV(I+1)*SV(I+1)-HV(I)*V(I)
   80 HTC(I)=HTC(I)/(V(I+1)*(T(I+1)-T(I))+SV(I+1)*(TSV(I+1)-T(I)))
      HTC(NT)=HSV(NT+1)*SV(NT+1)-HV(NT)*V(NT)
      HTC(NT)=HTC(NT)/(SV(NT+1)*(TSV(NT+1)-T(NT)))
      DO 555 J9=1,NT
  555 IF(HTC(J9).LT.0.1) HTC(J9)=1.0
      WRITE(2,90)(HTC(I),I=1,NT)
   90 FORMAT(11H0TRAY HTC-S/(1H ,7G15.5))
      CALL PARAM(1)
C
      RETURN
```

```
      END
      SUBROUTINE TEST(N,X,LEVEL)
      DIMENSION X(N)
C
C  ROUTINE TO MONITOR VARIOUS VECTORS FOR OVER AND UNDERFLOW, PROVIDE
C  MONITOR PRINTOUTS AND REDUCE RISK OF FAILURE BY ZEROING SUSPECT
C  VALUES.
C
      DO 1 I=1,N
      IFLAG = 0
      IF(ABS(X(N)).LT.10.0) IFLAG = IFLAG+1
      IF(ABS(X(N)).GT.1.0E-50) IFLAG=IFLAG+1
      IF(ABS(X(N)).EQ.0.0) IFLAG = IFLAG+1
      IF(IFLAG.EQ.2) GO TO 1
      GO TO 2
    1 CONTINUE
      RETURN
C
    2 CONTINUE
      WRITE(2,3) LEVEL,(X(I),I=1,N)
      DO 4 I=1,N
      IFLAG =0
      IF(ABS(X(N)).GT.1.0E50) IFLAG = 1
      IF(ABS(X(N)).LT.1.0E-50) IFLAG = 1
    4 IF(IFLAG.EQ.1) X(N) = 0.0
    3 FORMAT(25H0ERROR TEST MONITOR LEVEL,I2/(1H ,7E15.6))
      RETURN
      END
      SUBROUTINE UPDATE(IZERO,DELTA2)
      REAL L,LD
      DIMENSION DELTA2(174)
      COMMON L(44),V(44),LD(44),T(44),TD(44),WL(44),WD(44),PSI(44),
     1PSID(44),PSIW(44),EPS(44),RHOL(44),RHOLD(44),RHOV(44),AVL(44),
     2AD(44),AT(44),AP(44),AUD(44),HL(44),HV(44),HLD(44),HSR(44),
     3HSV(45),SL(44),SV(45),SR(44),DELV(44),DELSL(44),DELSV(45),
     4DELSR(44),ITYPE(44),INDEX(44),C(50),NT,TSV(45),HTC(44)
      IF(IZERO.EQ.-1) GO TO 5
      IF(IZERO.EQ.0) GO TO 2
      L(1)=L(1)+DELTA2(1)
      T(1)=T(1)+DELTA2(2)
      V(1)=V(1)+DELV(1)
      DO 1 I=2,NT
      J=4*I-5
      LD(I)=LD(I)+DELTA2(J)
      TD(I)=TD(I)+DELTA2(J+1)
      L(I) =L(I) +DELTA2(J+2)
      T(I) =T(I) +DELTA2(J+3)
      V(I) =V(I) +DELV(I)
    1 CONTINUE
      RETURN
```

```
C
    2 CONTINUE
      DO 3 I=1,4*NT-2
    3 DELTA2(I)=0.0
      DO 4 I=1,NT+1
      SV(I) = SV(I)+DELSV(I)
      DELSV(I)=0.0
      IF(I.GT.NT) GO TO 4
      SL(I) = SL(I)+DELSL(I)
      DELSL(I) = 0.0
      SR(I) = SR(I)+DELSR(I)
      DELSR(I) = 0.0
    4 DELV(I)=0.0
      RETURN
C
    5 CONTINUE
      L(1)=L(1)-DELTA2(1)
      T(1)=T(1)-DELTA2(2)
      V(1)=V(1)-DELV(1)
      DO 10 I=2,NT
      J=4*I-5
      LD(I)=LD(I)-DELTA2(J)
      TD(I) = TD(I)-DELTA2(J+1)
      L(I) = L(I)-DELTA2(J+2)
      T(I)=T(I)-DELTA2(J+3)
      V(I)=V(I)-DELV(I)
   10 CONTINUE
      RETURN
      END
      FINISH
```

A2.7 Sample data for the program.

```
CRUDE OIL DISTILLATION SIMULATION    DYNAMIC HEAT AND MASS BALANCE     G472
RELINEARISATION INCLUDED    15-PLATE TR2 DATA                        12/8/70.
NO OF TRAYS                  15
TRAY TYPES                    10    10    20    20    20
20    20    20    20    20      20    20    10    10    10
LIQUID DENSITY               44.7   45.1   48.5   48.8   49.1   49.6   51.4
51.6   51.7   52.0   53.8   54.2   56.8   57.5   59.7
VAPOUR DENSITY               .498   .515   .525   .546   .548
.569   .603   .648   .641   .662   .699   .708   .744   .767   .778
TRAY AREAS                    119    119    128    128    128
128    128    128    128    128   128    128    119    119    119
AREA UD                     0    8.52   7.58   8.52   7.58   8.52   7.58   8.52
7.58   8.52   7.58   8.52   8.52   7.58   8.52
HOLE AREA                    18.3   18.3    9     9     9
9   9    12    12    12    12    12    18.3   18.3   18.3
DOWNCOMER AREA                0    12.2   17.8   10.8   17.8
10.8   17.8   10.8   17.8   10.8   17.8   10.8   12.2   19.2   11.2
WEIR HEIGHT                  0.148   0.148   0.164   0.164   0.131
0.131   0.131   0.164   0.164   0.131   0.131   0.131   0.148   0.148   0.148
AV FLOW WIDTH                 11.8   11.8   11.4   11.4   11.4
11.4   11.4   11.4   11.4   11.4   11.4   11.4   11.8   11.8   11.8
TRAY TEMPS                    258    290    311    349    370    393    425
461    503    526    580    594    627    640    667
SIDESTREAM PLATES            9
REFLUX RETURN                1   0    32.0    136.0    0    0    0
VIR RETURN                   3   0    76.5    198.0    0    0    0
VIR W/D                      4   76.5   0    0    0    0    0
KERO W/D + SV RETURN         6   24.4   0    0    5.6   381   376
LIR RET + LGO SV RET         8   0    60.7   271   5.26   352   314
LIR W/D                      9   60.7   0    0    0    0    0
LGO W/D                       10   26.3   0    0    0    0    0
HGO W/D + SV RETURN          12   11.0   0    0    2.2   483   578
```

```
FEEDPLATE                     14   0   70.9   40.8   90.3   526   654
BOTTOMS STEAM                 1.2   1150   815
NO. .F CONSTANTS             28
VAP LIN ENTH COEFF          1   0.26
VAP LIN ENTH COEFF           2   241.5
LIQ LIN ENTH COEFF        3   0.582
LIQ LIN ENTH COEFF          4   27.2
TIME INCREMENT                5      1.0
XMU IMPLICIT PARAM            6        0.85
PRINTOUT TIME                 7      1.0
MAXIMUM PRINTOUT                8        7200.0
VAPOUR ENTH               10     0.00025
VAPOUR ENTH                 11   0.26
VAPOUR ENTH                 12   241.5
E1 BUBBLE TRAY              13   0.0
E2 BUBBLE TRAY              14   0.0
E3 BUBBLE TRAY                15     0.89
                                16   3.38
E10 BUBBLE TRAY             17   0.211
E11 BUBBLE TRAY               18     0.0
E1 SIEVE TRAY              25   0.204
E2 SIEVE TRAY              26   1.65
E3 SIEVE TRAY                 27   0.24
                              28   3.38
E10 SIEVE TRAY              29   0.0
E11 SIEVE TRAY                30   0.0
RELINEARISATION CON           37     1.0
NO OF CORRNS TO DELV          38   30
DOUBLING RATE                 39     100000
DELV DAMPING COEFF          40   1.0
NO INITIAL HB CALCN.        41    -1.0
32.0   60.5     73.1   60.5     120.6   66.6     126.6   72.6
56.1   78.6     56.1   79.0     31.7   79.0     102.4   73.7
112.4   83.7     51.7   93.7     25.4   93.7     25.4   91.7
14.4   91.5     85.3   1.2     85.3   1.2
NO. OF STEPS                   1
REFLUX STEP INCREASE             1   0   3.96   136   0   0   0
```

The initial steady state for the 15-plate column example was based on the initial state measured during the refinery experiment TR2 for the full size 44-plate column. The fact that the initial state as indicated by the instruments on the unit is not truly steady (that is it is not in heat and mass balance) is not important. The computer program calculates only the deviation from the initial state due to the input disturbance. A diagram showing the internal flowsand temperatures follows - Fig. A2-1.

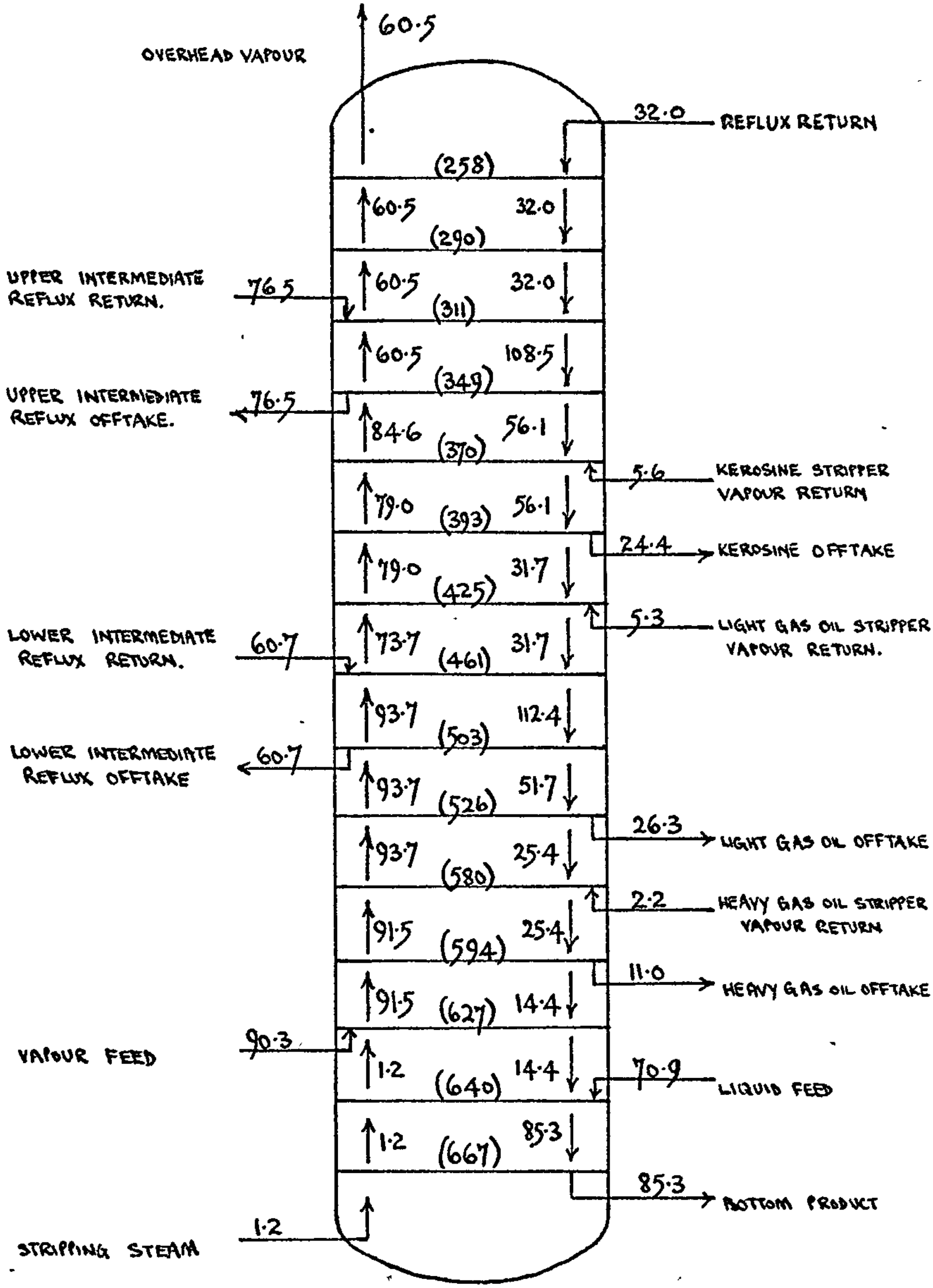

60·5
OVERHEAD VAPOUR
32·0
REFLUX RETURN
(258)
60·5
32·0
(290)
UPPER INTERMEDIATE REFLUX RETURN.
76·5
60·5
32·0
(311)
60·5
108·5
(349)
UPPER INTERMEDIATE REFLUX OFFTAKE.
76·5
84·6
56·1
(370)
5·6
KEROSINE STRIPPER VAPOUR RETURN
79·0
(393)
56·1
24·4
KEROSINE OFFTAKE
79·0
(425)
31·7
5·3
LIGHT GAS OIL STRIPPER VAPOUR RETURN.
LOWER INTERMEDIATE REFLUX RETURN.
60·7
73·7
(461)
31·7
93·7
(503)
112·4
LOWER INTERMEDIATE REFLUX OFFTAKE
60·7
93·7
(526)
51·7
26·3
LIGHT GAS OIL OFFTAKE
93·7
(580)
25·4
2·2
HEAVY GAS OIL STRIPPER VAPOUR RETURN
91·5
(594)
25·4
11·0
HEAVY GAS OIL OFFTAKE
91·5
(627)
14·4
VAPOUR FEED
90·3
1·2
(640)
14·4
70·9
LIQUID FEED
1·2
(667)
85·3
85·3
BOTTOM PRODUCT
STRIPPING STEAM
1·2

FIG. A2-1.

APPENDIX 3. A MATHEMATICAL MODEL OF A CRUDE OIL DISTILLATION UNIT - VALUES OF THE CONSTANTS FOR THE EMPIRICAL CORRELATIONS.

A3.1 The Francis weir formula.

The same equation was used for both bubble and sieve plates:-

$$L_n = e_9 \, \ell_n \, \varepsilon_n \, \rho_{Ln} \, \psi_n^{3/2}$$

(The symbols have the meaning assigned to them in Chapter 4.)

From Perry (2):-

$$L_n / (\varepsilon_n \rho_{Ln}) = 0.42 \, \ell_n \, \psi_n^{1.5} \sqrt{2g}$$

From which :-

$$e_9 = 0.42\sqrt{2g} = \underline{3.38}$$

A3.2 Froth height correlation.

A3.2.1 Bubble cap plates.

Bubble Tray Design Manual (7) gives:-

$$\underset{\substack{\text{froth height}\\ \text{(inches)}}}{Z_f} = 2.53 \underset{\text{ft/sec}\sqrt{\text{lb/ft}^3}}{F^2} + 1.89 \underset{\substack{\text{weir height}\\ \text{(inches)}}}{W} - 1.6$$

In the units and nomenclature of Chapter 4 this becomes:-

$$\psi_n = (0.211 V_{n+1}^2) / (A_{Tn}^2 \rho_{Vn+1}) + 0.89 \psi_w - 0.13$$

This equation was found to give negative values of ψ_n at high vapour rates and a simpler form that retained sensible values for the vapour rate dependence was used:-

$$\psi_n = (0.211 V_{n+1}^2) / (A_{Tn}^2 \rho_{Vn+1}) + 1.0 \psi_w$$

A3.2.2 Sieve plates.

Thomas and Campbell (9) give:-

$$\underset{\substack{\text{froth height}\\ \text{(inches)}}}{Z_f} = 2.45 \underset{\text{ft/sec lb/ft}}{F} + 0.053 \underset{\text{gpm/ft}}{L} + 1.24 \underset{\substack{\text{weir height}\\ \text{(inches)}}}{W}$$

In the units and nomenclature of Chapter 4 this becomes:-

$$\phi_n = (0.204\, V_{n+1}) / (A_{Tn} \sqrt{\rho_{Vn+1}}) + 1.65\, L / (\rho_{Ln}\, \ell_n) + 0.24$$

APPENDIX 4. TABULATED RESULTS FOR THE EXPERIMENTS AT BP REFINERY (LLANDARCY) LTD.

A4.1 Reference numbers.

In the following tables of raw data temperature indicator readings are referred to by a number prefixed by T, the key to which is given in the main body of the thesis, Fig. 5-2. Chart readings are referred to by a number prefixed by C, the key to which is given below. The flowrates are obtained from the data readings by the relation:-

True flow = (Reading/1000) x M

where M is the maximum attainable value for each particular flow for this crude distillation unit.

Reference	Variable
C13 C14 C15	Crude oil feedrate, A,B and C passes.
C16 C17 C18	Crude oil feed temperature, A,b and C passes.
C19	Tower top temperature.
C21	Tower top pressure.
C22	Overhead reflux flowrate.
C23	Re-run tower feedrate.
C36	Upper intermediate reflux flowrate.
C37	Lower intermediate reflux flowrate.
C38	Level in crude tower base.
C39	Reduced crude product flowrate.
C41	Heavy naphtha flowrate.
C42	Kerosine flowrate.
C43	Light gas oil flowrate.
C44	Heavy gas oil flowrate.

A4.2 Results for run TR3.

A4.2.1 Run TR3 temperature indicator readings.

(Step change input at 1400 hrs.)

Time	1400	1406	1409	1412	1415	1418	1421	1424	1427	1432	1435	1438
T18	638	638	638	638	638	638	638	638	638	639	640	639
T19	608	615	619	622	623	628	629	630	630	629	629	630
T20	530	543	546	547	549	549	550	551	551	548	551	552
T21	380	401	404	406	406	406	406	406	404	401	403	403
T22	103	103	104	104	104	104	104	105	105	104	105	105
T23	327	328	331	331	331	333	334	335	335	335	335	337
T24	493	500	502	503	504	506	506	507	506	506	506	508
T25	309	310	310	310	310	312	313	311	311	312	313	314
T26	234	237	237	237	236	236	237	237	237	237	237	237
T27	107	107	107	107	108	108	108	109	109	109	109	109
T28	193	197	197	197	199	199	200	199	199	201	203	203
T46	646	646	646	647	647	647	647	648	647	647	647	647
T47	648	650	650	652	650	651	650	651	651	650	651	651
T48	647	650	650	651	650	650	650	650	650	646	650	650
T49	644	644	646	647	647	647	646	646	646	646	646	646
T50	264	269	269	271	269	270	271	270	269	270	271	270
T71	790	788	787	787	787	785	782	783	784	782	782	782
T72	797	795	794	794	793	793	793	790	789	787	787	787
TA1	284				293				289			
TA2	301				301				303			
TA3	297				299				299			
TA4	297				299				299			
TA5	332				326				339			
TA6	362				378				377			
TA7	416				430				429			
TA8	448				451				452			
TA9	437				442				441			
TA10	539				551				552			
TA11	560				572				571			
TA12	622				638				639			
TA13	638				644				643			
TA14	638				642				641			
TA15	262				263				264			
TA16	72				72				71			
TA17	382				390				387			
TA18	347				364				363			
TA19	526				536				535			
TA20	600				606				617			

Time	1441	1445	1448	1451	1454	1459	1509	1517	1530	1540	1550	1600
T18	639	639	639	639	639	640	640	640	640	639	640	640
T19	631	631	632	632	632	632	626	622	618	618	618	618
T20	552	553	553	552	551	551	546	545	542	540	540	539
T21	404	406	406	404	403	401	396	391	392	392	391	390
T22	104	104	104	104	104	104	105	105	105	105	105	106
T23	337	338	339	339	339	339	340	339	339	338	338	338
T24	507	508	509	508	508	508	505	504	502	501	501	500
T25	314	315	316	316	316	316	315	312	310	310	310	310
T26	237	237	237	237	237	237	237	237	237	236	236	236
T27	109	109	109	109	109	108	108	108	107	106	106	106
T28	203	204	205	205	205	205	202	201	200	199	201	201
T46	646	646	647	645	646	647	647	647	646	646	646	646
T47	650	650	651	651	651	650	651	650	650	650	650	650
T48	649	649	651	651	651	650	650	650	650	649	649	649
T49	644	644	646	646	646	647	646	647	646	646	646	644
T50	270	270	270	270	269	270	266	266	266	266	264	264
T71	779	779	780	778	780	781	784	785	786	786	786	785
T72	786	786	788	787	789	789	790	790	792	792	793	792
TA1	293				292		289	286	288	288	286	286
TA2	303				305		307	305	306	306	304	305
TA3	300				301		302	302	301	.301	301	300
TA4	300				301		302	302	301	301	301	300
TA5	341				343		347	345	343	342	342	342
TA6	377				378		371	370	370	369	369	368
TA7	431				428		420	417	418	418	417	417
TA8	457				456		455	453	450	449	450	449
TA9	440				440		440	439	438	438	438	437
TA10	553				551		547	545	543	541	541	540
TA11	573				571		566	563	562	561	561	559
TA12	638				639		633	630	627	626	625	625
TA13	642				643		645	644	643	642	641	641
TA14	641				642		645	642	641	641	641	641
TA15	265				265		266	265	265	264	264	265
TA16	70				69		69	69	68	68	67	68
TA17	390				385		378	376	376	375	374	375
TA18	364				360		353	350	350	349	349	349
TA19	538				535		529	527	526	524	524	524
TA20	618				618		614	611	608	606	606	606

Time	1616	1627	1637	1647	1744	1803	1813	1828	1843	1902	1915	1927
T18	640	640	640	640	640	640	640	638	640	638	640	640
T19	618	617	616	616	617	618	619	617	616	615	618	618
T20	539	538	538	538	540	540	541	538	539	539	541	541
T21	390	390	390	391	393	393	394	387	392	390	393	394
T22	105	107	107	107	106	107	108	107	107	107	107	108
T23	337	338	338	337	337	338	339	337	337	336	337	338
T24	500	500	500	500	501	501	502	499	499	499	500	501
T25	309	309	309	309	310	311	311	309	309	308	308	310
T26	236	236	236	235	234	234	234	232	233	234	233	234
T27	106	107	108	108	106	106	106	106	106	106	105	106
T28	199	199	199	199	199	200	199	198	197	197	196	198
T46	647	648	648	647	647	648	647	647	647	647	648	647
T47	653	654	652	652	652	651	650	653	652	650	653	648
T48	650	649	648	649	649	650	649	647	646	645	652	641
T49	647	648	647	647	646	647	646	647	646	645	648	641
T50	264	265	265	266	266	267	267	264	264	264	267	266
T71	786	786	786	785	783	789	790	793	795	794	796	796
T72	792	794	794	791	793	796	796	795	796	795	798	798
TA1	287	288	288	287	289	291	289	286	290	288	290	290
TA2	305	306	306	306	306	306	307	305	306	306	307	307
TA3	300	301	301	301	300	300	301	300	300	299	300	299
TA4	300	301	301	301	300	300	301	300	300	299	300	299
TA5	342	342	342	342	342	342	343	342	342	342	342	342
TA6	369	369	369	370	370	370	371	368	370	369	372	371
TA7	418	417	419	420	422	421	422	416	421	419	423	421
TA8	450	449	449	447	449	450	449	449	449	448	451	449
TA9	440	438	440	439	439	440	441	439	440	439	441	439
TA10	542	540	540	540	543	543	543	540	541	540	545	543
TA11	561	560	560	560	562	561	562	559	561	560	565	562
TA12	626	625	624	624	627	626	626	624	624	624	629	623
TA13	643	643	642	642	642	642	642	642	642	641	646	638
TA14	643	643	642	642	642	642	642	641	641	641	644	634
TA15	265	265	266	266	265	266	266	264	264	266	268	269
TA16	69	68	69	69	68	67	67	66	67	67	67	69
TA17	377	376	375	376	377	377	377	373	377	375	378	376
TA18	349	348	349	350	352	351	351	346	350	349	351	351
TA19	524	524	524	524	525	525	526	523	525	525	526	525
TA20	607	606	604	604	606	606	607	604	605	605	608	606

Time	1937	1948	2000
T18	636	636	640
T19	615	615	619
T20	537	536	540
T21	389	388	391
T22	108	108	108
T23	337	336	336
T24	498	498	501
T25	309	307	307
T26	234	232	232
T27	106	104	104
T28	198	196	195
T46	647	647	648
T47	649	651	653
T48	641	646	653
T49	641	644	649
T50	263	263	265
T71	786	794	798
T72	796	795	801
TA1	286	285	288
TA2	304	304	305
TA3	297	297	299
TA4	297	297	299
TA5	341	342	342
TA6	367	367	370
TA7	417	417	421
TA8	447	447	449
TA9	437	437	440
TA10	539	539	543
TA11	558	558	563
TA12	623	623	628
TA13	638	639	645
TA14	636	641	644
TA15	269	269	270
TA16	69	70	72
TA17	371	373	378
TA18	347	346	351
TA19	521	522	526
TA20	603	605	608

A4.2.2 Results for Run TR3 - Chart readings.

Time	1416	1429	1441	1500	1520	1544	1601	1627	1644	1758	1820	1845
C13	855	860	860	860	860	860	855	858	858	858	858	858
C14	865	865	868	865	865	869	865	868	868	866	864	864
C15	855	855	860	855	855	858	856	856	858	855	856	856
C16	655	655	655	657	656	655	655	655	655	656	656	656
C17	650	650	650	650	650	648	647	647	647	649	648	648
C18	644	643	642	643	643	643	641	642	642	643	641	640
C19	262	260	261	260	255	256	255	255	255	256	257	256
C21	25	25	25	26	26	26	26	26	26	26	26	26
C22	342	360	340	330	350	350	350	350	345	341	343	340
C23	660	680	680	690	710	710	690	685	670	650	650	650
C36	550	545	550	550	555	555	555	550	555	555	555	550
C37	640	640	640	640	640	640	640	640	640	640	640	640
C38	790	790	790	790	790	790	790	790	790	790	790	790
C39	750	760	755	755	785	785	785	795	790	785	783	785
C42	515	510	510	510	510	510	510	505	510	510	508	504
C43	710	710	705	710	710	710	710	705	700	705	705	700
C44	370	365	365	365	365	365	365	365	365	370	365	362

Time	1905	1938	2011
C13	856	858	858
C14	864	868	862
C15	857	857	855
C16	655	655	656
C17	648	647	650
C18	640	636	645
C19	255	255	256
C21	26	26	26
C22	342	342	342
C23	650	665	650
C36	552	555	555
C37	640	640	640
C38	790	790	790
C39	790	790	780
C42	510	512	515
C43	705	705	705
C44	360	362	362

A4.2.3 Results for Run TR3 - Product properties.

Kerosine distillation points.

Time	10% pt.	90% pt.	Time	10% pt.	90% pt.
0915	100°F	217°F	1451	185	242
0943	167	218	1519	177	234
1011	169	223	1547	175	229
1039	166	218	1615	174	227
1107	166	218	1643	173	225
1135	167	220	1711	174	227
1203	167	220	1739	175	229
1231	167	220	1807	175	229
1259	166	218	1835	175	229
1327	167	218	1803	175	228
1355	167	218	1931	175	230
1423	181	236	1959	173	227

Cloud points.

Time	Kerosine	Light gas oil	Heavy gas oil
1010	-3°F	13°F	52°F
1100	+2	11	50
1145	-1	14	54
1230	-2	12	55
1355	-2	13	54
1408	-2	12	53
1420	+1	15	53
1435	+4	21	55
1450	-4	24	55
1510	+2	20	58
1530	+1	19	58
1550	+2	18	56
1610	0	16	57
1635	0	16	59
1655	-2	16	58
1750	-2	18	57
1810	0	20	53
1835	+4	18	56
1855	-6	17	51
1930	+2	19	60
1955	+1	15	60
2015	+2	16	58

Product specific gravities. (60°F/60°F.)

Time	Re-run feed	Kerosine	Light gas oil	Heavy gas oil	Residue
1010	0.6866	0.7877	0.8387	0.8769	0.9629
1100	0.6870	0.7841	0.8373	0.8764	0.9646
1145	0.6874	0.7857	0.8392	0.8776	0.9631
1230	0.6876	0.7856	0.8387	0.8779	0.9663
1355	0.6878	0.7854	0.8380	0.8780	0.9669
1408	0.6888	0.7908	0.8378	0.8779	0.9661
1420	0.6910	0.7967	0.8393	0.8786	0.9651
1435	0.6926	0.7957	0.8457	0.8697	0.9663
1450	0.6938	0.7982	0.8478	0.9039	0.9673
1510	0.6945	0.7922	0.8494	0.9135	0.9642
1530	0.6926	0.7898	0.8453	0.9029	0.9664
1550	0.6922	0.7894	0.8435	0.8886	0.9652
1610	0.6918	0.7894	0.8429	0.8857	0.9643
1635	0.6910	0.7887	0.8424	0.8844	0.9643
1655	0.6907	0.7897	0.8418	0.8826	0.9642
1750	0.6918	0.7908	0.8433	0.8848	0.9640
1810	0.6920	0.7904	0.8437	0.8849	0.9642
1835	0.6916	0.7882	0.8427	0.8854	0.9642
1855	0.6920	0.7900	0.8423	0.8833	0.9662
1930	0.6928	0.7914	0.8427	0.8834	0.9674
1955	0.6908	0.7888	0.8423	0.8850	0.9668
2015	0.6915	0.7906	0.8426	0.8840	0.9678

A4.3 Results for run TR4.

A4.3.1 Run TR4 temperature indicator readings.

(Step change input at 1602 hrs.)

Time	1310	1327	1350	1428	1439	1450	1510	1525	1540	1554	1603	1604
T18	650	648	650	650	648	648	651	649	650	649	649	649
T19	610	610	608	612	606	614	612	610	611	612	612	612
T20	528	528	528	529	526	532	530	528	528	530	529	528
T21	395	394	394	395	394	397	395	394	395	394	395	395
T22	326	326	326	327	326	325	328	327	328	326	327	328
T23	350	350	350	350	350	350	350	350	350	350	350	350
T24	503	502	502	504	501	505	504	502	502	503	504	503
T25	321	318	320	321	320	320	319	318	319	319	319	319
T26	236	235	235	236	237	235	236	236	236	236	236	236
T27	109	110	110	110	110	110	110	110	110	110	110	110
T28	206	204	205	206	206	206	206	206	206	207	206	206
T46	659	660	659	660	660	659	660	659	659	660	660	660
T47	660	661	659	661	663	662	661	662	661	660	662	662
T48	658	660	658	661	649	670	659	661	660	660	661	661
T49	654	656	655	657	653	660	657	658	656	655	658	658
T50	269	268	268	269	268	269	268	268	268	268	268	269
T71	855	853	856	845	840	842	844	844	845	842		845
T72	857	858	858	849	849	850	849	848	850	848		849
TA1	294	292	291	294	294	296	293	294	294	292		295
TA2	317	317	316	317	317	318	316	316	317	316		317
TA3	316	315	315	317	315	315	316	316	316	315		316
TA4	315	314	314	315	313	314	314	314	314	314		315
TA5	352	352	352	353	351	353	353	352	353	352		353
TA6	376	376	376	378	376	379	376	376	377	376		378
TA7	410	410	409	412	410	414	411	410	410			412
TA8	459	458	457	460	457	460	459	459	458			459
TA9	461	460	460	462	458	463	461	460	462			462
TA10	527	527	526	528	526	530	528	528	526			526
TA11	545	546	544	547	545	550	546	546	546			494
TA12	616	616	614	616	615	621	616	616	616			615
TA13	647	648	646	649	647	652	648	649	647			648
TA14	649	650	648	649	648	652	648	650	648			650
TA15	291	291	291	291	291	291	292	292	292			293
TA16	102	99	102	112	114	118	126	130	133			135
TA17	364	364	363	365	364	368	364	363	364			364
TA18	319	319	317	320	319	322	321	319	321			321
TA19	514	514	513	515	514	517	514	514	514			513
TA20	590	590	588	591	588	591	592	591	591			590

Time	1611	1619	1628	1638	1650	1658	1708	1719	1732	1747	1827	1839
T18	650	649	649	649	647	647	648	647	649	648	648	650
T19	608	605	605	601	600	600	600	603	603	603	602	604
T20	526	526	526	525	524	524	525	526	526	527	526	528
T21	396	395	396	395	393	394	395	396	395	396	395	398
T22	328	328	327	327	326	326	326	326	327	326	327	329
T23	350	350	350	351	350	350	350	350	351	350	351	352
T24	502	502	502	501	500	500	500	502	502	502	502	503
T25	318	318	320	321	318	318	318	318	318	318	321	320
T26	237	237	238	238	238	238	238	237	238	237	237	238
T27	110	110	110	110	110	110	110	111	111	111	111	111
T28	206	206	209	208	206	206	206	206	206	206	207	206
T46	660	659	661	659	659	660	658	659	658	658	660	660
T47	661	659	664	660	660	660	659	664	661	661	662	664
T48	661	659	662	660	659	660	658	663	660	661	665	664
T49	656	656	660	656	655	656	654	658	655	656	658	659
T50	268	268	270	268	268	268	268	269	268	268	269	269
T71	844	843	843	842	840	840	840	840	840	840	845	846
T72	848	848	850	846	847	846	845	846	846	846	850	851
TA1	296	295	293	291	294	294	294	294	294	295	292	296
TA2	318	317	318	318	318	317	317	317	317	318	317	318
TA3	316	316	318	317	316	316	316	316	316	317	317	317
TA4	315	315	316	316	315	314	314	314	315	316	315	316
TA5	354	353	354	353	352	353	353	353	354	353	355	354
TA6	378	378	379	378	376	377	377	378	378	378	378	378
TA7	413	412	414	412	410	411	411	412	413	412	414	413
TA8	459	459	460	459	457	457	458	459	459	459	461	460
TA9	461	461	463	461	460	460	460	460	460	460	462	461
TA10	526	524	526	524	523	524	523	525	524	524	526	525
TA11	542	540	542	539	536	538	538	540	539	540	542	540
TA12	612	610	611	607	606	606	606	609	608	608	610	610
TA13	646	645	646	644	643	643	642	644	642	644	647	646
TA14	650	650	651	650	650	650	648	651	648	651	652	652
TA15	293	293	292	292	292	288	292	292				
TA16	135	136	130	122	116	111						
TA17	365	364	366	363	362	364	365	366	366	365	367	366
TA18	322	322	322	320	319	319	320	322	322	322	322	323
TA19	512	512	513	510	509	510	510	511	510	511	512	512
TA20	590	588	586	583	581	580	581	581	582	582	581	584

Time	1900	1910	1920	1930
T18	650	649	650	649
T19	604	603	603	602
T20	527	526	526	526
T21	396	395	395	395
T22	328	328	328	328
T23	351	351	351	351
T24	504	502	502	502
T25	319	318	318	318
T26	238	237	237	237
T27	110	110	110	110
T28	207	207	207	206
T46	660	660	659	659
T47	662	662	662	662
T48	661	662	659	658
T49	657	658	656	656
T50	268	268	268	268
T71	848	848	844	844
T72	852	852	851	851
TA1	293	293	296	293
TA2	317	318	318	317
TA3	316	317	316	314
TA4	315	316	316	314
TA5	354	354	354	354
TA6	378	378	377	377
TA7	412	412	411	411
TA8	460	460	459	459
TA9	460	462	460	460
TA10	524	525	524	524
TA11	539	540	538	538
TA12	608	609	607	606
TA13	644	645	643	643
TA14	650	650	650	650
TA15				
TA16				
TA17	365	366	364	364
TA18	323	322	321	322
TA19	511	512	510	510
TA20	584	584	584	584

A4.3.2 Run TR4 chart readings.

Time	1315	1333	1357	1434	1446	1452	1520	1532	1546	1558	1609	1616
C13	843	843	843	840	840	839	840	840	840	840	840	840
C14	840	839	842	838	835	834	834	835	836	835	835	834
C15	842	840	842	840	839	839	839	839	839	839	839	839
C16	669	669	668	669	669	669	668	669	669	669	669	668
C17	660	660	659	660	660	660	660	660	660	660	660	660
C18	646	648	646	640	649	655	645	647	646	648	648	648
C19	262	262	263	262	261	262	262	261	262	262	262	262
C21	26.0	25.9	25.9	25.9	25.6	25.8	25.7	25.9	25.9	25.9	25.8	25.7
C22	500	500	500	515	500	510	505	505	500	500	502	510
C23	695	693	660	660	660	705	665	620	630	660	650	650
C36	540	540	540	540	540	540	540	540	540	540	540	540
C37	515	515	515	515	515	515	515	515	515	515	515	515
C38	790	790	788	795	789	791	790	790	790	790	792	792
C39	812	804	800	817	785	795	805	806	805	800	820	820
C42	402	402	402	402	402	402	402	402	402	402	402	402
C43	755	754	755	755	755	755	755	755	755	755	678	678
C44	530	530	530	530	530	530	530	530	530	530	530	530

Time	1625	1638	1645	1706	1715	1725	1740	1756	1807	1833	1845	1855
C13	840	840	840	840	840	840	840	840	840	840	840	840
C14	835	835	835	835	835	835	835	836	836	835	834	835
C15	840	840	840	840	839	838	839	838	839	839	839	839
C16	669	668	668	669	668	669						
C17	660	660	659	659	659	660						
C18	648	648	648	647	647	649						
C19	262	262	262	262	262	262	262	262	261	262	262	261
C21	25.8.	26.0	26.0	26.0	25.9	25.9	25.9	25.9	25.9	25.8	25.8	25.8
C22	502	508	511	505	500	505	500	505	508	510	515	510
C23	660	694	690	697	695	695	700	700	695	705	700	700
C36	540	540	540	540	540	540	540	540	540	540	543	543
C37	515	515	515	515	515	515	515	515	515	515	515	515
C38	790	790	790	795	790	790	790	792	792	790	792	792
C39	820	820	820	830	810	815	812	820	822	815	821	820
C42	402	402	402	402	403	403	403	403	403	403	403	403
C43	675	670	676	676	676	676	676	670	676	676	676	676
C44	530	530	530	530	530	530	530	530	530	530	530	530

Time	1907	1917	1927
C13	840	840	840
C14	835	835	835
C15	838	839	839
C19	262	262	262
C21	25.8	25.8	25.9
C22	515	511	510
C23	700	700	700

Time	1907	1917	1927
C36	543	543	543
C37	515	515	515
C38	792	790	791
C39	820	820	824
C42	403	403	403
C43	676	676	676
C44	530	530	530

A4.4 Run TR5 results.

A4.4.1 Run TR5 temperature indicator readings.

(Step changes in at 0923 hrs., 1010 hrs. and 1045 hrs.)

Time	0853	0908	0918	0926	0930	0940	0949	0958	1016	1028	1040	1050
T18	644	645	646	645	646	645	645	645	644	644	644	643
T19	606	606	606	604	601	598	599	599	596	594	596	594
T20	535	534	535	533	531	529	528	528	525	524	524	523
T21	402	403	404	399	395	393	397	396	392	392	393	391
T23	356	356	356	356	355	354	354	354	352	352	352	352
T24	509	510	510	508	507	505	504	504	502	501	501	500
T25	319	320	320	320	319	318	316	318	315	314	314	313
T26	252	253	253	253	252	253	251	252	252	252	252	252
T27	106	107	107	108	107	107	107	107	108	108	108	108
T46	655	656	656	656	656	655	655	655	655	655	655	656
T47	654	656	654	656	656	657	656	659	657	655	654	654
T48	656	656	655	656	656	657	656	655	656	655	654	654
T49	651	652	652	652	652	654	652	653	652	652	652	652
T50	276	276	276	269	270	271	269	269	266	265	265	263
T71	765						770			758		
T72	830						830			830		
TA1	304	300	300	295	294	295	295	294	291	291	294	288
TA2	324	325			322	322	321	321	320	319	318	317
TA3	320	322			320	320	321	320	320	319	318	317
TA4	320	321			320	320	320	320	319	318	318	317
TA5	358	358			357	356	356	356	354	352	352	351
TA6	378	378			374	375	375	374	372	372	371	370
TA7	417	418			408		410	409	406	406	406	403
TA8	464	464			462		460	460	458	457	456	455
TA9	456	456			454		453	453	452	450	450	450
TA10	530	530			525		523	523	522	520	519	518
TA11	542	543			535		534	534	531	530	529	528
TA12	613	613			606		605	605	603	602	602	600
TA13	646	648			644		642	644	642	642	642	640
TA14	646	648			647		646	646	646	645	646	645
TA17	385	385			376		377	377	374	373	374	370
TA18	347	347			340		340	339	337	336	336	335
TA19	522	522			517		515	514	512	511	511	509
TA20	596	596			589		588	588	586	585	583	583

Time	1057	1111	1120	1133	1143	1206	1229	1240
T18	644	644	644	643	644	644	644	644
T19	592	594	594	594	596	596	597	597
T20	522	522	523	523	524	526	525	524
T21	389	390	392	392	392	393	392	392
T23	350	350	350	350	349	349	348	348
T24	499	499	499	500	500	501	500	500
T25	312	313	313	313	313	314	315	314
T26	252	252	252	252	252	253	251	252
T27	108	108	108	109	109	109	109	109
T46	656	655	655	654	656	655	656	656
T47	655	653	655	654	656	655	657	656
T48	654	653	655	654	656	656	654	656
T49	652	650	652	650	652	652	652	651
T50	262	265	264	264	264	265	263	264
T71	770			770	770	770	770	770
T72	830			830	830	830	830	830
TA1	290	288	288	292	288	292	291	288
TA2	317	317	317	317	317	317	316	316
TA3	317	317	317	317	317	317	316	316
TA4	317	317	317	316	316	316	316	316
TA5	350	350	350	350	349	350	349	349
TA6	369	370	369	370	370	370	368	369
TA7	403	405	403	407	406	408	406	406
TA8	455	455	454	455	456	456	456	456
TA9	449	450	449	450	450	450	450	451
TA10	518	518	517	518	519	520	520	520
TA11	528	528	527	530	531	532	531	531
TA12	600	600	600	602	603	603	603	603
TA13	641	640	641	642	643	642	642	643
TA14	645	644	645	644	646	644	645	645
TA17	369	373	373	374	374	375	372	374
TA18	333	335	334	336	336	337	336	336
TA19	509	509	508	510	511	512	511	511
TA20	582	583	584	585	586	587	587	586

A4.4.2 <u>Run TR5 chart readings.</u>

Time	0858	0920	0923	0929	0936	0943	0954	1004	1012	1021	1034	1047
C13	885	885		885	885	885	885	885	885	885	885	885
C14	880	881		881	880	880	880	883	882	880	880	882
C15	875	875		875	874	873	875	875	875	875	873	873
C19	267	268		261	262	262	262	262	260	258	258	259
C21	23.3	23.2		23.1	23.2	23.1	23.0	23.0	23.1	23.1	23.1	23.1
C22	465	478	510	510	510	508	510	510	512	523	522	540
C23	752	750	750	750	750	750	750	750	750	750	740	700
C36	585		585	585	585	585	585	585	585	585	585	585
C37	575		575	575	575	575	575	578	575	575	575	575
C38	730		730	730	740	730	735	730	730	735	735	730
C39	830		830	830	845	845	844	845	845	845	850	850
C42	463		463	463	463	463	463	463	463	463	460	462
C43	693		693	693	693	693	695	695	693	693	693	693
C44	657		655	655	655	655	657	657	658	658	657	657

Time	1055	1103	1115	1126	1138	1148	1211	1221	1233
C13	885	885	885	885	885	885	885	885	885
C14	880	880	880	880	883	882	880	885	882
C15	873	874	872	875	874	874	872	874	875
C19	256	256	258	258	257	257	258	256	256
C21	23.2	23.2	23.2	23.2	23.3	23.3	23.1	23.1	23.1
C22	537	536	535	535	535	535	535	536	540
C23	705	705	680	680	690	680	685	685	685
C36	585	585	585	585	585	585	585	585	585
C37	575	575	575	575	575	575	575	575	575
C38	735	730	730	730	730	730	730	730	730
C39	855	856	857	858	852	852	852	851	860
C42	462	475	470	460	470	468	468	470	470
C43	693	693	693	693	693	693	693	693	693
C44	657	657	655	650	655	655	654	655	655

APPENDIX 5. TABULATED RESULTS AND COMPUTER PROGRAM LISTING FOR THE SINGLE SIEVE PLATE EXPERIMENTS.

A5.1 The dimensions of the unit.

Hole diameter	0.125 ins.
Perforated area	0.5625 ft .
Length of plate	5.0 ft.
Width of plate	1.5 ft.
Bubbling area	7.5 ft .
Downcomer area	1.125 ft .
Weir height	0.135 ft.
Area of exit pipe	0.0218 ft .

A5.2.1 Conversion of air rate (inches water gauge) to air rate (lb/sec.)

Inches water gauge	Volumetric flowrate (ft /sec.)	Mass flowrate (lb/sec.)
0.75	19.5	1.412
1.4	27.5	2.194
3.5	41.7	3.38
4.5	48.0	3.88
6.0	55.5	4.43
7.0	59.8	4.78
8.0	64.0	5.17

A5.2.2 Experimental values for tray hold up at various air and water rates.

Liquid rate	Air rate (ft /sec.) 27.2	42.0	48.0	55.0	60.0	64.0
400	49.66	56.16	71.66	57.66	101.6	141.2
800	61.40	69.90	84.90	71.40	118.9	157.9
1200	69.85	77.85	94.35	72.85	130.4	165.9
1600	76.20	85.20	101.7	92.20	141.2	172.7
2000	81.38	91.38	110.4	103.9	150.9	180.4
2400	86.40	95.90	114.9	108.9	155.9	184.4

A5.3 Liquid step-change results obtained by experiment.

A5.3.1 Liquid step-change from 1.11 to 5.55 lb/sec.

(Air rate 3.38 lb/sec.)

T (sec)	H (ft.)	WM (lb)	WT (lb)	WL (lb)
0	0.412	0.0	0.0	0.0
5	0.388	20.0	2.34	17.7
10	0.296	37.0	10.9	26.1
15	0.204	43.0	19.6	24.4
20	0.146	47.0	25.0	22.0
25	0.112	50.0	29.2	20.8
30	0.0875	51.0	30.5	20.5
35	0.0782	52.0	31.6	20.4
40	0.0710	52.0	32.0	20.0

(These figures correspond to Fig. 6-1.)

A5.3.2 Liquid step-change from 1.11 to 4.44 lb/sec.

(Air rate 3.38 lb/sec.)

T (sec)	H (Ft.)	WM (lb)	WT (lb)	WL (lb)
0	0.0375	0.0	0.0	0.0
5	0.0780	17.0	3.12	13.9
10	0.154	28.0	10.9	17.1
15	0.188	31.0	14.1	16.9
20	0.215	33.0	20.2	12.8
25	0.229	34.5	21.5	13.0
30	0.235	34.9	22.1	12.8
35	0.239	35.0	22.4	12.6
40	0.240	35.0	22.5	12.5

A5.3.3 <u>Liquid step-change from 5.55 to 1.66 lb/sec.</u>

(Air rate 4.78 lb/sec.)

T (sec)	H (ft.)	WM (lb)	WT (lb)	WL (lb)
0	0.412	0.0	0.0	0.0
5	0.404	15.5	7.98	7.52
10	0.296	33.5	10.95	22.55
15	0.196	42.5	20.15	22.35
20	0.146	44.0	24.8	18.15
25	0.112	45.5	28.2	17.3
30	0.0875	47.0	30.5	16.5
35	0.0792	48.5	31.3	17.2
40	0.0792	48.5	31.3	17.2

A5.3.4 <u>Liquid step-change from 2.22 to 6.66 lb/sec.</u>

(Air rate 4.78 lb/sec.)

T (sec)	H (ft.)	WM (lb)	WT (lb)	WL (lb)
0	0.0375	0	0	0
5	0.0541	25.5	1.56	23.9
10	0.0958	35.5	5.46	30.0
15	0.154	39.5	10.9	28.6
20	0.212	40.5	16.4	24.1
25	0.246	43.5	19.6	23.9
30	0.362	45.5	30.4	15.1
35	0.379	46.0	31.0	15.0
40	0.396	47.0	33.6	13.4
45	0.412	47.5	35.2	12.3
50	0.412	48.0	35.9	12.1

A5.4 <u>Vapour rate step-change results obtained by experiment.</u>

A5.4.1 <u>Vapour rate step-change from 2.40 to 6.52 lb/sec.</u>

(Liquid rate 4.44 lb/sec.)

T (sec)	H (ft.)	WM (lb)	WT (lb)	WL (lb)
0	0.129	0	0	0
5	0.138	3	0.797	2.203
10	0.142	6	1.18	4.82
15	0.142	8	1.18	6.82
20	0.1416	9	1.18	7.82

(These results correspond to Fig. 6-2.)

A5.4.2 Vapour rate step-change from 5.24 to 2.04 lb/sec.

(Liquid rate 4.44 lb/sec.)

T (sec)	H (ft.)	WM (lb)	WT (lb)	WL (lb)
0	0.138	0	0	0
5	0.129	0.50	0.078	0.42
10	0.129	4.50	0.078	4.42
15	0.129	5.50	0.078	5.42
20	0.129	6.0	0.078	5.92

A5.5 Predictions of the mathematical model.

A5.5.1 The computer program.

```
/---PROGRAM SIVMOD TO SIMULATE THE DYNAMIC BEHAVIOUR OF
/---THE DEPARTMENTAL SIEVE TRAY UNIT.   R.M.NEALE JAN 1970
/
REAL L1,L2,L20,L2Z,L3,L3Z
PAUSE
/
/---WRITE OUT TITLE AND USER LABEL.
/
2 WRITE(7,1)
READ(1,3) Z1, Z2, Z3*
WRITE(7,3) Z1, Z2, Z3*
/
/---READ DATA AND OUTPUT DATA CHECK.
/
*
READ(1,4) Z1,L1, Z2,L20, Z3,V, Z4,DELV
WRITE(7,4) Z1,L1, Z2,L20, Z3,V, Z4,DELV

READ(1,4) Z1, AT, Z2, AP, Z3, AV, Z4, HW
WRITE(7,4) Z1, AT, Z2, AP, Z3, AV, Z4, HW

/

READ(1,4) Z1, AX, Z2, AE, Z3, DL, Z4, DV
WRITE(7,4) Z1, AX, Z2, AE, Z3, DL, Z4, DV

READ(1,4) Z1, C1, Z2, C2, Z3, C3, Z4, C4
WRITE(7,4) Z1, C1, Z2, C2, Z3, C3, Z4, C4

/

READ(1,4) Z1, C5, Z2, C6, Z3, C7, Z4, DELT
WRITE(7,4) Z1, C5, Z2, C6, Z3, C7, Z4, DELT

READ(1,4) Z1, TMAX, Z2, TITST
WRITE(7,4) Z1, TMAX, Z2, TITST

TITST = TITST/DELT
 ITST= IFIX(TITST)
```

```
L3 = L20
/
/---COMPUTE EQUIVALENT L20 FOR DELV
/
HF = C2*(V+DELV) + C3*L1 + C4*HW + C5*(V+DELV)**2 + C6

IF(HF.LT.HW) HF=HW+0.01
FD = L20/(C1*AV*DL*(HF-HW)**1.5)

IF((ABS(DELV)-0.0001).LT.0.0)GO TO 5
HF1 = C2*V + C3*L1 + C4*HW + C5*V**2 + C6

FD1 = L20/(C1*AV*DL*(HF1-HW)****1.5)
FD = FD1*HF1/HF

L20 = C1*AV*FD*DL*(HF-HW)**1.5

/
/---COMPUTE THE LIQUID TRANSIENT
/

5 XJ = TMAX**/DELT + 0.5
J = IFIX(XJ)
TSUM = 0.0

/

E2 = AT*HF/(C1*AV*(HF-HW)**1.5)
HL = ((L3/(C7*DL*AE))**2)/(2.0*32.2)

L2 = L20
WT = AX*DL*HL

WL = HF*AT*DL*FD
WM1 = WT + WL

E3 = C7*DL*AE*SQRT(64.4)
/
WRITE(7,9)

WRITE(7,10)
10 FORMAT(51H   T      L2      L3      WL      WT      FD      HF      HL/)
*****
WRITE(7,7) TSUM,L2,L3,WL,WT,FD,HF,HL

ITS = 0

/
DO 6 I=1,J
/
/---CALCULATION OF THE TRANSIENT FOR THE PLATE
/
```

```
TSUM = TSUM + DELT
L2Z = L2
L3Z = L3
HLZ = HL
WTZ = WT

/
L2 = L1-(L1-L20)*EXP(-TSUM/E2)
FD = L2/(C1*AV*DL*(HF-HW)**1.5)

WL = FD*DL*AT*HF
/
/---AND FOR THE END TANK
/

HL = HLZ + (L2Z-E3*SQRT(HL))*DELT/(AX*DL)
L3 = E3*SQRT(HL)

WT = WTZ + (0.5*(L2Z+L2) - 0.5*(L3Z+L3))*DELT

/
/---OUTPUT RESULT
/

ITS = ITS + 1
IF(ITS.LT.ITST)GO TO 6
ITS = 0
WM = WM1 - WT - WL

WRITE(7,7) TSUM,L2,L3,WL,WT,FD,HF,HL,WM
6 CONTINUE
/

READ(1,8) ITRIG
IF(ITRIG.LT.0) STOP

GO TO 2

1 FORMAT(54HMATHEMATICAL MODEL OF HYDRODYNAMICS OF SIEVE TRAY UNIT/)

3 FORMAT(3A8)

4 FORMAT(A8,F12.6,5X,A8,F12.6/A8,F12.6,5X,A8,F12.6)

7 FORMAT(F5.1,2F7.3,2F7.3,3F7.4,F9.3)

9 FORMAT(18HTRANSIENT RESPONSE/)

8 FORMAT(I3)

END
*****************************
```

A5.5.2 Sample data.

SIVMOD TEST RUN 1 (Title)

L1	1.11	L20	1.11
V	2.40	DELV	4.12
AT	7.50	AP	0.5625
AV	1.50	HW	0.135
AX	1.50	AF	0.02182
DL	62.4	DV	0.0808
C1	3.38	C2	0.0122
C3	0.098	C4	0.999
C5	0.00	Co	0.200
C7	0.80	DELT	0.500
TMAX	40.0	TSTEP	2.00

A5.5.3 Sample results for this data.

T (sec)	WL (lb)	T (sec)	WL (lb)	T (sec)	WL (lb)	T (sec)	WL (lb)
0	4.404	10	20.61	20	21.91	30	22.01
2	11.38	12	21.17	22	21.95	40	22.02
4	15.60	14	21.51	24	21.98		
6	18.14	16	21.71	26	22.00		
8	19.68	18	21.83	28	22.01		

A5.5.4 Predicted results for a vapour rate step-change from 2.40 to 6.52 lb/sec.

(Liquid rate 1.11 lb/sec.)

T (sec)	WL (lb)
0	5.242
2	4.94
4	4.76
6	4.64
8	4.58
10	4.53
30	4.47

A5.5.5 Predicted results for a liquid rate step-change from 1.11 to 4.44 lb/sec.

(Vapour rate 3.38 lb/sec.)

T (sec)	WL (lb)	T (sec)	WL (lb)
0	4.54	12	17.4
2	9.81	14	17.7
4	13.0	16	17.9
6	15.0	18	18.0
8	16.2	20	18.1
10	17.0	22	18.1

APPENDIX 6. STEADY STATE RESULTS AND SYSTEM MATRIX FOR THE MODEL OF A THREE COMPONENT TEN PLATE DISTILLATION UNIT.

A6.1 Steady state results.

Feed composition vector = (0.30, 0.40, 0.30)

Plate	x	x	x	y	y	y	K	K	K
0	0.7337E0	0.2657E0	0.5214E-3						
1	0.4824E0	0.5142E0	0.3426E-2	0.7337E0	0.2657E0	0.5214E-3	0.1521E1	0.5168E0	0.1522E0
2	0.3416E0	0.6474E0	0.1092E-1	0.5966E0	0.4013E0	0.2106E-2	0.1746E1	0.6198E0	0.1928E0
3	0.2708E0	0.6949E0	0.2836E-1	0.5199E0	0.4739E0	0.6194E-2	0.1878E1	0.6821E0	0.2184E0
4	0.2459E0	0.6879E0	0.6623E-1	0.4845E0	0.4998E0	0.1571E-1	0.1971E1	0.7266E0	0.2371E0
5	0.2247E0	0.6356E0	0.1397E0	0.4676E0	0.4960E0	0.3636E-1	0.2081E1	0.7804E0	0.2603E0
6	0.2027E0	0.5404E0	0.2569E0	0.4561E0	0.4675E0	0.7644E-1	0.2250E1	0.8650E0	0.2976E0
7	0.1366E0	0.5967E0	0.2667E0	0.3335E0	0.5751E0	0.9136E-1	0.2443E1	0.9638E0	0.3425E0
8	0.8496E-1	0.6349E0	0.2801E0	0.2223E0	0.6698E0	0.1079E0	0.2616E1	0.1055E1	0.3853E0
9	0.4887E-1	0.6447E0	0.3064E0	0.1355E0	0.7341E0	0.1304E0	0.2773E1	0.1139E1	0.4256E0
10	0.2532E-1	0.6064E0	0.3683E0	0.7479E-1	0.7505E0	0.1747E0	0.2954E1	0.1238E1	0.4743E0
B	0.1084E-1	0.4895E0	0.4997E0	0.3519E-1	0.6861E0	0.2787E0	0.3247E1	0.1402E1	0.5578E0

Feed composition vector = (0.35, 0.35, 0.30)

Plate	x	x	x	y	y	y	K	K	K
0	0.8505E0	0.1493E0	0.1693E-3						
1	0.6479E0	0.3507E0	0.1431E-2	0.8505E0	0.1493E0	0.1693E-3	0.1313E1	0.4257E0	0.1183E0
2	0.4892E0	0.5051E0	0.5689E-2	0.7400E0	0.2592E0	0.8576E-3	0.1513E1	0.5130E0	0.1508E0
3	0.3923E0	0.5898E0	0.1789E-1	0.6534E0	0.3434E0	0.3180E-2	0.1665E1	0.5823E0	0.1778E0
4	0.3375E0	0.6131E0	0.4938E-1	0.6006E0	0.3896E0	0.9835E-2	0.1780E1	0.6354E0	0.1991E0
5	0.2997E0	0.5794E0	0.1208E0	0.5707E0	0.4023E0	0.2701E-1	0.1904E1	0.6943E0	0.2235E0
6	0.2624E0	0.4872E0	0.2504E0	0.5501E0	0.3839E0	0.6599E-1	0.2096E1	0.7880E0	0.2636E0
7	0.1875E0	0.5516E0	0.2609E0	0.4303E0	0.4895E0	0.8027E-1	0.2294E1	0.8875E0	0.3077E0
8	0.1219E0	0.6026E0	0.2755E0	0.3043E0	0.5978E0	0.9796E-1	0.2497E1	0.9919E0	0.3556E0
9	0.7207E-1	0.6249E0	0.3031E0	0.1939E0	0.6837E0	0.1225E0	0.2690E1	0.1094E1	0.4040E0
10	0.3790E-1	0.5956E0	0.3665E0	0.1101E0	0.7210E0	0.1689E0	0.2905E1	0.1211E1	0.4609E0
B	0.1632E-1	0.4838E0	0.4999E0	0.5261E-1	0.6719E0	0.2755E0	0.3224E1	0.1389E1	0.5511E0

(Note: 0.36E-2 denotes 0.36 x 10^{-2} etc.)

A6.2 The System Matrix.

ROW = 1	-0.3666600000E 01	0.0000000000E 00	0.0000000000E 00	0.1484940000E 01	-0.1390360000E 01
	-0.4094800000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 2	0.0000000000E 00	-0.3666600000E 01	0.0000000000E 00	-0.1482020000E 01	0.1391360000E 01
	-0.1433000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 3	0.0000000000E 00	0.0000000000E 00	-0.3666600000E 01	-0.2908000000E-02	-0.9880800000E-03
	0.5577600000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 4	0.3333333333E 02	0.0000000000E 00	0.0000000000E 00	-0.5808233333E 02	0.2317266667E 02
	0.6824666667E 01	0.4305566667E 02	-0.2259966667E 02	-0.7030000000E 01	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				

ROW = 5	0.0000000000E 00	0.3333333333E 02	0.0000000000E 00	0.2470033333E 02	-0.5652266667E 02
	0.2471666667E 01	-0.4283066667E 02	0.2267933333E 02	-0.4729666667E 01	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 6	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02	0.4846666667E-01	0.1646800000E-01
	-0.4262933333E 02	-0.2247300000E 00	-0.7977666667E-01	0.1175966667E 02	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 7	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02	0.0000000000E 00
	0.0000000000E 00	-0.7638900000E 02	0.2259966667E 02	0.7030000000E 01	0.5510633333E 02
	-0.2166733333E 02	-0.6937666667E 01	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 8	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02
	0.0000000000E 00	0.4283066667E 02	-0.5601266667E 02	0.4729666667E 01	-0.5439566667E 02
	0.2192566667E 02	-0.6326000000E 01	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				

ROW = 9	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.3333333333E 02	0.2247300000E 00	0.7977666667E-01	-0.4509300000E 02	-0.7108000000E 00
	-0.2581700000E 00	0.1326366667E 02	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 10	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.3333333333E 02	0.0000000000E 00	0.0000000000E 00	-0.8843966667E 02
	0.2166733333E 02	0.6937666667E 01	0.6206966667E 02	-0.2151200000E 02	-0.7019666667E 01
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 11	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02	0.0000000000E 00	0.5439566667E 02
	-0.5525900000E 02	0.6326000000E 01	-0.6017900000E 02	0.2220900000E 02	-0.7239333333E 01
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 12	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02	0.7108000000E 00
	0.2581700000E 00	-0.4659700000E 02	-0.1890666667E 01	-0.6969666667E 00	0.1425866667E 02
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				

ROW = 13	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02
	0.0000000000E 00	0.0000000000E 00	-0.9540300000E 02	0.2151200000E 02	0.7019666667E 01
	0.6770533333E 02	-0.2230066667E 02	-0.7438333333E 01	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 14	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.3333333333E 02	0.0000000000E 00	0.6017900000E 02	-0.5554233333E 02	0.7239333333E 01
	-0.6308066667E 02	0.2403466667E 02	-0.7890333333E 01	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 15	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.3333333333E 02	0.1890666667E 01	0.6969666667E 00	-0.4759200000E 02
	-0.4624666667E 01	-0.1734233333E 01	0.1532866667E 02	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 16	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02	0.0000000000E 00	0.0000000000E 00
	-0.1010786667E 03	0.2230066667E 02	0.7438333333E 01	0.7477900000E 02	-0.2407066667E 02
	-0.8281763333E 01	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				

ROW = 17	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02	0.0000000000E 00
	0.6308066667E 02	-0.5736800000E 02	0.7890333333E 01	-0.6417266667E 02	0.2814800000E 02
	-0.8438000000E 01	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 18	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02
	0.4624666667E 01	0.1734233333E 01	-0.4866200000E 02	-0.1060600000E 02	-0.4077333333E 01
	0.1074933333E 02	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 19	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.1081066667E 02	0.0000000000E 00	0.0000000000E 00	-0.5758933333E 02	0.7819333333E 01
	0.2690200000E 01	0.3225866667E 02	-0.6372666667E 01	-0.2264600000E 01	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 20	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.1081066667E 02	0.0000000000E 00	0.2084633333E 02	-0.4246333333E 02
	0.2757300000E 01	-0.2783733333E 02	0.8117000000E 01	-0.3902666667E 01	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				

ROW = 21	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.1081066667E 02	0.3409666667E 01	0.1310810000E 01
	-0.3078066667E 02	-0.4421333333E 01	-0.1744333333E 01	0.6167333333E 01	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 22	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02	0.0000000000E 00
	0.0000000000E 00	-0.6559200000E 02	0.6372666667E 01	0.2264600000E 01	0.4032466667E 02
	-0.4647333333E 01	-0.1697266667E 01	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 23	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02
	0.0000000000E 00	0.2783733333E 02	-0.4145033333E 02	0.3902666667E 01	-0.3472900000E 02
	0.6904000000E 01	-0.5115000000E 01	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 24	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.3333333333E 02	0.4421333333E 01	0.1744333333E 01	-0.3950066667E 02	-0.5595666667E 01
	-0.2256633333E 01	0.6812333333E 01	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				

ROW = 25	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.3333333333E 02	0.0000000000E 00	0.0000000000E 00	-0.7365800000E 02
	0.4647333333E 01	0.1697266667E 01	0.4750266667E 02	-0.3057800000E 01	-0.1142566667E 01
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 26	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02	0.0000000000E 00	0.3472900000E 02
	-0.4073733333E 02	0.5115000000E 01	-0.4033900000E 02	0.6000333333E 01	-0.6191333333E 01
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 27	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02	0.5595666667E 01
	0.2256633333E 01	-0.4014566667E 02	-0.7163666667E 01	-0.2942433333E 01	0.7333666667E 01
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				
ROW = 28	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.3333333333E 02
	0.0000000000E 00	0.0000000000E 00	-0.8083600000E 02	0.3057800000E 01	0.1142566667E 01
	0.5415800000E 02	-0.1834500000E 01	-0.7028333333E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00				

```
ROW = 29   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.3333333333E 02   0.0000000000E 00   0.4033900000E 02  -0.3933366667E 02   0.6191333333E 01
          -0.4393500000E 02   0.6119000000E 01  -0.7054333333E 01   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00

ROW = 30   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.3333333333E 02   0.7163666667E 01   0.2942333333E 01  -0.4066700000E 02
          -0.1022300000E 02  -0.4284333333E 01   0.7757000000E 01   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00

ROW = 31   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.3333333333E 02   0.0000000000E 00   0.0000000000E 00
          -0.8749133333E 02   0.1834500000E 01   0.7028333333E 00   0.3580533333E 02  -0.5639000000E 01
          -0.2243500000E 01

ROW = 32   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.3333333333E 02   0.0000000000E 00
           0.4393500000E 02  -0.3945233333E 02   0.7054333333E 01  -0.2546333333E 02   0.1010433333E 02
          -0.4374333333E 01
```

```
ROW = 33   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.3333333333E 02
           0.1022300000E 02   0.4284333333E 01  -0.4109033333E 02  -0.1034200000E 02  -0.4465333333E 01
           0.6617666667E 01

ROW = 34   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00

           0.5000000000E 01   0.0000000000E 00   0.0000000000E 00  -0.7397850000E 01   0.8458500000E 00
           0.3363250000E 00

ROW = 35   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.5000000000E 01   0.0000000000E 00   0.3819500000E 01  -0.3542700000E 01
           0.6561500000E 00

ROW = 36   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00   0.0000000000E 00
           0.0000000000E 00   0.0000000000E 00   0.5000000000E 01   0.1551300000E 01   0.6698000000E 00
          -0.3012700000E 01
```

APPENDIX 7. DATA AND RESULTS FOR TRANSFER FUNCTION CALCULATIONS.

A7.1 Data.

The system analysed was that described by the system matrix given in Appendix 6. The initial state vector, x(o), was that given in Chapter 8, section 8.5. No other data is necessary for the computer program of Bosley. Kropholler's program required the denominator polynomial coefficients which were obtained from the intermediate printout of the Bosley program.

A7.2 Numerator polynomial coefficients using the method of Bosley.

These are given overleaf in row order.

BOTTOM ROW OF BUSH MATRIX

```
-0.1050105487E 52   -0.3809739408E 52   -0.6209356714E 52   -0.6045981131E 52
-0.3949589263E 52   -0.1845364702E 52   -0.6428319004E 51   -0.1720558031E 51
-0.3622329299E 50   -0.6114268769E 49   -0.8406781408E 48   -0.9541540600E 47
-0.9039736096E 46   -0.7215944007E 45   -0.4890980047E 44   -0.2832881983E 43
-0.1409365723E 42   -0.6046959099E 40   -0.2244337649E 39   -0.7220894045E 37
-0.2016377275E 36   -0.4888518717E 34   -0.1028419201E 33   -0.1874615832E 31
-0.2953465631E 29   -0.4007483321E 27   -0.4660257225E 25   -0.4614704471E 23
-0.3858496820E 21   -0.2694410287E 19   -0.1548789463E 17   -0.7186753627E 14
-0.2619827523E 12   -0.7208597988E 09   -0.1404607824E 07   -0.1723878717E 04
```

S MATRIX

```
ROW =  1   -0.1143859583E 65    0.5646170939E 62   -0.2787008444E 60    0.1375708401E 58
           -0.6790679402E 55
            0.3356474525E 53   -0.1547608073E 51    0.2820638227E 49    0.2890654185E 48
            0.3420824193E 47

            0.3240697076E 46    0.2504914075E 45    0.1609400761E 44    0.8635525415E 42
            0.3392032089E 41
            0.1479360840E 40    0.4753566383E 38    0.1292305680E 37    0.2970098731E 35
            0.5756517714E 33
            0.9347650029E 31    0.1271471873E 30    0.1425912713E 28    0.1304016074E 26
            0.9547842289E 23
            0.5452204362E 21    0.2334935440E 19    0.7040192381E 16    0.1329936816E 14
            0.1131516442E 11
            0.0000000000E 00    0.0000000000E 00    0.0000000000E 00    0.0000000000E 00
            0.0000000000E 00
            0.0000000000E 00
```

ROW = 2	0.1142510347E 65	-0.5639511027E 62	0.2783721051E 60	-0.1374085700E 58
	0.6782629889E 55			
	-0.3352506519E 53	0.1545995314E 51	-0.2813501778E 49	-0.2881954645E 48
	-0.3410967196E 47			
	-0.3221718343E 46	-0.2498208278E 45	-0.1605252125E 44	-0.8614091534E 42
	-0.3382728680E 41			
	-0.1475954141E 40	-0.4743016497E 38	-0.1289540286E 37	-0.2963967698E 35
	-0.5745049128E 33			
	-0.9349629357E 31	-0.1269108592E 30	-0.1423350615E 28	-0.1301749629E 26
	-0.9531779736E 23			
	-0.5443319612E 21	-0.2331246823E 19	-0.7029400843E 16	-0.1327956727E 14
	-0.1179805827E 11			
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 3	0.1349170931E 62	-0.6659580215E 59	0.3287234107E 57	-0.1622622674E 55
	0.8009125013E 57			
	-0.3967814137E 50	0.1612682927E 48	-0.7136070327E 46	-0.8699072947E 45
	-0.9356468594E 44			
	-0.8978253607E 43	-0.6705439513E 42	-0.4148415310E 41	-0.2143274567E 40
	-0.9302916047E 38			
	-0.3406519287E 37	-0.1054933254E 36	-0.2765249462E 34	-0.6130713193E 32
	-0.1146799049E 31			
	-0.1802063909E 29	-0.2363158740E 27	-0.2561966262E 25	-0.2266328497E 23
	-0.1606173381E 21			
	-0.8884298229E 18	-0.3688430491E 16	-0.1079099427E 14	-0.1979989939E 11
	-0.1710528864E 08			
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 4	0.7220797361E 66	-0.3909739647E 64	0.1929874596E 62	-0.9526059253E 59
	0.4702203843E 57			
	-0.2720998209E 55	0.1148654684E 53	-0.5025099600E 50	0.1354330338E 49
	0.1447394566E 48			
	0.1607839863E 47	0.1448324370E 46	0.1080177454E 45	0.6720821467E 43
	0.3510732544E 42			

	0.1346894803E 41	0.5767670320E 39	0.1822968924E 38	0.4885806379E 36
	0.1109002038E 35			
	0.2126430400E 33	0.3427639642E 31	0.4613494322E 29	0.5135616321E 27
	0.4665733562E 25			
	0.3396204903E 23	0.1929248012E 21	0.8223591573E 18	0.2469212297E 16
	0.4647144467E 13			
	0.4114325263E 10	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 5	-0.7899048194E 66	0.3899448445E 64	-0.1924794810E 62	0.9500935047E 59
	-0.4689326004E 57			
	0.2314390123E 55	-0.1145601379E 53	0.5018170452E 50	-0.1340490650E 49
	-0.1430314718E 48			
	-0.1589334715E 47	-0.1432816229E 46	-0.1069154231E 45	-0.6655533949E 43
	-0.3478295089E 42			
	-0.1533309402E 41	-0.5719542054E 39	-0.1808520471E 38	-0.4849036042E 36
	-0.1101158240E 35			
	-0.2112017683E 33	-0.3405586249E 31	-0.4585334758E 29	-0.5105884146E 27
	-0.4640116147E 25			
	-0.3378521559E 23	-0.1919721559E 21	-0.8185074432E 18	-0.2458238559E 16
	-0.4627536179E 13			
	-0.4098376898E 10	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 6	-0.2081630172E 64	0.1027498016E 62	-0.5071778935E 59	0.2503468021E 57
	-0.1235742891E 55			
	0.6098436292E 52	-0.3048518171E 50	0.6912797515E 47	-0.1382636222E 47
	-0.1706341023E 46			
	-0.1800714019E 45	-0.1549211103E 44	-0.1101145895E 43	-0.6521574652E 41
	-0.3239991691E 40			
	-0.1356966003E 39	-0.4807119721E 37	-0.1443095271E 36	-0.3672492201E 34
	-0.7913834614E 32			
	-0.1440023069E 31	-0.2202476165E 29	-0.2812247925E 27	-0.2969249205E 25
	-0.2558279057E 23			
	-0.1765915665E 21	-0.9513273578E 18	-0.3846326655E 16	-0.1095822500E 14
	-0.1958028009E 11			
	-0.1647456184E 08	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			

ROW = 7	-0.1460462847E 67	0.7208856505E 64	-0.3558309627E 62	0.1756398138E 60
	-0.3649708299E 57			
	0.4279571877E 55	-0.2109195215E 53	0.1115376140E 51	0.7690123447E 48
	0.1831932896E 48			
	0.2055033730E 47	0.1918046763E 46	0.1481584253E 45	0.9561065436E 43
	0.5120133022E 42			
	0.2382585143E 41	0.9285065475E 39	0.3079360789E 38	0.8700999198E 36
	0.2094222422E 35			
	0.4286700024E 33	0.7438861099E 31	0.1089017954E 30	0.1335508352E 28
	0.1358626673E 26			
	0.1151302003E 24	0.7568903617E 21	0.3963011650E 19	0.1561441464E 17
	0.4346205183E 14			
	0.7605727050E 11	0.6282063792E 08	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 8	0.1452309206E 67	-0.7169054497E 64	0.3538663374E 62	-0.1746700780E 60
	0.3621841738E 57			
	-0.4255940981E 55	0.2097638096E 53	-0.1107332065E 51	-0.7332642455E 48
	-0.1730100483E 48			
	-0.1990171674E 47	-0.1868509255E 46	-0.1445237781E 45	-0.9338171172E 43
	-0.5075070317E 42			
	-0.2332812709E 41	-0.9098447906E 39	-0.3020359607E 38	-0.8541956589E 36
	-0.2057081819E 35			
	-0.4215276918E 33	-0.7320437729E 31	-0.1072452466E 30	-0.1316096879E 28
	-0.1339760498E 26			
	-0.1116299689E 24	-0.7473087032E 21	-0.3915155894E 19	-0.1543470600E 17
	-0.4298576067E 14			
	-0.7526430737E 11	-0.6219850821E 08	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			

ROW = 9	0.8062562774E 64	-0.3979668685E 62	0.1964362604E 60	-0.9696111223E 57
	0.4736016009E 55			
	-0.2362773782E 53	0.1155553207E 51	-0.8043940027E 48	-0.3575999567E 47
	-0.5184897812E 46			
	-0.5593130166E 45	-0.4955573535E 44	-0.3636070800E 43	-0.2229867305E 42
	-0.1151138857E 41			
	-0.5029545064E 39	-0.1867064884E 38	-0.5903027446E 36	-0.1591232688E 35
	-0.3655954623E 33			
	-0.7146972533E 31	-0.1184863277E 30	-0.1657432183E 28	-0.1942178727E 26
	-0.1387609849E 24			
	-0.1301105817E 22	-0.9586489481E 19	-0.4787910408E 17	-0.1797927403E 15
	-0.4764938626E 12			
	-0.7930940976E 09	-0.6223704928E 06	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 10	0.1632139862E 67	-0.8056192104E 64	0.3976516764E 62	-0.1962802194E 60
	0.9688382354E 57			
	-0.4782091290E 55	0.2363547836E 53	-0.1094216415E 51	0.1866463775E 49
	0.1045398839E 48			
	0.2203602140E 47	0.2124526789E 46	0.1701016391E 45	0.1140431020E 44
	0.6449039023E 42			
	0.3093400966E 41	0.1263935011E 40	0.4411851680E 38	0.1317775028E 37
	0.3369521283E 35			
	0.7369515225E 33	0.1375659303E 32	0.2183722212E 30	0.2931992178E 28
	0.3304910295E 26			
	0.3095822687E 24	0.2377036544E 22	0.1468047015E 20	0.7100894710E 17
	0.2585822001E 15			
	0.6653686158E 12	0.1076408976E 10	0.8218103668E 06	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 11	-0.1613700040E 67	0.7965174158E 64	-0.3931590809E 62	0.1940626993E 60
	-0.9578926604E 57			
	0.4728072169E 55	-0.2336661002E 53	0.1085921375E 51	-0.1775830258E 49
	-0.1729938031E 48			
	-0.2074612279E 47	-0.2006356148E 46	-0.1611098363E 45	-0.1083048495E 44
	-0.6139671066E 42			

	-0.2951702143E 41	-0.1208570337E 40	-0.4226811572E 38	-0.1264796266E 37
	-0.3239553013E 35			
	-0.7096693102E 33	-0.1326723152E 32	-0.2109079325E 30	-0.2835679455E 28
	-0.3200584182E 26			
	-0.3901929443E 24	-0.2307795115E 22	-0.1426995584E 20	-0.6910397131E 17
	-0.7519319144E 15			
	-0.6439779422E 12	-0.1051035234E 10	-0.8032927449E 06	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 12	-0.1844263802E 65	0.9103184506E 62	-0.4493281550E 60	0.2217858799E 58
	-0.1094774649E 56			
	0.5402737105E 53	-0.2689090576E 51	0.8297044782E 48	-0.9063460278E 47
	-0.1154608326E 47			
	-0.1290693196E 46	-0.1181703870E 45	-0.8991760333E 43	-0.5738206552E 42
	-0.3093645729E 41			
	-0.1416965172E 40	-0.5536351742E 38	-0.1850353792E 37	-0.5297717035E 35
	-0.1799638435E 34			
	-0.2729018803E 32	-0.4893418934E 30	-0.7463977963E 28	-0.9630867464E 26
	-0.1043218169E 25			
	-0.9783957688E 22	-0.6923896395E 20	-0.4105016364E 18	-0.1904928348E 16
	-0.6650167274E 13			
	-0.1639051489E 11	-0.2537372338E 08.	-0.1851778834E 05	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 13	-0.1231428761E 67	0.6078251539E 64	-0.3000183224E 62	0.1480868690E 60
	-0.7309431051E 57			
	0.3607977114E 55	-0.1777942338E 53	0.9476954243E 50	0.8507973077E 48
	0.1939455113E 48			
	0.2322907706E 47	0.2315763524E 46	0.1919177076E 45	0.1334943028E 44
	0.7851035709E 42			
	0.3926874792E 41	0.1677806656E 40	0.6143537147E 38	0.1931753460E 37
	0.5220721529E 35			
	0.1212421703E 34	0.2416083238E 32	0.4120476196E 30	0.5989424343E 28
	0.7377745722E 26			
	0.7641343074E 24	0.6585401094E 22	0.4656614393E 20	0.2650527551E 18
	0.1132225096E 16			
	0.3971306086E 13	0.9427930518E 10	0.1407169764E 08	0.9909971527E 04
	0.0000000000E 00			
	0.0000000000E 00			

ROW = 14	0.1205030773E 67	-0.5947953373E 64	0.2935869300E 62	-0.1449124026E 60
	0.7152763556E 57			
	-0.3530625889E 55	0.1740134931E 53	-0.9205707901E 50	-0.7134373459E 48
	-0.1731622047E 48			
	-0.2084578624E 47	-0.2090216249E 46	-0.1741188096E 45	-0.1216773094E 44
	-0.7186118923E 42			
	-0.3607924308E 41	-0.1546879354E 40	-0.5682012594E 38	-0.1791815033E 37
	-0.4855502439E 35			
	-0.1130414234E 34	-0.2257906814E 32	-0.3859152227E 30	-0.5621199552E 28
	-0.6937332029E 26			
	-0.7199287851E 24	-0.6215715967E 22	-0.4402942708E 20	-0.2510430598E 18
	-0.1121612663E 16			
	-0.3773889246E 13	-0.8973788695E 10	-0.1341532357E 08	-0.9462741974E 04
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 15	0.2639790081E 65	-0.1302980341E 63	0.6431385884E 60	-0.3174463165E 58
	0.1566873363E 56			
	-0.7735114633E 53	0.3780738251E 51	-0.2712428551E 49	-0.1373536945E 48
	-0.2078235175E 47			
	-0.2782072813E 46	-0.2255353025E 45	-0.1779789103E 44	-0.1181628563E 43
	-0.6648749606E 41			
	-0.3188796079E 40	-0.1309184588E 39	-0.4614926734E 37	-0.1390286247E 36
	-0.3651933479E 34			
	-0.3200169135E 32	-0.1581653540E 31	-0.2613058883E 29	-0.3681997006E 27
	-0.4398342583E 25			
	-0.4420271343E 23	-0.3696613981E 21	-0.2536557589E 19	-0.1400883539E 17
	-0.6060969160E 14			
	-0.1974052717E 12	-0.4541248491E 09	-0.6563374680E 06	-0.4472052952E 03
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 16	0.5752034373E 66	-0.2839151736E 64	0.1401376595E 62	-0.6917035435E 59
	0.3414160974E 57			
	-0.1685092279E 55	0.8344949618E 52	-0.3441243381E 50	0.1474514893E 49
	0.1938274330E 48			
	0.2426984246E 47	0.2490470475E 46	0.2130197712E 45	0.1532388057E 44
	0.9340676914E 42			
	0.4853387317E 41	0.2159683201E 40	0.8258779251E 38	0.2720475975E 37
	0.7720373582E 35			

	-0.1894676739E 34	0.4003924935E 32	0.7280960613E 30	0.1135829761E 29
	0.1513330950E 27			
	0.1711659089E 25	0.1630245549E 23	0.1293588614E 21	0.8430684756E 18
	0.4426573550E 16			
	0.1322498073E 14	0.5653936505E 11	0.1240060302E 09	0.1710336303E 06
	0.1113175751E 03			
	0.0000000000E 00			
ROW = 17	-0.5540996009E 66	0.2744813347E 64	-0.1354812344E 62	0.6687201049E 59
	-0.3300718216E 57			
	0.1629115276E 55	-0.8064393909E 52	0.3401135480E 50	-0.1294140987E 49
	-0.1687829366E 48			
	-0.2141803222E 47	-0.2203298821E 46	-0.1396564116E 45	-0.1371956537E 44
	-0.3403387162E 42			
	-0.4735505849E 41	-0.1958906345E 40	-0.7516126545E 38	-0.2483187201E 37
	-0.7973746065E 35			
	-0.1738020375E 34	-0.3680535487E 32	-0.6705400642E 30	-0.1047801242E 29
	-0.1393168195E 27			
	-0.1583391829E 25	-0.1510183065E 23	-0.1199726327E 21	-0.7827539151E 18
	-0.4114153830E 16			
	-0.1695560060E 14	-0.5265241443E 11	-0.1155916160E 09	-0.1595813113E 06
	-0.1039650724E 03			
	0.0000000000E 00			
ROW = 18	-0.1911187225E 65	0.9433410196E 62	-0.4656213488E 60	0.2298239902E 58
	-0.1134376020E 56			
	0.3597645867E 53	-0.2805429470E 51	0.4010655255E 48	-0.1803644659E 48
	-0.2504312353E 47			
	-0.2951642389E 46	-0.2871548089E 45	-0.2336195560E 44	-0.1604217174E 43
	-0.9367319076E 41			
	-0.4678525803E 40	-0.2007645142E 39	-0.7426074993E 37	-0.2372745276E 36
	-0.6355873983E 34			
	-0.1546472729E 33	-0.3233710128E 31	-0.5755277193E 29	-0.8802366448E 27
	-0.1151564931E 26			
	-0.1280603837E 24	-0.1200561062E 22	-0.9385734567E 19	-0.6031140938E 17
	-0.3123934997E 15			
	-0.1269314605E 13	-0.3886750669E 10	-0.8413982792E 07	-0.1145173315E 05
	-0.7352127393E 01			
	0.0000000000E 00			

ROW = 19	-0.4916405622E 65	0.2426678506E 63	-0.1197774865E 61	0.5912023511E 58
	-0.2918044512E 56			
	0.1441048293E 54	-0.6362442235E 51	0.9642881096E 49	0.1182659650E 49
	0.1382193468E 48			
	0.2402574683E 47	0.2533245893E 46	0.2229974940E 45	0.1654108756E 44
	0.1041777177E 43			
	0.5604337133E 41	0.2588058426E 40	0.1029687071E 39	0.3538869566E 37
	0.1052378737E 36			
	0.2709794276E 34	0.6040266138E 32	0.1164146718E 31	0.1935602694E 29
	0.2766976037E 27			
	0.3384713770E 25	0.3520620739E 23	0.3088072872E 21	0.2259403781E 19
	0.1759179017E 17			
	0.6592992059E 14	0.2509624788E 12	0.7202691222E 09	0.1462251747E 07
	0.1847652877E 04			
	0.1126130000E 01			
ROW = 20	0.4698860637E 65	-0.2319301587E 63	0.1144775523E 61	-0.5650429915E 58
	0.2788929524E 56			
	-0.1777284192E 54	0.6557870893E 51	-0.9283379014E 49	-0.1151433918E 49
	-0.1843280581E 48			
	-0.2345703823E 47	-0.2506138020E 46	-0.2215062976E 45	-0.1648726550E 44
	-0.1041367456E 43			
	-0.5616067435E 41	-0.2598699941E 40	-0.1035614028E 39	-0.3563874717E 37
	-0.1059377602E 36			
	-0.2773684343E 34	-0.6096518252E 32	-0.1175308997E 31	-0.1954305207E 29
	-0.2793407237E 27			
	-0.3416009315E 25	-0.3551737005E 23	-0.3113585197E 21	-0.2276473062E 19
	-0.1768320033E 17			
	-0.6631222375E 14	-0.2521604393E 12	-0.7229104237E 09	-0.1465897212E 07
	-0.1379016674E 04			
	-0.1126130007E 01			
ROW = 21	0.2175355531E 64	-0.1073722637E 62	0.5299704487E 59	-0.2615822540E 57
	0.1791093893E 55			
	-0.6776134460E 52	0.3045483818E 50	-0.3595035465E 48	-0.3122740234E 47
	-0.3391550182E 46			
	-0.3687425890E 45	-0.2711151100E 44	-0.1491520916E 43	-0.5384636130E 41
	-0.3612545136E 39			
	0.1172202784E 39	0.1063772626E 38	0.5925473725E 36	0.2500017890E 35
	0.3497440873E 37			

	0.2388654572E 32	0.5624467250E 30	0.1116093248E 29	0.1870043290E 27
	0.2642757073E 25			
	0.3138250669E 23	0.3111343077E 21	0.2551012804E 19	0.1706788593E 17
	0.9146309047E 14			
	0.3822747588E 12	0.1197875266E 10	0.2641120965E 07	0.3645224381E 04
	0.2363596719E 01			
	0.0000000000E 00			
ROW = 22	0.1399963078E 65	-0.6909941794E 62	0.3410581030E 60	-0.1683362965E 58
	0.8308609021E 55			
	-0.4005182370E 53	0.2196440854E 51	0.3131695744E 49	0.7800698814E 48
	0.1163075867E 48			
	0.1419357754E 47	0.1427085170E 46	0.1195805996E 45	0.8427966481E 43
	0.5033686579E 42			
	0.2562973153E 41	0.1117656684E 40	0.4188580910E 38	0.1352144936E 37
	0.3746628254E 35			
	0.9041880798E 33	0.1871858901E 32	0.3333692262E 30	0.5091567911E 28
	0.6658783782E 26			
	0.7344518363E 24	0.6837905882E 22	0.5300019652E 20	0.3371273343E 18
	0.1725978776E 16			
	0.6921546257E 13	0.2088950768E 11	0.4451149697E 08	0.5955371025E 05
	0.3753766667E 02			
	0.0000000000E 00			
ROW = 23	-0.1321184949E 65	0.6521108937E 62	-0.3218665425E 60	0.1588640898E 58
	-0.7341009025E 55			
	0.3364667454E 53	-0.2077659075E 51	-0.3112802477E 49	-0.7730447447E 48
	-0.1162870050E 48			
	-0.1429518167E 47	-0.1446302261E 46	-0.1218212105E 45	-0.8622191018E 43
	-0.5166933046E 42			
	-0.2637546066E 41	-0.1152301513E 40	-0.4323648746E 38	-0.1396640916E 37
	-0.3389003634E 35			
	-0.9337406818E 33	-0.1931600184E 32	-0.3436242450E 30	-0.5240541935E 28
	-0.6821017403E 26			
	-0.7530350016E 24	-0.6995548732E 22	-0.5408858243E 20	-0.3431439777E 18
	-0.1751904544E 16			
	-0.7905233287E 13	-0.2107938921E 11	-0.4478086543E 08	-0.5973299014E 05
	-0.3753766667E 02			
	0.0000000000E 00			

ROW = 24	-0.7877729354E 63	0.3888242904E 61	-0.1919113768E 59	0.9471998023E 56
	-0.4674987057E 54			
	0.2305098198E 52	-0.1187796511E 50	-0.1890381063E 47	-0.7026904350E 46
	-0.2585129251E 44			
	0.1015709052E 45	0.1921373146E 44	0.2240328712E 43	0.1942046963E 42
	0.1332356123E 41			
	0.7456702482E 39	0.3464232799E 38	0.1350587924E 37	0.4449319354E 35
	0.1243730566E 34			
	0.2055966050E 32	0.5974714882E 30	0.1025451007E 29	0.1489670809E 27
	0.1822755236E 25			
	0.1863238112E 23	0.1576365656E 21	0.1088344780E 19	0.6016427736E 16
	0.2592488624E 14			
	0.8368432632E 11	0.1898757014E 09	0.2693605761E 06	0.1792748910E 03
	0.0000000002E 00			
	0.0000000000E 00			
ROW = 25	-0.4317453608E 64	0.2130916225E 62	-0.1051710372E 60	0.5190564735E 57
	-0.2561555389E 55			
	0.1267634369E 53	-0.5185130538E 50	0.2745548896E 49	0.4398662015E 48
	0.6378327503E 47			
	0.7475547865E 46	0.7205805219E 45	0.5775889643E 44	0.3885209372E 43
	0.2209317720E 42			
	0.1048227457E 41	0.4411051626E 39	0.1560469536E 38	0.4738615342E 36
	0.1236185013E 35			
	0.2769551783E 33	0.5320760659E 31	0.8741158810E 29	0.1227811199E 28
	0.1448031321E 26			
	0.1439977753E 24	0.1189770232E 22	0.8052344517E 19	0.4378379627E 17
	0.1861443831E 15			
	0.5945079415E 12	0.1338021997E 10	0.1887143692E 07	0.1251255556E 04
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 26	0.4018890048E 64	-0.1983561166E 62	0.9789357618E 59	-0.4831657213E 57
	0.2384439064E 55			
	-0.1180160091E 53	0.4756085915E 50	-0.2757657986E 49	-0.4522912086E 48
	-0.6634659406E 47			
	-0.7852662373E 46	-0.7628698971E 45	-0.6151646275E 44	-0.4156078397E 43
	-0.2370268314E 42			
	-0.1147943793E 41	-0.4742740004E 39	-0.1677048943E 38	-0.5085879389E 36
	-0.1324000423E 35			

	-0.2958075525E 33	-0.5663823707E 31	-0.9268566948E 29	-0.1290965081E 28
	-0.1521516825E 26			
	-0.1505423462E 24	-0.1237261416E 22	-0.8327702920E 19	-0.4502638809E 17
	-0.1903377073E 15			
	-0.6044333206E 12	-0.1352695512E 10	-0.1897297630E 07	-0.1251255556E 04
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 27	0.2935616483E 63	-0.1473541154E 61	0.7272414481E 58	-0.3589052224E 56
	0.1771142889E 54			
	-0.3746683153E 51	0.4290375056E 49	0.1209381481E 47	0.1242308052E 47
	0.2543038025E 46			
	0.3770815913E 43	0.4228623394E 44	0.3757319240E 43	0.2708528630E 42
	0.1609417437E 41			
	0.2971220522E 39	0.3316815318E 38	0.1165741961E 37	0.3472495340E 35
	0.8781198429E 33			
	0.1835168089E 32	0.3430424917E 30	0.5273917031E 28	0.6315192354E 26
	0.7348356193E 24			
	0.6544412409E 22	0.4748113290E 20	0.2753528451E 18	0.1242569010E 16
	0.4193254257E 13			
	0.9929229286E 10	0.1467331483E 08	0.1015381371E 05	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 28	0.1406629666E 64	-0.6941926539E 61	0.3425786034E 59	-0.1690497059E 57
	0.8341814643E 54			
	-0.4096386644E 52	0.2590888372E 50	0.1158419300E 49	0.2211102139E 48
	0.3081066094E 47			
	0.3435623347E 46	0.3236677159E 45	0.2494319183E 44	0.1609473031E 43
	0.3756930873E 41			
	0.4039545021E 40	0.1586226585E 39	0.5316528164E 37	0.1523138239E 36
	0.3731129813E 34			
	0.7806239763E 32	0.1391651496E 31	0.2105869894E 29	0.2689780977E 27
	0.2377662826E 25			
	0.2551904569E 23	0.1849857701E 21	0.1075169598E 19	0.4877050873E 16
	0.1653032503E 14			
	0.3969332306E 11	0.5940570361E 08	0.4170851852E 05	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			

ROW = 29	-0.1287980315E 64	0.6356443577E 61	-0.3136870593E 59	0.1547938119E 57
	-0.7638456903E 54			
	0.3748364449E 52	-0.2451602048E 50	-0.1270921486E 49	-0.2442455770E 48
	-0.3461075454E 47			
	-0.3964336689E 46	-0.3713427977E 45	-0.2877357334E 44	-0.1861497996E 43
	-0.1013029874E 42			
	-0.4664486118E 40	-0.1825141475E 39	-0.6086924421E 37	-0.1733184421E 36
	-0.4215268056E 34			
	-0.8749231056E 32	-0.1546386068E 31	-0.2318750044E 29	-0.2933613366E 27
	-0.3107906283E 25			
	-0.2728784663E 23	-0.1958194488E 21	-0.1126753081E 19	-0.5060457893E 16
	-0.1704621412E 14			
	-0.4040300525E 11	-0.5992022545E 08	-0.4170851852E 05	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 30	-0.1186499011E 63	0.5854856755E 60	-0.2889167799E 58	0.1425596004E 56
	-0.7033610035E 53			
	0.3475236765E 51	-0.1392908446E 49	0.1124937330E 48	0.2313387487E 47
	0.3729838699E 46			
	0.4786357735E 43	0.4767306419E 44	0.3830233464E 43	0.2520159732E 42
	0.1373272413E 41			
	0.6749219091E 39	0.2389081070E 38	0.7703761579E 36	0.2099911885E 35
	0.4841287519E 33			
	0.9420732279E 31	0.1547310596E 30	0.2128770249E 28	0.2438293252E 26
	0.2302310339E 24			
	0.1767385739E 22	0.1083360417E 20	0.5158321238E 17	0.1834063345E 15
	0.4568879564E 12			
	0.7094813917E 09	0.5145218456E 06	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 31	-0.4172697666E 63	0.2059062454E 61	-0.1015987188E 59	0.5012605296E 56
	-0.2472532183E 54			
	0.1228308135E 52	-0.3542236291E 49	0.5651144419E 48	0.9038889904E 47
	0.1219450813E 47			
	0.1329963717E 46	0.1190402839E 45	0.8837637677E 43	0.5488510388E 42
	0.2870238698E 41			
	0.1770216819E 40	0.4773498160E 38	0.1526487662E 37	0.4156830376E 35
	0.9633216812E 33			

-259-

```
         0.1895967305E 32   0.3157711832E 30   0.4426347761E 28   0.5182668336E 26
         0.5016482729E 24
         0.3958065159E 22   0.2497104827E 20   0.1225930640E 18   0.4499189155E 15
         0.1157597869E 13
         0.1356001843E 10   0.1390283951E 07   0.0000000000E 00   0.0000000000E 00
         0.0000000000E 00
         0.0000000000E 00

ROU = 32 0.3758907571E 63  -0.1854884229E 61   0.9152480839E 58  -0.4515630987E 56
         0.2227374250E 54
        -0.1108814094E 52   0.2432403810E 49  -0.6959731064E 48  -0.1161906886E 48
        -0.1599572547E 47
        -0.1749313651E 46  -0.1596350979E 45  -0.1188190231E 44  -0.7363394307E 42
        -0.7827133653E 41
        -0.1677654024E 40  -0.6227519831E 38  -0.1962610209E 37  -0.5257426364E 35
        -0.1196346822E 34
        -0.2311540711E 32  -0.3775190915E 30  -0.5187243589E 28  -0.5952750804E 26
        -0.5648055547E 24
        -0.4370013152E 22  -0.2705183156E 20  -0.1304151742E 18  -0.4704516284E 15
        -0.1194065449E 13
        -0.1881408777E 10  -0.1390283951E 07   0.0000000000E 00   0.0000000000E 00
         0.0000000000E 00
         0.0000000000E 00
```

ROU = 33	0.4137944591E 62	-0.2041803787E 60	0.1007401669E 58	-0.4969795482E 55
	0.2451605120E 53			
	-0.1194944847E 51	0.1109818637E 49	0.1308542667E 48	0.2580106634E 47
	0.3801123840E 46			
	0.4793453261E 45	0.4059401740E 44	0.3044210793E 43	0.1874854104E 42
	0.9568364035E 40			
	0.4074321570E 39	0.1454006328E 38	0.4361187727E 36	0.1100588588E 35
	0.2735240194E 33			
	0.4155721883E 31	0.6174873787E 29	0.7608962338E 27	0.7700840695E 25
	0.6315759143E 23			
	0.4119549490E 21	0.2080795505E 19	0.7822163812E 16	0.2053287154E 14
	0.3346786438E 11			
	0.2540716114E 08	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROU = 34	0.1072809317E 62	-0.5293901121E 59	0.2611850938E 57	-0.1288416740E 55
	0.6365639672E 52			
	-0.2748464360E 50	0.1156975052E 49	0.1963037972E 48	0.3006098100E 47
	0.3635121431E 46			
	0.3547340038E 45	0.2832416586E 44	0.1871077156E 43	0.1031472396E 42
	0.4776417020E 40			
	0.1846720306E 39	0.6176353624E 37	0.1732708582E 36	0.4121681851E 34
	0.8300364282E 32			
	0.1410883002E 31	0.2013667864E 29	0.2395772312E 27	0.2352208812E 25
	0.1879615646E 23			
	0.1190315543E 21	0.5947547195E 18	0.2202418331E 16	0.5711892317E 13
	0.2222703820E 10			
	0.6951419753E 07	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			

ROW = 35	-0.9641642550E 61	0.4757417363E 59	-0.2347189695E 57	0.1157866525E 55
	-0.5726009152E 52			
	0.2762300812E 50	-0.1619748617E 49	-0.2951143668E 48	-0.4542812884E 47
	-0.5489922591E 46			
	-0.5321754634E 45	-0.4201172271E 44	-0.2733825970E 43	-0.1480359495E 42
	-0.6718867087E 40			
	-0.2569403347E 39	-0.8309108377E 37	-0.2276400718E 36	-0.5285477535E 34
	-0.1038788836E 33			
	-0.1723008589E 31	-0.2400705043E 29	-0.2789575292E 27	-0.2676721130E 25
	-0.2092187464E 23			
	-0.1307007410E 21	-0.6354117265E 18	-0.2309471348E 16	-0.5886868727E 13
	-0.9355860144E 10			
	-0.4951419753E 07	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			
ROW = 36	-0.1087361360E 61	0.5364890561E 58	-0.2646638568E 56	0.1305515039E 54
	-0.6796370551E 51			
	0.4851607073E 49	0.4627591764E 48	0.9880803884E 47	0.1536680200E 47
	0.1354764025E 46			
	0.1774382683E 45	0.1368733478E 44	0.8627362129E 42	0.4488812569E 41
	0.1942428862E 40			
	0.7027602431E 38	0.2132737910E 37	0.5436888279E 35	0.1163790706E 34
	0.2087038839E 32			
	0.3122144263E 30	0.3870374629E 28	0.3938038392E 26	0.3245134519E 24
	0.2125728107E 22			
	0.1077824897E 20	0.4065727631E 17	0.1070538110E 15	0.1749778294E 12
	0.1731634822E 09			
	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00	0.0000000000E 00
	0.0000000000E 00			
	0.0000000000E 00			

A7.3 Numerator polynomial coefficients using the modification of Kropholler.

-0.1212503073E 51	-0.3290971509E 51	-0.3956629628E 51	-0.2803028430E 51
-0.1315504439E 51			
-0.4367207279E 50	-0.1071115898E 50	-0.2003791291E 49	-0.2930978587E 48
-0.3418834352E 47			
-0.3230789305E 46	-0.2504948630E 45	-0.1609141611E 44	-0.8652567944E 42
-0.3780158729E 41			
-0.2213396428E 40	0.4339781080E 39	-0.3171225361E 39	0.2071171704E 39
-0.1358619129E 39			
0.8910718016E 38	-0.5844287803E 38	0.3833130010E 38	-0.2514078382E 38
0.1648948883E 38			
-0.1081529441E 38	0.7093684767E 37	-0.4652725635E 37	0.3051720044E 37
-0.2001627870E 37			
0.1312874303E 37	-0.8611204687E 36	0.5648140140E 36	-0.3704654075E 36
0.2429911133E 36			
-0.1593792022E 36			

Row 1.

0.1208821213E 51	0.3280630469E 51	0.3943883634E 51	0.2793884989E 51
0.1311210647E 51			
0.4353104103E 50	0.1067725739E 50	0.1997618321E 49	0.2922231485E 48
0.3408979499E 47			
0.3221810564E 46	0.2498242750E 45	0.1604993472E 44	0.8631104119E 42
0.3771043355E 41			
0.2208776035E 40	-0.4332957892E 39	0.3166054608E 39	-0.2067806951E 39
0.1356414685E 39			
-0.8896207276E 38	0.5834817934E 38	-0.3826916676E 38	0.2510003514E 38
-0.1646276355E 38			
0.1079776590E 38	-0.7082188048E 37	0.4645185006E 37	-0.3046774159E 37
0.1998383356E 37			
-0.1310744543E 37	0.8597248596E 36	-0.5638936249E 36	0.3698649970E 36
-0.2425977991E 36			
0.1591215960E 36			

Row 2.

0.3681664573E 48	0.1034048317E 49	0.1274030712E 49	0.9142947451E 48
0.4293760029E 48			
0.1410241510E 48	0.3389976414E 47	0.6172637448E 46	0.8746633089E 45
0.9854122422E 44			
0.8978358515E 43	0.6705503149E 42	0.4147973518E 41	0.2146120259E 40
0.9118433541E 38			
0.4608030775E 37	-0.6792784474E 36	0.5162292640E 36	-0.3362346830E 36
0.2203922479E 36			
-0.1444834370E 36	0.9473934533E 35	-0.6212895066E 35	0.4074626682E 35
-0.2672388374E 35			
0.1752753084E 35	-0.1149612816E 35	0.7540242888E 34	-0.4945633903E 34
0.3243848708E 34			
-0.2127652248E 34	0.1395538302E 34	-0.9153426089E 33	0.6003800084E 33
-0.3937941692E 33			
0.2582930319E 33			

Row 3.

-0.1552620213E 51	-0.4638344133E 51	-0.6217660566E 51	-0.4972956235E 51
-0.2664488093E 51			
-0.1019017460E 51	-0.2897581733E 50	-0.6307634661E 49	-0.1075130647E 49
-0.1461177619E 48			
-0.1607178077E 47	-0.1448360921E 46	-0.1080156387E 45	-0.6722095712E 43
-0.3592372225E 42			
-0.1601683009E 41	-0.2174230249E 39	-0.2539079584E 39	0.1540825893E 39
-0.1013883082E 39			
0.6648978107E 38	-0.4360903437E 38	0.2860227131E 38	-0.1875979551E 38
0.1230435009E 38			
-0.8070337313E 37	0.5293306358E 37	-0.3471874555E 37	0.2277206812E 37
-0.1493626887E 37			
0.9796706517E 36	-0.6425755608E 36	0.4214696594E 36	-0.2764451502E 36
0.1813226607E 36			
-0.1180311339E 36			

Row 4.

0.1553780867E 51	0.4579791525E 51	0.6136851597E 51	0.4907192771E 51
0.2629076182E 51			
0.1005568871E 51	0.2860020905E 50	0.6228060531E 49	0.1062025815E 49
0.1444061494E 48			
0.1589155622E 47	0.1432852673E 46	0.1069133274E 45	0.6656801627E 43
0.3469984596E 42			
0.1587826905E 41	0.2143803456E 39	0.2526059561E 39	-0.1533282819E 39
0.1008914013E 39			
-0.6616412146E 38	0.4339543673E 38	-0.2846222482E 38	0.1866794611E 38
-0.1224410862E 38			
0.8030827809E 37	-0.5267391017E 37	0.3454876721E 37	-0.2266057902E 37
0.1486314271E 37			
-0.9748812661E 36	0.6394295787E 36	-0.4194061853E 36	0.2750917002E 36
-0.1804349207E 36			
0.1183488560E 36			

Row 5

0.1882470046E 49	0.5850710997E 49	0.8074590625E 49	0.6571138222E 49
0.3538412861E 49			
0.1343737677E 49	0.3752844305E 48	0.7950297093E 47	0.1309266438E 47
0.1709962056E 46			
0.1800534058E 45	0.1549221495E 44	0.1101135534E 43	0.6522213487E 41
0.3235848036E 40			
0.1383967532E 39	0.3042432937E 37	0.1299408925E 37	-0.7530788577E 36
0.4961043477E 36			
-0.3252135421E 36	0.2132655393E 36	-0.1398634095E 36	0.9172986606E 35
-0.6016321372E 35			
0.3946021721E 35	-0.2588170988E 35	0.1697577775E 35	-0.1113444396E 35
0.7303127130E 34			
-0.4790162459E 34	0.3141900345E 34	-0.2060796763E 34	0.1351693990E 34
-0.8865882425E 33			
0.5815215019E 33			

Row 6

-0.1312043784E 51	-0.4113113716E 51	-0.5785514728E 51	-0.4850480743E 51
-0.2710088446E 51			
-0.1085388610E 51	-0.3213092527E 50	-0.7264742249E 49	-0.1283732333E 49
-0.1806524456E 48			
-0.2056337771E 47	-0.1917986436E 46	-0.1481576899E 45	-0.9561745698E 43
-0.5185665023E 42			
-0.2411877530E 41	-0.7364313733E 39	-0.1567536884E 39	0.8173770540E 38
-0.5419924067E 38			
0.3553325433E 38	-0.2330570478E 38	0.1528582984E 38	-0.1002581478E 38
0.6575869383E 37			
-0.4313093791E 37	0.2828957286E 37	-0.1855518518E 37	0.1217041365E 37
-0.7982635287E 36			
0.5235800263E 36	-0.3434238075E 36	0.2252543861E 36	-0.1477462708E 36
0.9690811344E 35			
-0.6356294257E 35			

Row 7.

0.1264478693E 51	0.3967743775E 51	0.5579666183E 51	0.4678691010E 51
0.2624283614E 51			
0.1048512249E 51	0.3107643710E 50	0.7036011920E 49	0.1245142602E 49
0.1754832310E 48			
0.2000418796E 47	0.1868449244E 46	0.1445230562E 45	0.9338842013E 43
0.5070662572E 42			
0.2361215043E 41	0.7203111535E 39	0.1545022915E 39	-0.8066581292E 38
0.5348605651E 38			
-0.3506594829E 38	0.2299927560E 38	-0.1508487211E 38	0.9894016931E 37
-0.6489426736E 37			
0.4256397197E 37	-0.2791770273E 37	0.1831127558E 37	-0.1201043258E 37
0.7877763378E 36			
-0.5167034403E 36	0.3389094666E 36	-0.2222933920E 36	0.1458041281E 36
-0.9563424370E 35			
0.6272740392E 35			

Row 8.

0.4557395624E 49	0.1453989568E 50	0.2058910828E 50	0.1718268266E 50
0.9482641125E 49			
0.3688527959E 49	0.1054760797E 49	0.2287938044E 48	0.3860124704E 47
0.5170872364E 46			
0.5593822092E 45	0.4955541679E 44	0.3636058006E 43	0.2229959686E 42
0.1150541280E 41			
0.5068421696E 39	0.1613220954E 38	0.2251110231E 37	-0.1071902189E 37
0.7133131609E 36			
-0.4674141099E 36	0.3065081102E 36	-0.2010116883E 36	0.1318338463E 36
-0.8646641873E 35			
0.5671223085E 35	-0.3719723084E 35	0.2439769852E 35	-0.1600252720E 35
0.1049614081E 35			
-0.6884489282E 34	0.4515583517E 34	-0.2961812485E 34	0.1942679443E 34
-0.1274221909E 34			
0.8357745747E 33			

Row 9.

-0.1024766092E 51	-0.3330262833E 51	-0.4848463481E 51	-0.4200357271E 51
-0.2429442768E 51			
-0.9994046094E 50	-0.3046882861E 50	-0.7093745146E 49	-0.1291335467E 49
-0.1873787790E 48			
-0.2202280705E 47	-0.2124596699E 46	-0.1701008184E 45	-0.1140462470E 44
-0.6446993162E 42			
-0.3106897560E 41	-0.1170062311E 40	-0.1017327558E 39	0.3646382265E 38
-0.2481196702E 38			
0.1625039828E 38	-0.1065882270E 38	0.6991022143E 37	-0.4585396310E 37
0.3007569254E 37			
-0.1972677346E 37	0.1293890731E 37	-0.8486721302E 36	0.5566508331E 36
-0.3651121027E 36			
0.2394803802E 36	-0.1570774784E 36	0.1030286763E 36	-0.6757755820E 35
0.4432487326E 35			
-0.2907312034E 35			

Row 10.

0.9391592135E 50	0.3052766897E 51	0.4449211159E 51	0.3861697660E 51
0.2239347865E 51			
0.9241120072E 50	0.2827298291E 50	0.6606968909E 49	0.1207199033E 49
0.1758006298E 48			
0.2073226678E 47	0.2006425246E 46	0.1611090375E 45	0.1083078831E 44
0.6137695533E 42			
0.2964653003E 41	0.1123662000E 40	0.9794637538E 38	-0.3524984821E 38
0.2398066461E 38			
-0.1570637612E 38	0.1030210477E 38	-0.6757096054E 37	0.4431980417E 37
-0.2906949596E 37			
0.1906682032E 37	-0.1250605626E 37	0.8202815685E 36	-0.5380294402E 36
0.3548982663E 36			
-0.2314692601E 36	0.1518220317E 36	-0.9958217924E 35	0.6531697202E 35
-0.4284708467E 35			
0.2810057317E 35			

Row 11.

0.8560643663E 49	0.2774947450E 50	0.3992509791E 50	0.3386588024E 50
0.1900946371E 50			
0.7529256885E 49	0.2195846533E 49	0.4867766971E 48	0.8413652759E 47
0.1157813747E 47			
0.1290539831E 46	0.1181711968E 45	0.8991739174E 43	0.5738315845E 42
0.3092945217E 41			
0.1421506767E 40	0.5240343751E 38	0.3785125569E 37	-0.1213629687E 37
0.8311967544E 36			
-0.5430860384E 36	0.3567032864E 36	-0.2339189495E 36	0.1534118840E 36
-0.1006172120E 36			
0.6599285086E 35	-0.4328400884E 35	0.2838990573E 35	-0.1862096366E 35
0.1221355516E 35			
-0.8010935754E 34	0.5254425815E 34	-0.3446417799E 34	0.2260534168E 34
-0.1482704519E 34			
0.9725197061E 33			

Row 12.

-0.8343619744E 50	-0.2784635040E 51	-0.4157756456E 51	-0.3690439957E 51
-0.2135841442E 51			
-0.9203578697E 50	-0.2876724018E 50	-0.6870119296E 49	-0.1284658834E 49
-0.1918040287E 48			
-0.2323854650E 47	-0.2315711675E 46	-0.1919177577E 45	-0.1334956349E 44
-0.7850153037E 42			
-0.3932553403E 41	-0.1640253365E 40	-0.8604401007E 38	0.1420288655E 38
-0.1063396592E 38			
0.6938293434E 37	-0.4551573971E 37	0.2985391253E 37	-0.1958161466E 37
0.1284392504E 37			
-0.8424566089E 36	0.5525826782E 36	-0.3624486629E 36	0.2377361364E 36
-0.1559349146E 36			
0.1022800776E 36	-0.6708698999E 35	0.4400329549E 35	-0.2886235703E 35
0.1893119055E 35			
-0.1241721674E 35			

Row 13.

0.7033151436E 50	0.2355059327E 51	0.3532363475E 51	0.3153132259E 51
0.1879920677E 51			
0.7977186905E 50	0.2510902561E 50	0.6041813231E 49	0.1137999103E 49
0.1710666225E 48			
0.2085612923E 47	0.2090165486E 46	0.1741188730E 45	0.1216785280E 44
0.7185313720E 42			
0.3613198557E 41	0.1512310596E 40	0.7948588853E 38	-0.1307245293E 38
0.9797582002E 37			
-0.6393287409E 37	0.4194239407E 37	-0.2751089577E 37	0.1804511857E 37
-0.1183623401E 37			
0.7763685307E 36	-0.5092375333E 36	0.3340194661E 36	-0.2190897909E 36
0.1437049162E 36			
-0.9425846503E 35	0.6182561896E 35	-0.4055235315E 35	0.2659887174E 35
-0.1744656324E 35			
0.1144343702E 35			

Row 14.

0.1310430449E 50	0.4295630517E 50	0.6253740119E 50	0.5372907731E 50
-0.3059106655E 50			
0.1231349334E 50	0.3658070622E 49	0.8282730906E 48	0.1466534543E 48
0.2073645031E 47			
0.2382299310E 46	0.2255342146E 45	0.1779787860E 44	0.1181639678E 43
0.6648049443E 41			
0.3193371935E 40	0.1279438906E 39	0.6556382746E 37	-0.1130012783E 37
0.8353377729E 36			
-0.5449475027E 36	0.3573063857E 36	-0.2342859629E 36	0.1536400585E 36
-0.1007609537E 36			
0.6608425031E 35	-0.4334259014E 35	0.2842752529E 35	-0.1864525030E 35
0.1222923049E 35			
-0.8021141684E 34	0.5261062179E 34	-0.3450739751E 34	0.2263352421E 34
-0.1484544155E 34			
0.9737216616E 33			

Row 15.

-0.7066874581E 50	-0.2401401961E 51	-0.3649007618E 51	-0.3296188619E 51
-0.1987835237E 51			
-0.8534793077E 50	-0.2720938354E 50	-0.6642195234E 49	-0.1271879527E 49
-0.1948275301E 48			
-0.2426499587E 47	-0.2490494980E 46	-0.2130195630E 45	-0.1532393739E 44
-0.9340312819E 42			
-0.4855759343E 41	-0.2144177313E 40	-0.9274134383E 38	0.3934119493E 37
-0.4440637773E 37			
0.2859736975E 37	-0.1876996223E 37	0.1231160623E 37	-0.8075759617E 36
0.5297282273E 36			
-0.3474732426E 36	0.2279224091E 36	-0.1495029735E 36	0.9806406796E 35
-0.6432318391E 35			
0.4219131344E 35	-0.2767430754E 35	0.1815218785E 35	-0.1190638556E 35
0.7809619463E 34			
-0.5122464419E 34			

Row 16.

0.5644009594E 50	0.1932102893E 51	0.2961186895E 51	0.2700731079E 51
0.1645766060E 51			
0.7143107087E 50	0.2302139786E 50	0.5679202675E 49	0.1098238201E 49
0.1697498544E 48			
0.2131325069E 47	0.2203322487E 46	0.1896562231E 45	0.1371961288E 44
0.8403530740E 42			
0.4387510192E 41	0.1945773222E 40	0.8377134431E 38	-0.3163657262E 37
0.3774820174E 37			
-0.2428155467E 37	0.1594080861E 37	-0.1045721823E 37	0.6859991611E 36
-0.4500104031E 36			
0.2951981613E 36	-0.1936409837E 36	0.1270206863E 36	-0.8331939661E 35
0.5465239114E 35			
-0.3584893860E 35	0.2351452779E 35	-0.1542387791E 35	0.1011692941E 35
-0.6635934196E 34			
0.4352652057E 34			

Row 17.

0.1422807053E 50	0.4692799159E 50	0.6877919883E 50	0.5954319381E 50
0.3420535603E 50			
0.1391622543E 50	0.4187783761E 49	0.9629440562E 48	0.1736321928E 48
0.2507635124E 47			
0.2951478347E 46	0.2871556438E 45	0.2336193682E 44	0.1604226227E 43
0.9366750517E 41			
0.4682179567E 40	0.1983972839E 39	0.8967980851E 37	-0.7700116261E 36
0.6656657229E 36			
-0.4315241419E 36	0.2828800767E 36	-0.1854246718E 36	0.1215683827E 36
-0.7971244419E 35			
0.5227167435E 35	-0.3427920779E 35	0.2248083746E 35	-0.1474372164E 35
0.9669670213E 34			
-0.6341906559E 34	0.4159511994E 34	-0.2728134310E 34	0.1789340949E 34
-0.1173609700E 34			
0.7697623060E 33			

Row 18.

-0.5867855783E 50	-0.2018702553E 51	-0.3106727926E 51	-0.2844407953E 51
-0.1740601685E 51			
-0.7594073005E 50	-0.2464276797E 50	-0.6134181063E 49	-0.1199977149E 49
-0.1881333767E 48			
-0.2402616855E 47	-0.2533243873E 46	-0.2229974672E 45	-0.1654111066E 44
-0.1041712367E 43			
-0.5605295773E 41	-0.2581812075E 40	-0.1070525038E 39	-0.8642733816E 36
-0.1858455661E 37			
0.1147038293E 37	-0.7542114719E 36	0.4947100484E 36	-0.3245320145E 36
0.2128940700E 36			
-0.1396576099E 36	0.9161334805E 35	-0.6009603043E 35	0.3942086789E 35
-0.2585834456E 35			
0.1696177318E 35	-0.1112590873E 35	0.7297883365E 34	-0.4786918114E 34
0.3150874050E 34			
-0.2059523269E 34			

Row 19.

0.5381437718E 50	0.1863516876E 51	0.2888466817E 51	0.2664866747E 51
0.1643773197E 51			
0.7229602894E 50	0.2364543342E 50	0.5929919158E 49	0.1167985242E 49
0.1842463691E 48			
0.2365744131E 47	0.2506136080E 46	0.2215062771E 45	0.1648728465E 44
0.1041355080E 43			
0.5616872357E 41	0.2593440544E 40	0.1070061450E 39	0.1305012486E 37
0.1588119722E 37			
-0.9698299840E 36	0.6383258243E 36	-0.4188633757E 36	0.2748670533E 36
-0.1803616577E 36			
0.1183420071E 36	-0.7764425567E 35	0.5093995750E 35	-0.3341872157E 35
0.2192330306E 35			
-0.1438167453E 35	0.9434149828E 34	-0.6188528267E 34	0.4059428763E 34
-0.2662788434E 34			
0.1746640011E 34			

Row 20.

0.4864243812E 49	0.1551879369E 50	0.2182647160E 50	0.1795446188E 50
0.9682864380E 49			
0.3644847201E 49	0.9973667240E 48	0.2042701005E 48	0.3199354485E 47
0.3887769102E 46			
0.3687612272E 45	0.2711143027E 44	0.1491514949E 43	0.5385021860E 41
0.3588496009E 39			
-0.1156993709E 39	-0.1162269681E 38	0.4595808109E 35	-0.4405789993E 36
0.2792992347E 36			
-0.1771934293E 36	0.1158800794E 36	-0.7584415333E 35	0.4966361747E 35
-0.3253161479E 35			
0.2131510260E 35	-0.1396877133E 35	0.9155863472E 34	-0.6002009344E 34
0.3034951789E 34			
-0.2570995768E 34	0.1691720327E 34	-0.1109334793E 34	0.7274727536E 33
-0.4770756276E 33			
0.3128752177E 33			

Row 21.

-0.4877264711E 50	-0.1643865122E 51	-0.2470723578E 51	-0.2201915376E 51
-0.1307218809E 51			
-0.5515332096E 50	-0.1725617925E 50	-0.4130543406E 49	-0.7751404307E 48
-0.1163319134E 48			
-0.1410345739E 47	-0.1427085824E 46	-0.1195805602E 45	-0.8427989009E 43
-0.5033543735E 42			
-0.2563893153E 41	-0.1111671745E 40	-0.4579379684E 38	0.1205636343E 37
-0.1713728733E 37			
0.1098074466E 37	-0.7208103532E 36	0.4728108000E 36	-0.3101613752E 36
0.2034664294E 36			
-0.1334734783E 36	0.8757705667E 35	-0.5743549933E 35	0.3767583768E 35
-0.2471379005E 35			
0.1621102609E 35	-0.1063352272E 35	0.6974933199E 34	-0.4575091719E 34
0.3000937570E 34			
-0.1968393732E 34			

Row 22

0.4450134039E 50	0.1513239860E 51	0.2296715239E 51	0.2068577007E 51
0.1241809711E 51			
0.5299072172E 50	0.1676515463E 50	0.4055453947E 49	0.7683926113E 48
0.1163049632E 48			
0.1420506828E 47	0.1446302866E 46	0.1218211800E 45	0.8622208517E 43
0.5166821499E 42			
0.2638277614E 41	0.1147513864E 40	0.4637867163E 38	-0.6680802004E 36
0.1396118253E 37			
-0.8912099478E 36	0.5863372732E 36	-0.3852321788E 36	0.2530476781E 36
-0.1661854045E 36			
0.1091109751E 36	-0.7162761345E 35	0.4701411757E 35	-0.3085478797E 35
0.2024755499E 35			
-0.1328574282E 35	0.8717040259E 34	-0.5719097385E 34	0.3752023822E 34
-0.2461427121E 34			
0.1614710510E 34			

Row 23.

0.4271390006E 49	0.1306284669E 50	0.1740132953E 50	0.1334290064E 50
0.6542086023E 40			
0.2162716402E 49	0.4910627737E 48	0.7509876434E 47	0.6749593255E 46
0.2721977916E 44			
-0.1015776361E 45	-0.1921360319E 44	-0.2240337215E 43	-0.1941997752E 42
-0.1332657207E 41			
-0.7437868837E 39	-0.3583739477E 38	-0.5853975615E 36	-0.5373815018E 36
0.3175606423E 36			
-0.2063439445E 36	0.1344677093E 36	-0.8757623935E 35	0.5711248135E 35
-0.3728523146E 35			
0.2436206766E 35	-0.1592916422E 35	0.1042120063E 35	-0.6820931358E 34
0.4466161565E 34			
-0 2925232452E 34	0.1916449136E 34	-0.1255813952E 34	0.8230535562E 33
-0.5395010405E 33			
0.3536770517E 33			

Row 24.

-0.3437923726E 50	-0.1139352724E 51	-0.1679143271E 51	-0.1463056843E 51
-0.8466728059E 50			
-0.3472174192E 50	-0.1053124694E 50	-0.2437732237E 49	-0.4413849314E 48
-0.6377578291E 47			
-0.7475534223E 46	-0.7205803911E 45	-0.5775886767E 44	-0.3885227446E 43
-0.2209203818E 42			
-0.1068958523E 41	-0.4363649429E 39	-0.1869510507E 38	0.1546819522E 37
-0.1335626644E 37			
0.8669751431E 36	-0.5686298771E 36	0.3729055281E 36	-0.2445788325E 36
0.1604210109E 36			
-0.1052237361E 36	0.6901920205E 35	-0.4527170677E 35	0.2969498615E 35
-0.1947772182E 35			
0.1277590046E 35	-0.8380007127E 34	0.5496615505E 34	-0.3605334100E 34
0.2364802131E 34			
-0.1551112273E 34			

Row 25

0.3109306691E 50	0.1045205828E 51	0.1564501531E 51	0.1386067920E 51
0.8162025369E 50			
0.3406503494E 50	0.1030905173E 50	0.2471119029E 49	0.4537049720E 48
0.6633961057E 47			
0.7852696727E 46	0.7628697549E 45	0.6151644687E 44	0.4156089099E 43
0.2370193030E 42			
0.1148410389E 41	0.4711654948E 39	0.1884311408E 38	-0.8711056208E 36
0.9299366022E 36			
-0.6075927788E 36	0.4023921773E 36	-0.2659388483E 36	0.1755261993E 36
-0.1157226297E 36			
0.7622440808E 35	-0.5016948972E 35	0.3300002433E 35	-0.2169534486E 35
0.1425728266E 35			
-0.9366072473E 34	0.6151157003E 34	-0.4038832060E 34	0.2651385568E 34
-0.1740293122E 34			
0.1142136377E 34			

Row 26.

0.3286265360E 49	0.9415032183E 49	0.1146472003E 50	0.7699403812E 49
0.3047346783E 49			
0.6568440116E 48	0.2273870866E 47	-0.3337637969E 47	-0.1231811459E 47
-0.2563555673E 46			
-0.3770790603E 45	-0.4228622409E 44	-0.3757331679E 43	-0.2708456114E 42
-0.1609850287E 41			
-0.7944870304E 39	-0.3479644552E 38	-0.1486603894E 36	-0.6755106367E 36
0.4056283150E 36			
-0.2593615709E 36	0.1662294366E 36	-0.1069627550E 36	0.6905048374E 35
-0.4460710510E 35			
0.2899853141E 35	-0.1834910821E 35	0.1227135029E 35	-0.7999425534E 34
0.5220298646E 34			
-0.3409739300E 34	0.2228786244E 34	-0.1457744298E 34	0.9539229256E 33
-0.6244902504E 33			
0.4089654249E 33			

Row 27.

-0.2098376026E 50	-0.6842751771E 50	-0.9896749101E 50	-0.8439000927E 50
-0.4766345341E 50			
-0.1902954032E 50	-0.5607000036E 49	-0.1258554430E 49	-0.2206164223E 48
-0.3081309542E 47			
-0.3485616279E 46	-0.3236673119E 45	-0.2494317056E 44	-0.1609485684E 43
-0.8756183043E 41			
-0.4044594144E 40	-0.1553611143E 39	-0.7437216661E 37	0.1231584165E 37
-0.9086549483E 36			
0.5923218485E 36	-0.3830675475E 36	0.2543131578E 36	-0.1667014314E 36
0.1092893334E 36			
-0.7165854151E 35	0.4608835244E 35	-0.3081326166E 35	0.2020711647E 35
-0.1345213076E 35			
0.8691196186E 34	-0.5700101997E 34	0.3738465688E 34	-0.2451943300E 34
0.1608173171E 34			
-0.1054772561E 34			

Row 28.

0.1872797500E 50	0.6271923595E 50	0.9328414376E 50	0.8188461888E 50
0.4762940873E 50			
0.1957293012E 50	0.5925575737E 49	0.1362616982E 49	0.2437933930E 48
0.3461298382E 47			
0.3964325714E 46	0.3713428456E 45	0.2877357591E 44	0.1861497102E 43
0.1013029550E 42			
0.4664879577E 40	0.1820414847E 39	0.6517623116E 37	-0.1759882609E 36
0.2690446230E 36			
-0.1941452817E 36	0.1382119850E 36	-0.9649974519E 35	0.6645082886E 35
-0.4528716321E 35			
0.3062093341E 35	-0.2057816932E 35	0.1376313600E 35	-0.9170384702E 34
0.6091903861E 34			
-0.4037150554E 34	0.2670288700E 34	-0.1763457541E 34	0.1163119788E 34
-0.7663724803E 33			
0.5045387202E 33			

Row 29

0.2255884028E 49	0.5708631967E 49	0.5683892596E 49	0.2505886171E 49
0.3454013049E 47			
-0.5432577353E 48	-0.3185294018E 48	-0.1040540597E 48	-0.2317548255E 47
-0.3799683512E 46			
-0.4786863583E 45	-0.4767301789E 44	-0.3830256806E 43	-0.2520025613E 42
-0.1374056359E 41			
-0.6202765637E 39	-0.2667683505E 38	0.9188096104E 36	-0.1055360792E 37
0.6386363067E 36			
-0.3981505284E 36	0.2493446853E 36	-0.1578080495E 36	0.1002476112E 36
-0.6400087479E 35			
0.4103643353E 35	-0.2640947127E 35	0.1704966856E 35	-0.1103643655E 35
0.7160044577E 34			
-0.4653921325E 34	0.3029732396E 34	-0.1974955414E 34	0.1288789104E 34
-0.8417772170E 33			
0.5502191521E 33			

Row 30.

-0.1091743651E 50	-0.3490873623E 50	-0.4934225818E 50	-0.4097700047E 50
-0.2246639663E 50			
-0.8683234141E 49	-0.2471937332E 49	-0.5354659923E 48	-0.9053500452E 47
-0.1219378857E 47			
-0.1329967213E 46	-0.1190407901E 45	-0.8837624494E 43	-0.5488589434E 42
-0.2860749573E 41			
-0.1273313716E 40	-0.4574733775E 38	-0.2812373572E 37	0.7942319513E 36
-0.5457560636E 36			
0.3557166273E 36	-0.2325537127E 36	0.1521451040E 36	-0.9959439767E 35
0.6522140999E 35			
-0.4272491712E 35	0.2799484480E 35	-0.1834673238E 35	0.1202559561E 35
-0.7883313126E 34			
0.5168387689E 34	-0.3388733077E 34	0.2222025471E 34	-0.1457084556E 34
0.9555203675E 33			
-0.6266308040E 33			

Row 31.

0.9872929531E 49	0.3333869833E 50	0.4966147600E 50	0.4336919103E 50
0.2494111092E 50			
0.1007769655E 50	0.2985769053E 49	0.6692620544E 48	0.1163223240E 48
0.1599507689E 47			
0.1769321949E 46	0.1596350215E 45	0.1188193682E 44	0.7363201070E 42
0.3828213749E 41			
0.1671621534E 40	0.6565010865E 38	0.6773853895E 35	0.1121896153E 37
-0.6060873445E 36			
0.3474659440E 36	-0.2004258760E 36	0.1166534395E 36	-0.6853617022E 35
0.4065750559E 35			
-0.2435504054E 35	0.1473006329E 35	-0.8991819420E 34	0.5537434807E 34
-0.3438154201E 34			
0.2150795060E 34	-0.1354600673E 34	0.8582998438E 33	-0.5467221647E 33
0.3498603277E 33			
-0.2247754228E 33			

Row 32.

0.1044562426E 49	0.1570290874E 49	-0.3188975387E 48	-0.2391900084E 49
-0.2474543029E 49			
-0.1394393430E 49	-0.5138115968E 48	-0.1337916952E 48	-0.2578659604E 47
-0.3801194847E 46			
-0.4393451191E 45	-0.4059393674E 44	-0.3044257930E 43	-0.1874583339E 42
-0.9584514167E 40			
-0.5983143581E 39	-0.1939940429E 38	0.2743732207E 37	-0.1915861918E 37
0.1151758077E 37			
-0.7031520512E 36	0.4329663085E 36	-0.2687919431E 36	0.1681268264E 36
-0.1058766479E 36			
0.6707853561E 35	-0.4272400099E 35	0.2733796817E 35	-0.1756265301E 35
0.1132122253E 35			
-0.7319023637E 34	0.4743230162E 34	-0.3080257781E 34	0.2003762650E 34
-0.1305352009E 34			
0.8513874119E 33			

Row 33.

-0.6611536926E 49	-0.2020690424E 50	-0.2709383251E 50	-0.2115787243E 50
-0.1080401906E 50			
-0.3851731659E 49	-0.1002496577E 49	-0.1970650422E 48	-0.3005723124E 47
-0.3635149057E 46			
-0.3547333220E 45	-0.2832421487E 44	-0.1871050649E 43	-0.1031620378E 42
-0.4767972383E 40			
-0.1915883510E 39	-0.3263437783E 37	-0.1926826055E 37	0.1066199079E 37
-0.6612594543E 36			
0.4126597214E 36	-0.2598182843E 36	0.1647954754E 36	-0.1051696108E 36
0.6745993076E 35			
-0.4345308003E 35	0.2808565922E 35	-0.1820382477E 35	0.1182571070E 35
-0.7696471319E 34			
0.5016522001E 34	-0.3273694996E 34	0.2138433470E 34	-0.1397959388E 34
0.9144688078E 33			
-0.5985023700E 33			

Row 34.

0.6775695890E 49	0.2286258110E 50	0.3328003196E 50	0.2777818142E 50
0.1494471071E 50			
0.5539477693E 49	0.1480912480E 49	0.2957985523E 48	0.4542475990E 47
0.5489938496E 46			
0.5321757358E 45	0.4201149461E 44	0.2733953122E 43	0.1479656477E 42
0.6757741889E 40			
0.2353656781E 39	0.2037375298E 38	-0.6574229644E 37	0.3878203796E 37
-0.2229053536E 37			
0.1297718247E 37	-0.7642933907E 36	0.4553613694E 36	-0.2743631855E 36
0.1670813871E 36			
-0.1027650056E 36	0.6378335548E 35	-0.3991313762E 35	0.2515735313E 35
-0.1595727382E 35			
0.1017709432E 35	-0.6521052277E 34	0.4195008880E 34	-0.2707686552E 34
0.1752583771E 34			
-0.1137030284E 34			

Row 35

-0.1640242382E 48	-0.2655275396E 49	-0.6185683767E 49	-0.6619928549E 49
-0.4140510190E 49			
-0.1687686234E 49	-0.4784016657E 48	-0.9873097995E 47	-0.1536718180E 47
-0.1854761857E 46			
-0.1774384789E 45	-0.1368720741E 44	-0.8628146200E 42	-0.4484052325E 41
-0.1971145353E 40			
-0.5298192357E 38	-0.1256128800E 38	0.6254742114E 37	-0.3835624787E 37
0.2343142637E 37			
-0.1440385736E 37	0.8908959369E 36	-0.5544283824E 36	0.3471021742E 36
-0.2185394040E 36			
0.1383221493E 36	-0.8707257330E 35	0.5619399317E 35	-0.3603392327E 35
0.2318518094E 35			
-0.1496226410E 35	0.9680475229E 34	-0.6276970616E 34	0.4077732893E 34
-0.2653244105E 34			
0.1728695418E 34			

Row 36.

APPENDIX 8. COMPUTER PROGRAM FOR THE CHEN-SHIEH CALCULATION.

A8.1 The Fortran source program.

```
      LIST
      SEND TO (ED,ICLA-DEFAULT.AXXX)
      LIBRARY (ED,SUBGROUPUSUB)
      LIBRARY (ED,SUBGROUPFSCE)
      DUMP ON (ED,PROGRAM OVLY)
      RUN
      PROGRAM (C394)
      PRIORITY 45
      COMPRESS INTEGER AND LOGICAL
      INPUT  1=CR0
      OUTPUT 2=LP0
      TRACE  2
      END

      TRACE 0
      MASTER CRUNCH
C
C     THIS ROUTINE READS IN THE ZEROES AND POLES OF A TRANSFER FUNCTION,
C     MULTIPLIES OUT TO GIVE A RATIO OF TWO POLYNOMIALS (INTERMEDIATE
C     OUTPUT),  CONVERTS TO RUNNING FRACTION FORM (INTERMEDIATE OUTPUT),
C     FORMS THE CHEN-SHIEH MATRIX ( INTERMEDIATE OUTPUT), AND FINALLY
C     CALCULATES THE REQUIRED TIME SOLUTION.
C
      DIMENSION A(50),B(50),C(50),ZP(50),H(100),BA(36,36)
C
      READ(1,1) INUM
      DO 4 IT = 1,INUM
      I = 1
      READ(1,1) IP
      IF (IP.EQ.2) GO TO 11
      READ(1,16) ALPHA
    3 READ(1,1)KC,KT,(ZP(J),J=1,KT)
      WRITE(2,9) IT,KC,KT,(ZP(J), J=1,KT)
      IF(I EQ 2) GO TO 2
      CALL FUDDLE(B,KC,KT,ZP)
      N=KT+1
      I = I+1
      GO TO 3
    2 CALL FUDDLE(A,KC,KT,ZP)
      M=KT+1
      GO TO 12
   11 CONTINUE
C
C     THIS SECTION READS THE NO. OF POLES AND ZEROES AND THE COEFFICIENTS
C     OF THE NUMERATOR AND THEN THE DENOMINATOR POLYNOMIALS.
C     COEFFICIENTS ARE IN ASCENDING POWERS OF S.
C
      READ(1,1)   N,M,ALPHA,
     1            (B(I),I=1,N+1), (A(I), I=1,M+1)
      DO 13 I=1,N
      I1 = N-I+1
   13 B(I) = B(I)/(ALPHA**I1)
C
      DO 14 I=1,M
      I1=M-I+1
   14 A(I) = A(I)/(ALPHA**I1)
      KT = M
      M=M+1
```

```
      N=N+1
   12 CONTINUE
      WRITE(2,5) IT, (B(I),I=1,N)
      WRITE(2,10) (A(I),I=1,M)
      CALL CHACHA(A,B,C,M,N,H,IH,IT)
      DO 15 I=1,KT
   15 H(2*I) = H(2*I)*ALPHA
C
      CALL CHMAT(H,BA,KT)
      WRITE(2,8)
      DO 7 I=1,KT
    7 WRITE(2,6) I,(BA(I,J),J=1,KT)
      CALL RESPON(H,BA)
    4 CONTINUE
      STOP
    1 FORMAT(2I0,150F0.0)
    5 FORMAT(24H0INTERMEDIATE OUTPUT RUN,I3,
     1       5X,22HNUMERATOR COEFFICIENTS//(6F15.6))
    6 FORMAT(4H0ROW,I3,6E15.6/(7X,6E15.6))
    8 FORMAT(19H0CHEN-SHIEH MATRIX./)
    9 FORMAT(15H0DATA CHECK RUN,I3/ 5H0KC =,I3,5X,4HKT =,I3/
     1       5H0ZP =,5F15.6/(5X,5E15.6))
   10 FORMAT(1H0,31X,24HDENOMINATOR COEFFICIENTS//(6F15.6))
   16 FORMAT(1000F0.0)
      END

      SUBROUTINE CHACHA(A,B,C,M,N,H,IH,J)
C
C  THIS ROUTINE ORGANISES THE REPEATED DIVISION OF A TRANSFER FUNCTIO
C  FORMED AS A RATIO OF TWO POLYNOMIALS, GIVING THE CHEN SHIEH H
C  COEFFICIENTS AS INTERMEDIATE OUTPUT.
C
      DIMENSION A(50),B(50),C(50),H(100)
C
      DO 12 I=1,2*M
   12 H(I) = 0.0
      IH = 0
      ICOEFF = 0
    2 K = M
      IF(N.GT.M) K=N
C
      ICOEFF = ICOEFF+1
      N1 = N
      M1 = M
      CALL SHUSH(A,B,C,N1,M1,K)
      WRITE(2,3) ICOEFF,C(1)
C
      IH = IH+1
      H(IH) = C(1)
C
      IF(ABS(C(2)).LT.1.0E-30) GO TO 10
      IF(K.EQ.2) GO TO 5
C
      DO 6 I=1,N
    6 A(I) = B(I)
```

```
      M=N
C
      DO 7 I=1,K-1
    7 B(I) = C(I+1)
      N=K-1
      GO TO 2
C
    5 ICOEFF = ICOEFF+1
      C(1) = B(1)/C(2)
      WRITE(2,8)  ICOEFF,C(1)
C
      IH = IH+1
      H(IH) = C(1)
C
      ICOEFF = ICOEFF+1
      C(3) = C(2)/B(2)
      WRITE(2,8) ICOEFF,C(3)
C
      IH = IH+1
      H(IH) = C(3)
C
    9 CONTINUE
   10 WRITE(2,11) J
    3 FORMAT(27H0CHEN-SHIEH COEFFICIENT NO.,I3,3H = ,E15.6/)
    4 FORMAT(1H0,50X,21HREMAINDER DENOMINATOR,3F15.6/(72X,3F15.6))
    8 FORMAT(27H0CHEN-SHIEH COEFFICIENT NO.,I3,3H = ,E15.6)
   11 FORMAT(23H0END OF CALCULATION NO.,I3/////)
      RETURN
      END

      SUBROUTINE CHMAT(H,B,M)
C
C  SUBROUTINE TO FORM THE CHEN-SHIEH MATRIX (BA) GIVEN THE
C  2M CHEN-SHEIH COEFFICIENTS (H).
C
      DIMENSION A(50),B(36,36),H(100)
C
      DO 2 I=1,M
    2 A(I) = H(2*I)
C
      DO 3 I=1,M
      B(I,I) = 0.0
      DO 4 J=1,I
    4 B(I,I) = B(I,I) + H(2*J-1)
    3 CONTINUE
C
      DO 5 K=1,M
      DO 6 L=1,M
      IF(K.EQ L) GO TO 6
      IF(K.GT L) B(K,L) = B(L,L)
      IF(K.LT L) B(K,L) = B(K,K)
    6 CONTINUE
    5 CONTINUE
C
      DO 7 K=1,M
      DO 8 L=1,M
    8 B(K,L) =-B(K,L)*A(L)
    7 CONTINUE
C
      RETURN
      END
```

```
      SUBROUTINE FIDDLY(A,B,C,M,N,IPT)
C
C  SUBROUTINE TO MULTIPLY TWO POLYNOMIALS A,B OF LENGTH M,N
C  RESPECTIVELY TO FORM A THIRD POLYNOMIAL C OF LENGTH IPT,
C  WHERE IPT IS SET TO BE M+N-1 BY THE USER.
C
      DIMENSION A(M),B(N),C(IPT)
C
      DO 1 I=1,IPT
    1 C(I) = 0.0
C
      JC = 0
    2 JC = JC+1
      IP = JC+1
      IF(JC.GT.IPT) RETURN
      IA = 0
    3 IA = IA+1
      IF(IA.GT M) GO TO 2
      IB = 0
    4 IB = IB+1
      IF(IB.GT.N) GO TO 3
      IF((IA+IB).NE.IP) GO TO 4
      C(JC) = A(IA)*B(IB) + C(JC)
      GO TO 3
      END
      SUBROUTINE FUDDLE(C,KC,KT,ZP)
C
C  THIS ROUTINE ORGANISES THE MULTIPLYING OUT OF A TRANSFER FUNCTION
C  IN POLE ZERO FORM TO A RATIO OF TWO POLYNOMIALS.
C
      DIMENSION A(50),B(3),C(50),ZP(50)
C
      K = 0
      IF(KC.EQ.0) GO TO 1
C
    2 K = K+2
      IF(K.NE 2) GO TO 3
      A(1),C(1) = ZP(K-1)**2 + ZP(K)**2
      A(2),C(2) = -2.0*ZP(K-1)
      A(3),C(3) = 1.0
      M,IPT = 3
C
    4 IF(K.EQ KC) GO TO 1
      GO TO 2
C
    3 B(1) = ZP(K-1)**2 + ZP(K)**2
      B(2) = -2.0*ZP(K-1)
      B(3) = 1.0
      N=3
      IPT = M+N-1
C
      CALL FIDDLY(A,B,C,M,N,IPT)
C
      M = IPT
      DO 5 I=1,M
    5 A(I) = C(I)
      GO TO 4
C
```

```
    1 K = K+1
      IF(K.GT KT) RETURN
      IF(K.EQ 1) GO TO 7
C
      B(1) = -ZP(K)
      B(2) = 1.0
      N=2
      IPT = M+N-1
      CALL FIDDLY(A,B,C,M,N,IPT)
      M = IPT
      DO 8 I=1,M
    8 A(I) = C(I)
      GO TO 1
    7 A(1),C(1) = -ZP(K)
      A(2),C(2) = 1.0
      M,IPT = 2
      GO TO 1
      END

      SUBROUTINE MARGOT(N,BA,V,H,THAX,NR,IV,VX,CHEN)
C
C
      DIMENSION QC(400),CHEN(100),VX(40),BA(36,36)
      DIMENSION Q(40,40),R(40,40), F(40,40,2)
      DIMENSION D(40),IV(40),V(40),REINT(20)
      EQUIVALENCE (Q(1),F(1601)),(R(1),F(1))
C
C  LOAD QC WITH THE REQUIRED PARTITION OF THE SYSTEM MATRIX.
C
      DO 300 IA=1,N
      IC = N*(IA-1)
      DO 300 IB=1,N
  300 QC(IB+IC) = BA(IB,IA)
C
C  FORM THE INITIAL STATE VECTOR AS VX/QC.
C
      NA = N*N
      N1 = N
      CALL F4SOLVE(QC,VX,N,NA,N1,1,DUM,IDUM,IT,REINT)
C
C  LOAD Q WITH THE REQUIRED PARTITION OF THE SYSTEM MATRIX.
C
      DO 301 IA=1,N
      DO 301 IB=1,N
  301 Q(IA,IB) = BA(IA,IB)
C
      NT = N
      NL=NT-N-1
      QTHRO = 1.0
      VTOT = 1.0
      STAYP = 0.04
  203 CC=1.0E+76
      DO 1 I=1,N
      D(I)=-Q(I,I)
C
C     CC IS MINIMUM STAGE TIME CONSTANT
C     POSITIVE STAGE THROUGH FLOWS IN D, DIAGONALS OF Q MADE ZERO
C
      IF(ABS(V(I)).GE.1.0E-10)  CC=AMIN1(CC,ABS(V(I)/D(I)))
```

```
    1 Q(I,I)=0.
C      CALCULATION OF TIME INCREMENT
C.     CONSTRAIN DT TO FIT IN WITH NORMALISED TIME PRINT OUT INTERVAL
       WRITE(2,399) H, VTOT, STAYP, CC, QTHRO
  399 FORMAT(21H0PRINTOUT INCREMENT =,G15.5/
    1         17H V-SCALE FACTOR =,G15.5/
    2         18H ACCURACY FACTOR =,G15.5/
    3         27H MINIMUM DIAGONAL ELEMENT =,G15.5/
    4         17H Q-SCALE FACTOR =,G15.5)
       IX=(1.+DIM (ALOG(H*VTOT/(-ALOG(STAYP)*CC*QTHRO))/ALOG(2.),0.))
       DT=H/(2.**IX)*VTOT/QTHRO
       STAYP=EXP(-DT/CC)
C      IF V IS ZERO MAKE EXP(-D/V*DT) ZERO,  (1-EXP(-D/V*DT/2))/D IS
       DO 3 I=1,N                                                PUT IN
       IF(ABS(V(I)).GE.1.0E-10)  V(I)=EXP(-D(I)*DT/(2.*V(I)))
    3 D(I)=(1.-V(I))/D(I)
C      MAKE TRANSITION MATRIX, CC IS (1.0-EXP(-D/V*DT/2.))/D
       DO 4 I=1,NT
       IF(I-N-1)0,8,10
       CC=(1.0-V(I))*D(I)
       GO TO 9
    8  CC=DT
   10  R(I,I),V(I)=1.0
    9 DO 5 J=1,N
       CD=0.
       DO 6 K=1,N
    6 CD=CD+D(K)*Q(I,K)*Q(K,J)
    5 R(I,J)=CC*(CD+V(J)*Q(I,J))
    4 R(I,I)=R(I,I)+V(I)*V(I)
C      FINDING THE 2**H TH POWER OF THE TRANSITION MATRIX R IN F
       L=1
       DO 37 M=1,IX
       L=3-L
       LI=3-L
       DO 37 I=1,NT
       ATR=FLOAT((I+NL)/NT)
       DO 37 J=1,N
       CA=0.
       DO 38 K=1,N
   38 CA=CA+F(I,K,LI)*F(K,J,LI)
   37 F(I,J,L)=CA+ATR*F(I,J,LI)
       NS=N-NR+1
C      WRITE OUT COLUMN HEADINGS
       WRITE(2,103) QTHRO,VTOT,STAYP,IX
  103 FORMAT(17H0THROUGHPUT RATE=, G12.4/
    1  14H TOTAL VOLUME=,G12.4/7H STAYP=,G12.4////
    2  3H M=,I3//3X,4HTIME,6X,8HRESPONSE/)
C
C  LOAD ISV FROM VX INTO V.
C
       DO 303 I=1,NT
  303 V(I) = VX(I)
C
       TIME=0.
       DO 32 I=1,NT
   32  D(I)=V(I)
       DUM = 0.0
   97 WRITE(2,102) TIME,DUM
       DO 45 I=1,NT
   45 V(I)=D(I)
```

```
  102 FORMAT(F8.2,4X,10G12.4)
      IF(TIME GE.TMAX) RETURN
C     CALCULATE RESPONSES
      DO 42 I=1,NT
      CB=0.
      DO 43 J=1,N
   43 CB=CB+V(J)*F(I,J,L)
   42 D(I)=CB+FLOAT((I+NL)/NT)*V(I)
      TIME=TIME+H
      DO 304 I=NS,NT
  304 OC(I) = D(IV(I)) - VX(I)
      DUM = 0.0
      DO 302 I=NS,NT
      J=I-NS+1
  302 DUM = DUM + OC(I)*CHEN(2*J)
      GO TO 97
      END

      SUBROUTINE RESPON(H,BA)
C
C
      DIMENSION H(100),BA(36,36),V(40),IV(40),VX(40)
C
      READ(1,1) NMIN, NMAX, TSTEP, TMAX
C
      DO 2 I=NMIN,NMAX
C
      WRITE(2,4) I
      DO 3 J=1,I
      VX(J) = 1.0
      V(J) = 1.0
    3 IV(J) = J
C
      NR = I
      CALL MARGOT(I,BA,V,TSTEP,TMAX,NR,IV,VX,H)
C
    2 CONTINUE
      STOP
    1 FORMAT(2I0,2F0.0)
    4 FORMAT(49H1PREDICTED RESPONSE FOR CHEN-SHIEH MODEL OF ORDER,I3
      END                                                          ///)

      SUBROUTINE SHUSH(A,B,C,N,M,K)
C
C  THIS ROUTINE PERFORMS THE DIVISION OF ONE POLYNOMIAL BY ANOTHER.
C  THE POLYNOMIALS ARE IN ASCENDING POWERS OF S.   RESULT IS HELD IN C
C
      DIMENSION A(M),B(N),C(K)
C
      J1 = N
      IF(N.GT.M) J1=M
C
      C(1) = A(1)/B(1)
      D = C(1)
      DO 1 I=2,J1
    1 C(I) = A(I)-D*B(I)
C
      IF(M.EQ.N) RETURN
      IF(M.GT.N) GO TO 2
```

```
C
      DO 3 I = J1+1,N
    3 C(I) = -D*B(I)
      RETURN
C
    2 DO 4 I=J1+1,M
    4 C(I) = A(I)
C
      RETURN
      END
```

A8.2 Data.

The program accepts as data the following information:-

1) The number of calculations to be performed.
2) A parameter IP. If the polynomials are to be entered in factored (pole-zero) form then IP is set to 1. If the starting point is to be the polynomial coefficients then IP is set to 2.
3) For IP = 1 :-

ALPHA	a scaling factor normally set to 1.
KC	the number of complex poles.
KT	the total number of poles.
ZP	the poles themselves. This item consists of KT numbers. For a complex pair $a \pm ib$ only a and b need be given.

For IP = 2 :-

N	the order of the numerator polynomial.
M	the order of the denominator polynomial.
ALPHA	a scaling factor normally set to 1.

4)

NMIN	the lowest order Chen-Shieh model response required.
NMAX	the highest order model required.
TSTEP	the printout interval.
TMAX	maximum response time.

If more than one calculation is to be performed the above data is repeated from item 2).

A8.3 Results.

These are self-explanatory and include a data check. An abbreviated example is given overleaf.

```
INTERMEDIATE OUTPUT RUN  1      NUMERATOR COEFFICIENTS

 -0.677570E 40  -0.278626E 50  -0.332800E 50  -0.277782E 50  -0.149447E 50  -0.553948E 49
 -0.148091E 49  -0 295799E 48  -0.454248E 47  -0.548994E 46  -0.532176E 45  -0.420117E 44
 -0.273383E 43  -0.148036E 42  -0.671887E 40  -0.256949E 39  -0.830911E 37  -0.227640E 36
 -0.528548E 34  -0.103872E 33  -0.172310E 31  -0.240071E 29  -0.278958E 27  -0.267672E 25
 -0.209219E 23  -0 130710E 21  -0.635412E 18  -0.230947E 16  -0.588687E 13  -0.935587E 10
 -0.695142E 07

                                DENOMINATOR COEFFICIENTS

 -0.105011E 52  -0 380974E 52  -0.620936E 52  -0.604598E 52  -0.394959E 52  -0.184536E 52
 -0.642832E 51  -0.172056E 51  -0.362233E 50  -0.611427E 49  -0.840678E 48  -0.954154E 47
 -0.903974E 46  -0.721594E 45  -0.489098E 44  -0.283288E 43  -0.140937E 42  -0.604696E 40
 -0.224434E 39  -0.722089E 37  -0.201638E 36  -0.488852E 34  -0.102842E 33  -0.187462E 31
 -0.295347E 29  -0 400748E 27  -0.466026E 25  -0.461470E 23  -0.385850E 21  -0.269441E 19
 -0.154879E 17  -0.718675E 14  -0.261983E 12  -0.720859E 09  -0.140461E 07  -0.172383E 04
 -0.100000E 01

CHEN-SHIEH COEFFICIENT NO.  1 =    0.154981E 03

CHEN-SHIEH COEFFICIENT NO.  2 =    0.254277E-01

CHEN-SHIEH COEFFICIENT NO.  3 =   -0.687377E 02

CHEN-SHIEH COEFFICIENT NO.  4 =   -0.130799E-01
```

etc.

CHEN-SHIEH MATRIX

ROW 1	-0.394081E 01	0.202714E 01	0.342586E 01	0.659798E-02	-0.118098E 01	-0.566395E 00
	0.358181E-01	-0.145787E-01	-0.150987E 00	0.183509E 00	0.138603E 00	0.504274E-01
	0.676025E-02	-0.100590E-01	-0.491859E-02	0.103633E-02	0.307365E-01	-0.350391E-01
	-0.856683E-02	0.798650E-02	-0.252776E-02	0.104317E-02	-0.869423E-03	0.170081E-03
	0.396547E-04	-0.114140E-05	0.173187E-04	-0.853228E-05	-0.150249E-07	0.401903E-06
	-0.464362E-07	0.927386E-08	-0.291847E-09	0.753511E-10	-0.905769E-12	0.382802E-11
ROW 2	-0.394081E 01	0.112806E 01	0.190641E 01	0.367162E-02	-0.657187E 00	-0.315186E 00
	0.190320E-01	-0.811269E-02	-0.840208E-01	0.102119E 00	0.771294E-01	0.280617E-01
	0.376192E-02	-0.559763E-02	-0.273708E-02	0.576691E-03	0.171041E-01	-0.194985E-01
	-0.476727E-02	0.444430E-02	-0.140664E-02	0.580500E-03	-0.483814E-03	0.946460E-04
	0.220667E-04	-0.635163E-06	0.963745E-05	-0.474802E-05	-0.836104E-08	0.223650E-06
	-0.254407E-07	0.516069E-08	-0.162406E-09	0.419312E-10	-0.504040E-12	0.213021E-11
⋮						
ROW 35	-0.394081E 01	0.112806E 01	-0.930720E 01	0.362051E 00	-0.112204E 02	-0.158641E 02
	-0.469462E 01	0.641195E 01	0.508454E 02	-0.546644E 02	-0.474661E 02	-0.242897E 02
	-0.122441E 02	-0.339098E 00	-0.125858E 02	-0.128963E 02	0.528910E 03	-0.600169E 03
	-0.325341E 03	0.268650E 03	-0.104235E 03	-0.282841E 03	0.216733E 03	-0.648396E 02
	-0.134850E 03	-0.865679E 01	-0.182841E 03	0.509986E 02	-0.127969E 02	-0.122337E 03
	-0.859824E 02	-0.124286E 03	-0.820398E 02	-0.143188E 03	0.173578E 03	-0.733587E 03
ROW 36	-0.394081E 01	0.112806E 01	-0.930720E 01	0.362051E 00	-0.112204E 02	-0.158641E 02
	-0.469462E 01	0.641195E 01	0.508454E 02	-0.546644E 02	-0.474661E 02	-0.242897E 02
	-0.122441E 02	-0.339098E 00	-0.125858E 02	-0.128963E 02	0.528910E 03	-0.600169E 03
	-0.325341E 03	0.268650E 03	-0.104235E 03	-0.282841E 03	0.216733E 03	-0.648396E 02
	-0.134850E 03	-0.865679E 01	-0.182841E 03	0.509986E 02	-0.127969E 02	-0.122337E 03
	-0.859824E 02	-0.124286E 03	-0.820398E 02	-0.143188E 03	0.173578E 03	-0.537579E 03

PREDICTED RESPONSE FOR CHEN-SHIEH MODEL OF ORDER 2

PRINTOUT INCREMENT = 0.50000E-01
V-SCALE FACTOR = 1.0000
ACCURACY FACTOR = 0.94000
MINIMUM DIAGONAL ELEMENT = 0.25375
Q-SCALE FACTOR = 1.0000

THROUGHPUT RATE= 1.000
TOTAL VOLUME= 1.000
STAYP= 0.9510

M= 2

TIME	RESPONSE
0.00	0.0000E 00
0.05	0.6024E-03
0.10	0.1174E-02
0.15	0.1714E-02
0.20	0.2223E-02
0.25	0.2700E-02
0.30	0.3145E-02
0.35	0.3559E-02
0.40	0.3943E-02
0.45	0.4297E-02
0.50	0.4622E-02
0.55	0.4920E-02
0.60	0.5194E-02
0.65	0.5438E-02
0.70	0.5660E-02
0.75	0.5859E-02
0.80	0.6038E-02
0.85	0.6196E-02
0.90	0.6336E-02
0.95	0.6458E-02
1.00	0.6565E-02
1.05	0.6656E-02
1.10	0.6734E-02
1.15	0.6799E-02
1.20	0.6853E-02
1.25	0.6896E-02
1.30	0.6930E-02
1.35	0.6956E-02
1.40	0.6974E-02
1.45	0.6985E-02
1.50	0.6991E-02
1.55	0.6991E-02
1.60	0.6987E-02
1.65	0.6979E-02
1.70	0.6968E-02
1.75	0.6954E-02
1.80	0.6937E-02
1.85	0.6919E-02
1.90	0.6899E-02
1.95	0.6878E-02
2.00	0.6857E-02

APPENDIX 9. SAMPLE CONVERGENCE FOR THE ZERO ESTIMATION METHOD OF DAVISON.

$K = -10^4$

EIGENVALUE PRODUCT = 0.12088211971E 55

-1.85772
-2.02705
-2.90746
-3.64507
-3.80107
-7.47372
-11.4153
-16.3374
-20.2181
-27.7684
-40.0644
-49.5135
-57.0219
-60.0242
-70.7442
-75.5392
-87.2043
-105.833
-148.566
-218.654

28.1565	+35.7039 i
28.1565	-35.7039 i
-21.4856	+5.25407 i
-21.4856	-5.25407 i
-27.3838	+10.0654 i
-27.3838	-10.0654 i
-34.0044	+11.1350 i
-34.0044	-11.1750 i
-39.9422	+8.83434 i
-39.9422	-3.83434 i
-43.9776	+3.54308 i
-43.9776	-3.54308 i
-53.7556	+77.0118 i
-53.7556	-77.0118 i
-162.402	+56.3943 i
-162.402	-56.3943 i

$K = -10^5$

EIGENVALUE PRODUCT = 0.12088217452E 56

-1.85772
-2.02705
-2.90745
-3.66396
-3.77652
-7.47571
-11.4234
-16.9043
-20.0818
-27.7633
-40.0462
-49.4932
-56.9947
-60.0341
-70.7450
-75.5391
-87.2047
-105.856
-148.585
-248.254

58.6408	+55.0467 i
58.6408	-55.0467 i
-23.9400	+3.64954 i
-23.9400	-3.64954 i
-28.3987	+7.95015 i
-28.3987	-7.95015 i
-33.7305	+3.97138 i
-33.7305	-3.97138 i
-38.6661	+7.09185 i
-38.6661	-7.09185 i
-41.8099	+2.78791 i
-41.8099	-2.78791 i
-47.6747	+121.850 i
-47.6747	-121.850 i
-184.160	+94.8261 i
-184.160	-94.8261 i

$K = -10^6$

EIGENVALUE PRODUCT = 0.12088212933E 57

-1.85773
-2.02705
-2.90744
-3.66632
-3.77360
-7.47591
-11.4242
-16.9863
-20.0421
-27.7125
-39.9319
-49.4011
-56.9020
-60.0351
-70.7450
-75.5392
-87.2047
-105.858
-148.587
-297.123

104.467	+80.7338 i
104.467	-80.7338 i
-25.9960	+2.66686 i
-25.9960	-2.66686 i
-29.2954	+6.25700 i
-29.2954	-6.25700 i
-33.6300	+7.19776 i
-33.6300	-7.19776 i
-37.1798	+180.367 i
-37.1798	-180.367 i
-37.6172	+5.68579 i
-37.6172	-5.68579 i
-40.1136	+2.20812 i
-40.1136	-2.20812 i
-216.046	+143.146 i
-216.046	-143.146 i

$K = -10^7$

EIGENVALUE PRODUCT = 0.12124995043E 58

-1.85772
-2.02705
-2.90159
-3.66660
-3.77424
-7.49138
-11.4283
-16.9951
-20.0416
-26.7905
-28.3744
-49.5002
-56.9009
-60.0403
-70.7446
-75.5386
-87.2046
-105.858
-148.587
-369.904

170.817	+115.522 i
170.817	-115.522 i
-21.1305	+258.921 i
-21.1305	-258.921 i
-28.4978	+3.68029 i
-28.4978	-3.68029 i
-31.6947	+5.61594 i
-31.6947	-5.61594 i
-35.1737	+5.42665 i
-35.1737	-5.42665 i
-37.9038	+3.45005 i
-37.9038	-3.45005 i
-39.6325	+0.557516 i
-39.6325	-0.557516 i
-262.032	+206.704 i
-262.032	-206.704 i

$K = -10^8$

EIGENVALUE PRODUCT = 0.12100907515E 59

-1.85777
-2.02765
-2.90742
-3.66715
-3.77329
-7.47492
-11.4242
-16.9983
-20.0300
-49.4926
-56.9846
-60.0478
-70.7044
-75.5718
-87.2009
-105.859
-148.589
-473.756

264.924	+162.833 i
264.924	-162.833 i
1.75253	+365.552 i
1.75253	-365.552 i
-27.1478	+1.43378 i
-27.1478	-1.43378 i
-29.4013	+3.70513 i
-29.4013	-3.70513 i
-31.9350	+4.99232 i
-31.9350	-4.99232 i
-34.8519	+5.01231 i
-34.8519	-5.01231 i
-37.5820	+3.40124 i
-37.5820	-3.40124 i
-39.5628	+0.631971 i
-39.5628	-0.631971 i
-327.119	+292.990 i
-327.119	-292.990 i

$K = -10^9$

-1.85893	
-2.04731	
-2.88729	
-3.60537	
-3.82436	
-7.49462	
-11.4878	
-16.8467	
-21.3426	
-21.8047	
-41.9879	
-49.2970	
-56.8758	
-60.4362	
-70.2946	
-75.9048	
-87.1796	
-105.858	
-148.604	
-619.490	
397.228	+228.026 i
397.228	-228.026 i
34.0357	+512.244 i
34.0357	-512.244 i
-26.3230	+5.14668 i
-26.3230	-5.14668 i
-30.2529	+7.00125 i
-30.2529	-7.00125 i
-34.2533	+6.87711 i
-34.2533	-6.87711 i
-37.0161	+5.85909 i
-37.0161	-5.85909 i
-40.1218	+3.64976 i
-40.1218	-3.64976 i
-418.833	+413.308 i
-418.833	-413.308 i

EIGENVALUE PRODUCT =

0.12189417069E 60

$K = -10^{10}$

1937.72	
110.672	
-1.78215	
-2.01720	
-2.83729	
-3.65231	
-4.00087	
-7.61103	
-11.0758	
-16.9743	
-20.1450	
-23.1480	
-36.2509	
-39.7146	
-40.8036	
-43.7701	
-56.5481	
-61.1431	
-72.2301	
-73.8584	
-87.1261	
-105.852	
-148.662	
-2348.27	
42.6790	+1999.49 i
42.6790	-1999.49 i
-26.7791	+3.96045 i
-26.7791	-3.96045 i
-29.7266	+8.74161 i
-29.7266	-8.74161 i
-34.9100	+6.97182 i
-34.9100	-6.97182 i
-39.2435	+4.40615 i
-39.2435	-4.40615 i
-190.060	+151.274 i
-190.060	-151.274 i

EIGENVALUE PRODUCT =

0.12117802899E 61

APPENDIX 10. A DISTILLATION SYSTEM USED TO DEMONSTRATE A POINT IN CHAPTER 10.

Feed composition vector = (0.60, 0.01, 0.39).

Plate	x	x	x	y	y	y	K	K	K
0	0.9999E0	0.1454E-3	0.1797E-5						
1	0.9995E0	0.4865E-3	0.2420E-4	0.9999E0	0.1454E-3	0.1797E-5	0.1000E1	0.2977E0	0.7424E-1
2	0.9987E0	0.1116E-2	0.1886E-3	0.9997E0	0.3325E-3	0.1402E-4	0.1001E1	0.2980E0	0.7432E-1
3	0.9903E0	0.2259E-2	0.1391E-2	0.9992E0	0.6749E-3	0.1037E-3	0.1003E1	0.2987E0	0.7456E-1
4	0.9857E0	0.4293E-2	0.1002E-1	0.9979E0	0.1298E-2	0.7594E-3	0.1012E1	0.3025E0	0.7578E-1
5	0.9270E0	0.7400E-2	0.0560E-1	0.9921E0	0.2408E-2	0.5467E-2	0.1070E1	0.3254E0	0.8334E-1
6	0.7000E0	0.9199E-2	0.2846E0	0.9601E0	0.4102E-2	0.3578E-1	0.1360E1	0.4460E0	0.1256E0
7	0.7056E0	0.9352E-2	0.2850E0	0.9600E0	0.4173E-2	0.3583E-1	0.1361E1	0.4462E0	0.1257E0
8	0.7034E0	0.9898E-2	0.2807E0	0.9594E0	0.4431E-2	0.3620E-1	0.1364E1	0.4477E0	0.1263E0
9	0.6885E0	0.1168E-1	0.2998E0	0.9556E0	0.5349E-2	0.3901E-1	0.1388E1	0.4581E0	0.1301E0
10	0.5982E0	0.1567E-1	0.3861E0	0.9306E0	0.8340E-2	0.6106E-1	0.1556E1	0.5323E0	0.1582E0
B	0.3334E0	0.1057E-1	0.6500E0	0.7787E0	0.1505E-1	0.2062E0	0.2336E1	0.9086E0	0.3172E0

The molar flowrates are the same as for the system given in Chapter 8.