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Component Separation Efficiencies
and
Distillation Tower Dynamic Behavior

A dissertation
presented to
The Department of Chemical and Nuclear Engineering
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in partial fulfillment of
the requirements for
the degree of

Doctor of Philosophy
(Chemical Engineering)

by

William F. Huber, Jr.

M.S. Chemical Engineering
University of Cincinnati (1967)

B.S. Chemical Engineering
University of Notre Dame (1962)

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SUMMARY

This thesis concerns the effects of component separation efficiency upon distillation tower dynamic response. Matrix methods were used in formulating the solution and computer generated numerical solutions were compared to experimental results. The experimental unit was a ten tray, 4-inch diameter sieve tower distilling a mixture of benzene, toluene, and p-xylene at atmospheric pressure.

Inclusion of a Murphree efficiency for each component and each tray was done in a rigorous way and not through the use of a modified K value. The matrices of coefficients become supertriangular rather than tridiagonal in the unsteady state component balances when this is done. Mathematical and numerical solutions for sets of equations of the form $\frac{d\bar{X}_i}{dt} = \bar{A}_i \bar{X}_i + \bar{F}_i$ ($i = 1, 2, \dots, I$) were developed for the case where $\bar{A}_i$ are supertriangular. Sargent's (2) method was used in solving the equations along with Hyman's (33) method for locating the eigen values and vectors of the matrices. Solutions for both supertriangular and tridiagonal matrices were included for completeness and for comparison.

The method of incorporating efficiencies into the solution was tested numerically and found to be stable and reliable for a ten-stage system. Both Sargent's method and Hyman's method were easily programmed. Time for a dynamic solution covering up to 90 minutes of real time was 2 to 3 minutes of CPU time on an IBM-360 Model 65.

In all of the cases studied, speed of response on every tray decreased with a decrease in efficiency. For a hypothetical case the apparent time constant for change increased from 3.75 minutes, to 5.5 minutes, to 40 minutes for efficiencies of 100, 70, and 20 percent respectively.

When efficiencies are included in the proposed manner the characteristic roots of the solution may be complex numbers yielding sine and cosine solutions.

This is impossible when using a modified K value to account of the effects of efficiencies.

The predictions of the model were compared to experimental response curves for relatively large (10 - 30%) step changes in feed composition. The model was found to be capable of predicting the response of the experimental unit. For runs where a good match in initial and final compositions were computed the computed response deviates from the actual less than 3% over response curve.

I INTRODUCTION

The original idea of investigating the effects of component separation efficiencies upon distillation tower dynamic response came from Dr. Nathan Gilbert. (9) After observing the efforts of a major industrial concern in developing dynamic models Dr. Gilbert concluded fundamental knowledge was lacking as a firm basis for description. For large units distilling a range of components the present models predicted gross rates of change three and four times in excess of the observed rates.

Research was initiated to investigate two of the fundamental considerations which are usually disregarded in formulating a distillation model. The importance of heat transfer as the rate controlling phenomena was studied by Mr. Robert Milam and the importance of component separation efficiencies fell to this author. The four primary considerations to be answered by this thesis are:

1. Does mass transfer efficiency have a significant effect upon the response of distillation towers?
2. Can the effect be realistically simulated with the concept of a Murphree Tray Efficiency for each component?
3. What numerical techniques may best be used to incorporate this effect into the mathematical model?
4. Can the concept and the calculational methods be experimentally verified?

For reasons to be presented later in this thesis a matrix method of formulation was chosen for the numerical solution. Midway through the thesis it was discovered that through little additional effort the mathematics could be kept general enough to apply to quite a variety of chemical engineering problems. Beyond the usual distillation parallels of absorption and extraction the methods apply to staged processes with mass transfer or reaction where either by-pass or recycle occurs. Stated in its most succinct mathematical form the matrix methods apply to the steady-state and dynamic solutions of sets of linear and non-linear equations which may be expressed according to the matrix equation:

$$\frac{d\bar{X}}{dt} = \bar{A} \bar{X} + \bar{F} \quad i=1,2..I$$

Where: $\bar{A} = \bar{A}(t)$ an N by N coefficient matrix,

$\bar{F} = \bar{F}(t)$ a column vector of length N

t = the scalar independent variable, i.e. time,

$\bar{X} = \bar{X}(t)$ a column vector of length N and the dependent variables.

Note that there are N times I total equations represented by the I sets of N equations. The limitation of this method is that the matrix $\bar{A}$ must be at least supertriangular. That is, $\bar{A}$ must contain all zero elements on either side of the three central top to bottom diagonals.

Such a matrix is shown below.

	2	5	7	3	1	0	6
	1	7	6	5	4	9	1
	0	8	6	5	9	4	2
	0	0	4	7	1	3	2
	0	0	0	7	4	9	0
zero elements	0	0	0	0	8	2	8
	0	0	0	0	0	3	7

three central diagonals

While this may seem a rather restrictive limitation it should be noted that matrix application to staged chemical engineering problems has been previously limited to coefficient matrices containing elements only on the three central diagonals. In terms of stage processes this means a stage may communicate with any number of stages behind it but only with the first stage in front of it, or vice versa.

Two such situations are shown in Figure 1. The development of these matrix techniques was taken as an end in itself and a secondary purpose of this thesis.

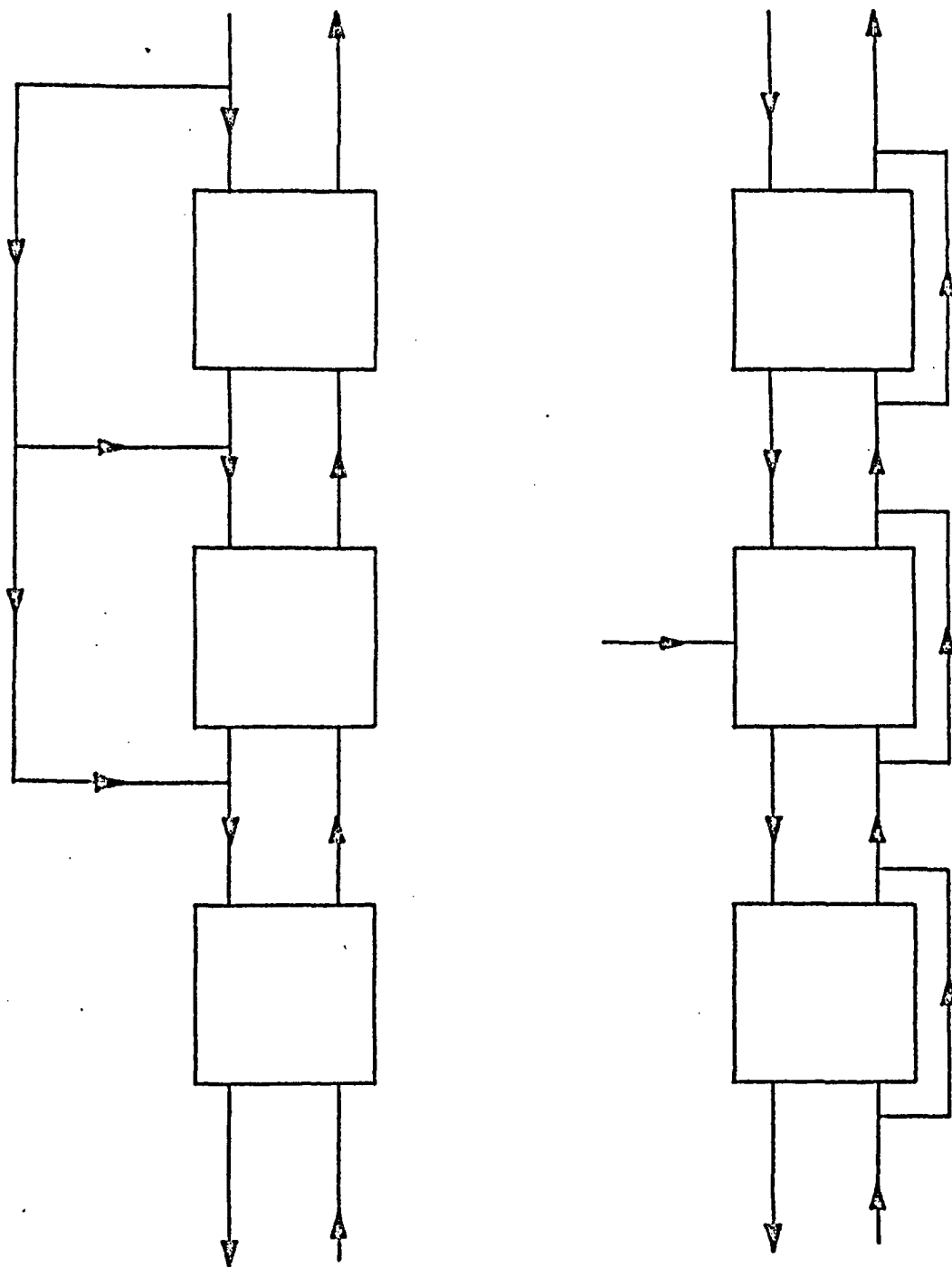
The Distillation Tower as a Dynamic System

The prediction of tower dynamic behavior finds application to a variety of distillation problems. Process start-up and batch operations are two familiar ones. Probably the widest application, however, is in the design of control systems. Whatever the application, the physical arrangement on which the model is based is much the same.

Figure 2 depicts a typical distillation tower under operating

FIGURE 1

Two examples of the types of staged processes which could be modeled using the proposed matrix mathematics and numerical methods.



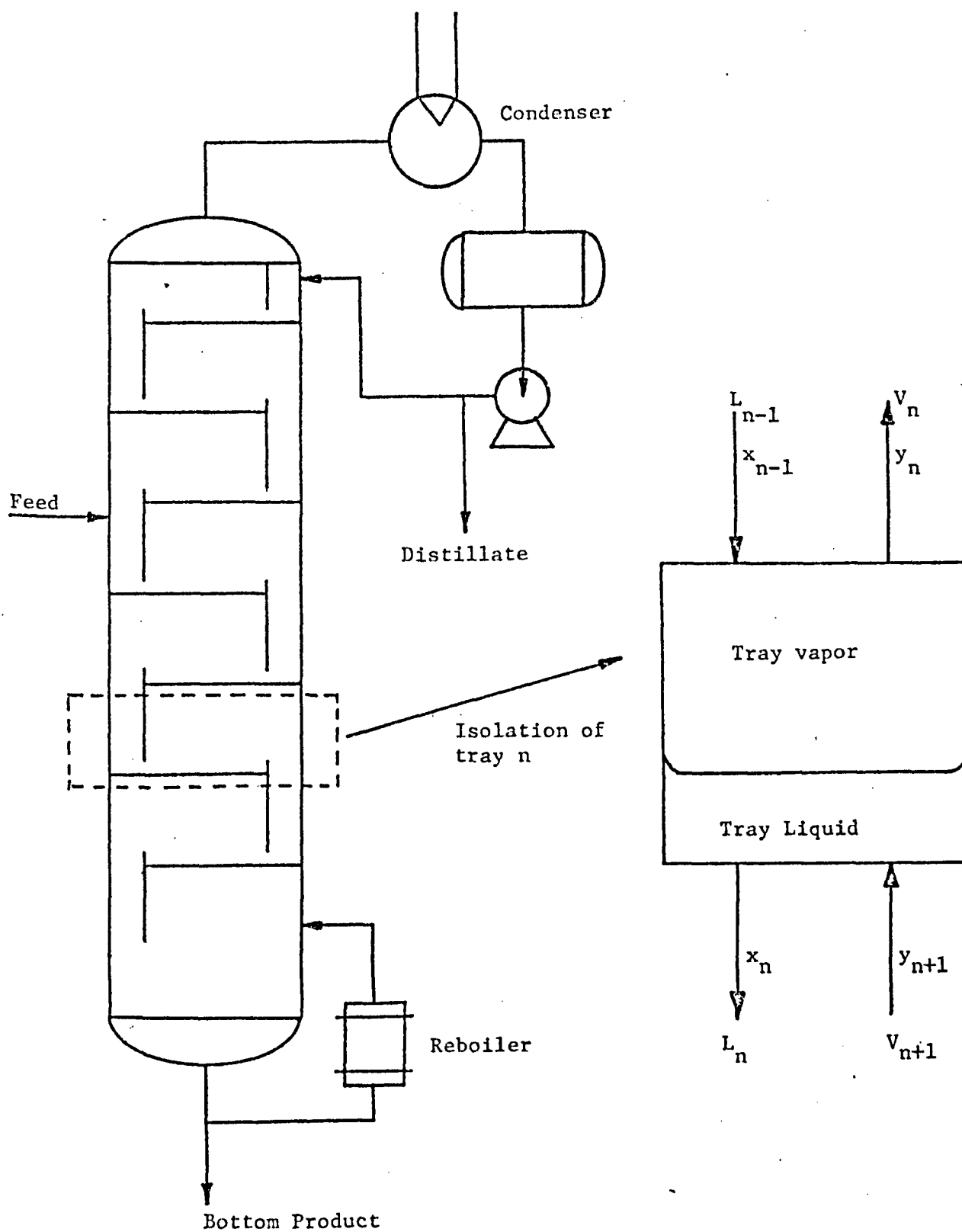
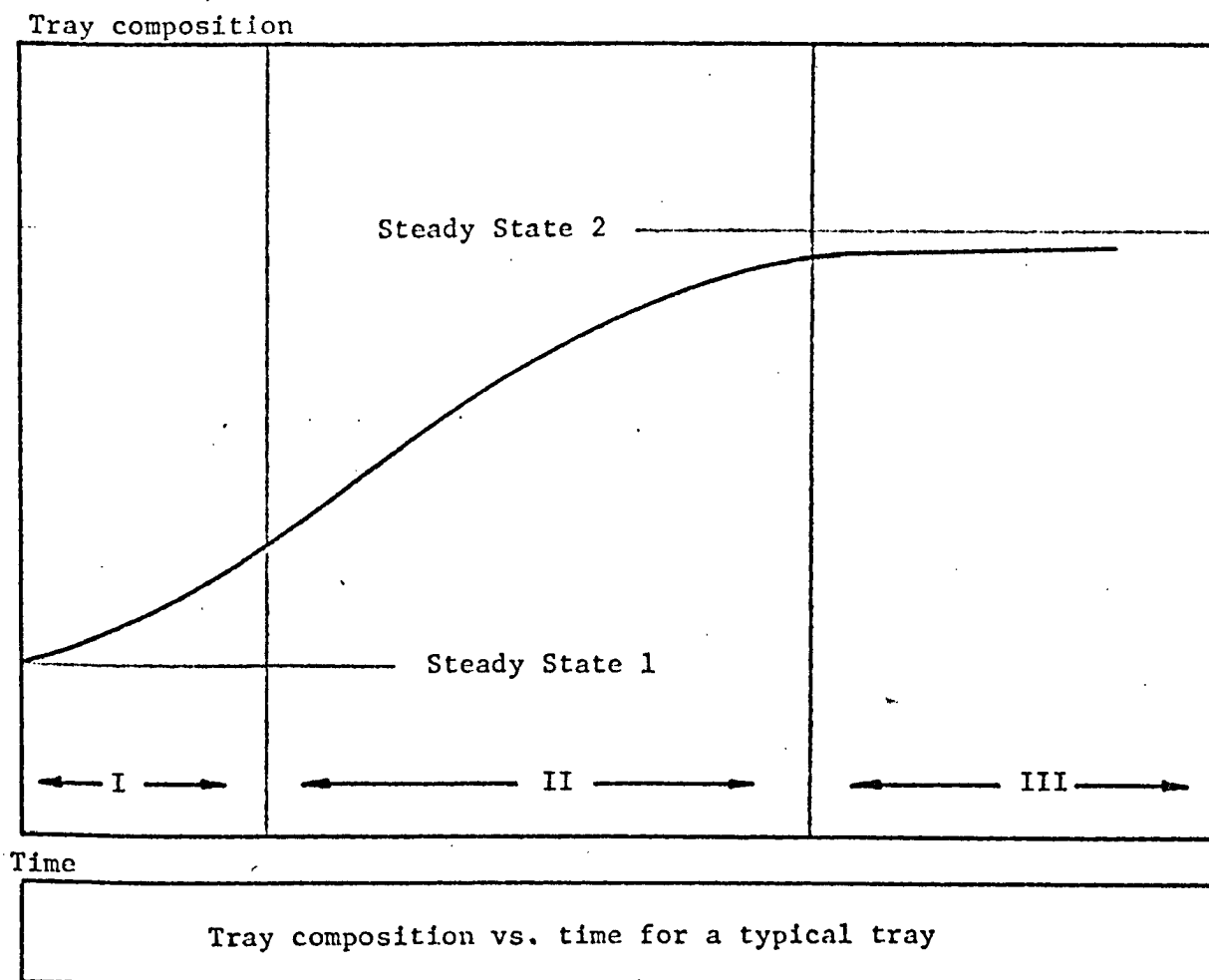


Figure 2

conditions. Vapor from the reboiler passes upward through the perforations or slots on the trays where it contacts the liquid which is cascading down across the trays. Feeds and products are being added and withdrawn from various trays and the condensed vapor is returned to the tower as liquid reflux. The dynamic description of the tower consists of the simultaneous description of each tray of the tower plus the reboiler and condenser. Figure 2 shows the model tray and adjacent trays with the streams labeled L for liquid, and V for vapor. Each tray contains liquid and vapor hold-up. The essential problem is to relate the variation of the exiting streams and the hold-ups to the variation of the inlet streams. The relationships which are used to determine this variation are; component mass balances, heat or enthalpy balance, liquid-vapor equilibrium, degree of approach to equilibrium, and the hydrodynamic relations. Each of these relationships takes on special importance in certain problems and in certain phases of every problem. Figure 3 shows the response of a single tray to a change in reflux ratio. The curve is broken into three regions. In region I (the initial response), the disturbance is propagated mainly by the liquid phase and the tray hydrodynamics play a dominant role in determining how fast the flow change becomes a concentration change. For control about a steady-state where small disturbances determine the corrective action this is the primary region of interest. In region II mass transfer becomes significant and liquid and vapor rates may change due to unequal heats of vaporization of the components. In region III mass transfer becomes completely controlling as the rates become fixed, hold-ups have stabilized and concentrations slowly approach their new steady state values.



Because of the complexity of the problem taken in its entirety, no general method of solution exists which proceeds from formulation, to computation to response prediction and control simulation. Nor is it the purpose of this thesis to do so. Whenever possible considerations other than mass transfer will be eliminated or their effects minimized to allow better examination of mass transfer considerations. This is particularly true in the experimental portion of the thesis.

Significant Past Work

According to Mah ⁽¹⁴⁾ the earliest chemical engineering investigation of column dynamics was that of Huffman and Urey ⁽³⁸⁾ on the separation of oxygen isotopes in 1935. Approximately fifteen years later detailed mathematical formulation of the model was proposed by a number of authors differing only in their emphasis or their particular notational procedures. Marshal and Pigford ⁽¹⁵⁾, Davidson ⁽⁶⁾, and Lapidus and Amundson ⁽¹³⁾ all published similar works which derive the basic mass and heat balances which make up the model. Amundson's works are particularly significant to this thesis since he emphasizes a matrix approach which greatly simplifies the bookkeeping of large numbers of variables. His more recent book ⁽²⁾ provides an excellent summary of his method of formulation and shows how analytical solutions to the matrix equations may be developed (providing certain simplifying assumptions may be made).

The advent of the computer brought on a variety of solutions to these sets of equations. Since the problem is one of solving a large set of differential difference equations, it is not surprising that both analog and digital computer solutions have been proposed. Both techniques require a large machine for a practical problem. The non-linear nature of the

equations complicates the analog solutions and the sensitivity of the solutions makes the numerical integration of the digital solution a difficult undertaking. Analog solutions using active and passive circuits have been devised by Acrivos and Amundson ⁽¹⁾, Rijasdorp ⁽²¹⁾, and Rose and Williams ⁽²³⁾ to name but a few. The analog solution is superior for analyzing control problems about a steady state where the equations may be linearized and controllers may be connected directly into the electrical model. Once programmed the parameters of the controllers may be varied and new solutions generated with little additional effort.

While the digital computer allows the non-linear nature of the problem to be preserved it does require the numerical integration of large sets of differential equations. This requires a large memory, an extremely detailed and well organized notational procedure, and the choice of a suitable time interval of integration. Various numerical integration techniques such as Euler's Method, Runge-Kutta, and predictor-corrector methods have been tried ^(26,14,16). These methods suffer from the common numerical malady of step length choice. Too large a step length in this highly non-linear problem leads rapidly to an accumulating error and a meaningless solution. Another disadvantage is that these techniques reveal little other than a once through solution of the specific problem. No fundamental measure of response is directly obtained. The main advantage of this method is the ability to incorporate new concepts into the solution regardless of the arithmetic complexity.

Probably the finest collection of recent work on unsteady state processes may be found in Holland's text ⁽¹²⁾. Here all of the modern numerical and matrix methods are presented. Until this work all of the work which included efficiencies in the solution has been done with the purely numerical approach rather than the matrix approach. Rosenbrock ⁽²⁵⁾ included Murphree efficiencies in a numerical model for a binary system for the sake of completeness, however, he made no investigation of their effects. For multicomponent mixtures a simplified definition of efficiency has usually been used to incorporate efficiencies into the model. This consists of defining a modified K-value and using the modified K value in the solution usually used for ideal trays. Thus the effect of efficiencies is accounted for in the tray equilibrium relations - through the K values. With matrix methods the only mention of tray efficiencies appears in Sargent's article ⁽²⁶⁾. He suggested, in a post script, how efficiencies might be incorporated into the matrix solution using the modified K-value approach and assumed that a physical basis did not exist for the estimation of component efficiencies.

The modern matrix methods of Mah and Sargent are lacking in two important respects. There is little numerical testing of the methods and no experimental verification. In fact, Holland ⁽¹²⁾ states that as of 1966 they had been tried on only one problem. Solutions with the matrix method including efficiencies have, to this author's knowledge, never been attempted nor has any experimental verification of these methods been done.

A Plan of Attack

As will be shown later in Section II it was discovered that using the concept of a Murphree Efficiency for each component on each tray, the general matrix model of Amundson and of Mah ⁽¹⁴⁾ could be modified to include efficiencies with no compromise as to mathematical rigor. The matrices, however, take on a more complex form containing many more elements than they would with ideal trays. Mah had already developed a numerical method of solution for the simpler matrix equations. If his solutions could be modified to apply to the matrix containing tray efficiencies, a method yielding both numerical response and a fundamental measure of response in terms of the eigen values and eigen vectors of these matrices could be obtained. Although this model was designed to solve the distillation problem in its most general form, heat and hydrodynamic calculations were eliminated whenever possible by holding vapor and liquid rates constant and column hold ups constant. In this way the mass-transfer should not be masked by these phenomena. This was true in both experimental and numerical investigations.

After developing this matrix model and the appropriate mathematics for solution, the model was tested under steady-state conditions. Then the model was applied to simplified situations using simplified vapor-liquid equilibrium data and varying efficiencies to determine the gross effects efficiency might be expected to have on response. The model was then tested under completely general vapor-liquid equilibrium relations to determine appropriate time intervals of integration and convergence properties. Finally the model was tested

against a real system - a ten tray sieve tower distilling a mixture of benzene, toluene and p-xylene.

II PROBLEM FORMULATION

Introduction

The most general mathematical formulation for distillation tower dynamics consists of a component mass balance and a heat balance for each stage of the unit. For N stages, including the reboiler and condenser, and I components this gives N times I simultaneous differential equations relating components; that is, a mass balance for each component on each stage. A differential heat (enthalpy) balance may be written about each stage yielding N additional equations. To these basic sets may be added the problem dependent relationships such as vapor-liquid equilibrium, tray hydrodynamics, and tray pressure drop including its influence on tray boiling temperature. The main idea in this case was to isolate the $N \times I$ component balances and to explore ways of solving these equations simultaneously, including in the solution the added complexity of non-ideal trays.

Generalized Component Balance

For a tower containing N total stages (with the overhead condenser being stage 1) and I components the unsteady-state mole balance on a tray n for component i is:

$$\frac{d}{dt} (g_{n,i,n} y_{n,i,n} + G_{n,i,n} x_{n,i,n}) = L_{n-1,i,n-1} x_{n-1,i,n-1} - (L_{n,i,n} x_{n,i,n} + V_{n,i,n} y_{n,i,n} + P_{n,i,n} x_{n,i,n}) + V_{n+1,i,n+1} y_{n+1,i,n+1} + f_{i,n} \quad (2.1)$$

where: g_n , G_n = Vapor and liquid holdup on tray n ,

V_n , L_n = Vapor and liquid rates leaving tray n ,

$y_{i,n}, x_{i,n}$ = Vapor and liquid mole fractions of component i
leaving tray n .

P_n = Liquid Product rate leaving tray n .

$f_{i,n}$ = Feed rate of component i onto tray n .

Written for trays 1 thru N and for components 1 thru I , N times I
differential equations may be obtained. How, or if, these equations may
be solved depends upon how the vapor compositions on the tray are related
to the liquid compositions. Most equilibrium data is correlated in the
f
$$y_{i,n}^* = K_{i,n} x_{i,n} \quad (2.2)$$

where $y_{i,n}^*$ is the equilibrium vapor composition for liquid composition
 $x_{i,n}$. The $K_{i,n}$ are functions of the total pressure, temperature, component
 $x_{i,n}$. The $K_{i,n}$ are functions of the total pressure, temperature, component
and liquid composition. For a given pressure and liquid composition the
 $K_{i,n}$ are functions of temperature and can be determined by the bubble
point calculation

$$\sum K_{i,n} x_{i,n} = 1.0 \quad (2.3)$$

Let us first consider the mass balance for ideal trays which by
definition are equilibrium stages where; $y_{i,n} = y_{i,n}^*$. Further assume that
the molar liquid holdup is much larger than the molar vapor holdup and that
the liquid holdup variation may be taken as zero over a time interval of
integration. Replacing $y_{i,n}$ by $K_{i,n} x_{i,n}$ Eq. (2.1) becomes

$$\frac{dx_n}{dt} = \frac{L_{n-1}x_{n-1}}{G_n} - \frac{(L_n + V_n K_n + P_n)x_n + V_{n+1}K_{n+1}x_{n+1} + f_n}{G_n} \quad (2.4)$$

where the (i) subscript has been omitted for simplicity. Combining the
quantities before the x_n into the terms a_n , b_n , and c_n respectively and

defining $f' = f/G$ Eq. (2.4) may be written in the more simplified form

$$\frac{dx}{dt} = a_n x_{n-1} - b_n x_n + c_n x_{n+1} + f'_n \quad (2.5)$$

Written for trays 1 thru N this set of equations for a single component may be conveniently put into the matrix form

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} b_1 & c_1 & 0 & 0 & 0 \dots 0 \\ a_2 & b_2 & c_2 & 0 & 0 \dots 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 \dots a_n & b_n & c_n & 0 \dots 0 \\ 0 & 0 & 0 & 0 & \dots a_N & b_N \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \\ \vdots \\ x_N \end{bmatrix} + \begin{bmatrix} f'_1 \\ f'_2 \\ \vdots \\ f'_n \\ \vdots \\ f'_N \end{bmatrix} \quad (2.6)$$

or more succinctly,

$$\frac{dX}{dt} = \Lambda X + F \quad (2.7)$$

Note that the matrix of the coefficients contains all of its non-zero elements on the three central diagonals. Thus the matrix Λ is termed tridiagonal or a Jacobi matrix. The properties of this type of matrix are well known and it is this unique form which makes the assumption of ideal trays so attractive. The solution of Eq. (2.7) will be shown in Sections III and IV for the tridiagonal form.

With the added complication of non-ideal trays the development is identical to the above up to the point where the equilibrium relationship, $y_{i,n} = y^*_{i,n} = K_{i,n} x_{i,n}$ is substituted into the component mass balance. If the Murphree tray efficiency is used to describe the degree of approach to equilibrium, the efficiency relation and the liquid-vapor phase equilibrium together determine the variation of vapor compositions with liquid compositions. The Murphree tray efficiency for component i on tray n is defined as

$$E_{n,i} = \frac{y_{n,i} - y_{n+1,i}}{K_{n,i}x_{n,i} - y_{n+1,i}} \quad (2.8)$$

This relation may be used to relate the vapor composition leaving a tray to the liquid composition on that tray and the vapor composition from the tray below when re-arranged into the form

$$y_n = E_n K_n x_n + (1-E_n) y_{n+1} \quad (2.9)$$

Writing this equation for trays 1 to N gives the series:

$$y_1 = E_1 K_1 x_1 + (1-E_1) y_2 \quad (2.10)$$

$$y_2 = E_2 K_2 x_2 + (1-E_2) y_3 \quad (2.11)$$

$$y_N = K_N x_N \quad \text{.. For the reboiler} \quad (2.12)$$

Equations (2.10) thru (2.12) may be substituted into the component mole balance (in succession) and each vapor composition made a function of the liquid on the tray and trays further down the tower. That is,

$$y_n = y_n(x_n, x_{n+1}, x_{n+2} \dots x_N).$$

Written in matrix form, the N differential equations become

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} & \dots & a_{1,N} \\ a_{2,1} & a_{2,2} & a_{2,3} & \dots & \dots & a_{2,N} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & a_{n,n-1} & a_{n,n} & a_{n,n+1} & \dots & a_{n,N} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & a_{N,N-1} & a_{N,N} & \vdots \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \\ \vdots \\ x_N \end{bmatrix} + \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \\ \vdots \\ f_N \end{bmatrix} \quad (2.13)$$

The matrix of coefficients is now supertriangular having non-zero elements on, above, and one position below the main diagonal. This type of matrix is also referred to as an upper Hessenberg matrix or an almost-triangular matrix.

The appropriate algorithm for generating the matrix of coefficients is as follows:

$$a_{n-1,n} = L_{n-1,n} / G_n \quad n=2,3,4,\dots,N \quad (2.14)$$

$$a_{n',n} = -(V_{n,n} K_{n,n} E_{n,n} + L_{n,n} + P_{n,n}) / G_n \quad n=1,2,3,\dots,N \quad (2.15)$$

$$a_{n,n+p} = (V_{n+1,n} - V_{n,n} (1-E_{n,n})) E_{n,n+p} K_{n+p,n} / G_n \prod_{r=p-1}^{N-1} (1-E_r) \quad (2.16)$$

where $n=1,2,3,\dots,n-1$ and $p=n+1,\dots,N$ for each value of n .

The efficiencies and the K values are understood to have the subscript i indicating component. For I components there are I matrices identical in form. That is I matrix equations of the form

$$\frac{d\bar{X}_i}{dt} = \bar{A}_i \bar{X}_i + \bar{F}_i \quad i=1,2,3,\dots,I \quad (2.17)$$

In the following section the solution of these equations will be explored.

Heat Balance

Liquid and vapor rates through the tower are determined by the heat balance, which for stage n , may be written as

$$\frac{d}{dt} (H_n G_n + h_n g_n + T'_n) = V_{n-1} h_{n-1} - (L_n H_n + V_n h_n) + L_{n+1} H_{n+1} - P_n H_n + F_n H_n + Q_n \quad (2.19)$$

where

T'_n = The heat content of the tray material,

H_n = the molar liquid enthalpy for the liquid on tray n ,

h_n = the molar vapor enthalpy for the vapor on tray n ,

Q_n = the rate of heat addition to tray n ,

H_f = the molar enthalpy of the feed to tray n ,

F_n = the molar feed rate to tray n

G_n, g_n = liquid and vapor holdups respectively.

An equation of this form may be written for each stage of the process, $n=1, 2, \dots, N$. This set of heat balances is related directly to the component balances since the composition on the tray determines the molar enthalpies in Eq. (2.19).

III SOLUTION OF THE MATRIX EQUATIONS

Introduction

In Section II the component mass balances for a tray were derived and it was shown how these equations could be put into the convenient matrix form.

$$\frac{d\bar{X}_i}{dt} = \bar{A}_i \bar{X}_i + \bar{F}_i \quad i=1,2..I \quad (3.1)$$

In this section the methods used to solve these equations for the dynamic and steady-state cases will be presented. Methods for ideal and non-ideal trays are included for comparison and completeness.

Steady-state Solutions

At steady state the equations representing the component balances become; $\bar{A}_i \bar{X}_i = -\bar{F}_i$ ($i=1,2..I$) where the elements of the coefficient matrices are functions of the liquid and vapor rates, equilibrium constants, and ultimately of the $\bar{X}_i$. For fixed feed rates, reflux ratio and product rates, Amundson (2) has developed an iterative method of solution to these equations. The basis of his solution is presented below, where the details of the computational techniques have been postponed until Section IV, "Numerical Methods."

As a first approximation, constant molar overflow is assumed and liquid and vapor rates computed accordingly. A rough guess of the top and bottom stage temperatures and the assumption that tray temperature varies linearly with tray number assigns a temperature to each tray of the tower. With the flow rates and temperatures in hand, K values may be

computed for each component on each tray and the coefficient matrix formed for each component. The equations $\bar{A}_i \bar{X}_i = -\bar{F}_i$, ($i=1,2..I$) are solved individually for the mole fraction of each component on each tray. Having the compositions, revised estimates of tray temperatures may be made along with revised estimates of liquid and vapor rates. Now new coefficient matrices may be computed and the whole process repeated until convergence is reached. Convergence is achieved when the sum of the X_i ($i=1,2..I$) as computed from the separate matrix equations equals the identity vector and the sum of the $K_i x_i$ ($i=1,2..I$) on every tray equal 1.0 (plus or minus a tolerance of convergence).

Many authors write the steady-state solution of Eq. (3.1) in the form $\bar{X}_i = -\bar{A}_i^{-1} \bar{F}_i$ ($i=1,2..I$). This is believed to be somewhat misleading in that it implies the way to compute the $\bar{X}_i$ is to invert the $\bar{A}_i$. While mathematically accurate this is a poor technique numerically. With or without tray efficiencies, the matrices ($\bar{A}_i$, $i=1,2..I$) contain large numbers of zero elements and the equations $\bar{A}_i \bar{X}_i = -\bar{F}_i$ may be more easily solved using elimination algorithms.

For ideal trays $\bar{A}_i$ is tridiagonal with all of its non-zero elements lying on the three central diagonals. With non-ideal trays $\bar{A}_i$ is super-triangular and contains all of its non-zero elements on and above the three central diagonals. Solving with the elimination algorithm proceeds in much the same way as one would solve the N linear, simultaneous equations represented by each matrix equation by hand computation. Starting with the last equation (the N th row), x_N may be made a function of

x_{N-1} and f_N . The variable x_N may then be eliminated in each of the other equations which contain it. Working up through the rows x_{N-1} , x_{N-2} , x_{N-3} ... x_2 are eliminated (in sequence) and the value of x_1 computed. Back substitution into the equations used to eliminate each x_n gives x_2 to x_N .

Elimination Algorithm for Tridiagonal $\bar{A}$

For the set of N linear equations represented by the equation, $\bar{A}\bar{X} = -\bar{F}$, where $\bar{A}$ is tridiagonal the following algorithm holds for solution:

$$\bar{A} = \begin{vmatrix} b_1 & c_1 & 0 & 0 & . & . & 0 \\ a_2 & b_2 & c_2 & 0 & . & . & 0 \\ 0 & a_3 & b_3 & c_3 & . & . & 0 \\ . & . & . & 0 & a_{N-1} & b_N \end{vmatrix}$$

As the coefficients of the matrix are operated upon, the old values are destroyed. Let the starred quantities stand for the new values and unstarred for the old.

$$\text{Define: } c_1^* = c_1 / b_1, f_1^* = f_1 / b_1 \quad (3.2)$$

Now operate upon each row of the matrix, letting:

$$c_{i+1}^* = c_{i+1} / (b_{i+1} - a_{i+1}c_i^*) \quad (3.3)$$

$$\text{and, } f_{i+1}^* = (f_{i+1} - a_{i+1}f_i^*) / (b_{i+1} - a_{i+1}c_i^*) \quad (3.4)$$

from $i=1$ to $i = N-1$.

Now back-substitute to obtain each x by:

$$x_N = f_N^* \quad (3.5)$$

$$\text{and, } x_i = f_i^* - c_i^* x_{i+1}, i = N-1 \text{ to } 1 \quad (3.6)$$

Elimination Algorithm for Supertriangular $\bar{A}$

The solution for the supertriangular matrix is entirely analogous to the solution presented for the triangular matrix. The only difference is in the number of operations which must be performed. This method is easily visualized by thinking of the matrix terms as coefficients in a system of linear equations. Each row of the $\bar{A}$ matrix contains the coefficients of a single equation. For the set of N linear equations given by the matrix equation

$$\bar{A}\bar{X} = -\bar{F} \quad (3.7)$$

where $\bar{X}$ and $\bar{F}$ are column vectors of length N , and $\bar{A}$ is a supertriangular matrix of order $N \times N$, the very last row contains only two non-zero elements, $a_{N,N-1}$ and $a_{N,N}$. The second last row contains only three non-zero elements and they are in the last three row positions, $a_{N-1,N-2}$, $a_{N-1,N-1}$, and $a_{N-1,N}$. And so it goes up the rows of the matrix, with each preceding row containing one more element to the left-hand side of the matrix than the previous row. Using the last row, the equation

$$a_{N,N-1} x_{N-1} + a_{N,N} x_N = -f_N \quad (3.8)$$

$$x_N = -f_N / a_{N,N} - a_{N,N-1} x_{N-1} / a_{N,N} \quad (3.9)$$

may be used to eliminate x_N in each equation (matrix row) above the last one (row N). Now the system contains $N-1$ equations and $N-1$ unknowns. If the process is repeated using row $N-1$, x_{N-1} may be eliminated and so on up to equation 1 where the process terminates with one equation and one unknown, x_1 . The value of x_1 may then be substituted into each succeeding equation which was used in the elimination steps and $x_2, x_3, x_4, \dots, x_N$

computed. In terms of operations upon the matrix $\bar{A}$ and the column vector $\bar{F}$, the sequence is as follows. Note that the original matrix is destroyed as the coefficients are eliminated. Let starred quantities refer to new values in the matrix and unstarred to the previous values.

For $i = N, N-1, \dots, 2$ define:

$$g_i = f_i/a_{i,i}, \text{ and } h_i = -a_{i,i-1}/a_{i,i} \quad (3.10-3.11)$$

For each i update the matrix and vector according to:

$$a_{j,i-1}^* = a_{j,i-1} + a_{j,i}h_i, \quad j=1,2,\dots,i-1 \quad (3.12)$$

$$f_j^* = f_j - a_{j,i}g_i, \quad j=1,2,\dots,i-1 \quad (3.13)$$

After eliminating all rows except the first, compute

$x_1 = f_1/a_{11}$ and back-substitute to obtain the

rest of the x_i according to

$$x_i = g_i + h_i x_{i-1}, \quad i=1,2,\dots,N. \quad (3.14)$$

Dynamic Solutions

The unsteady-state solution to the sets of matrix equations

$\frac{d\bar{X}_1}{dt} = \bar{A}_1 \bar{X}_1 + \bar{F}_1$ ($i=1,2,\dots,I$) must in general be iterative since each $\bar{A}_1$ is a

function of all components and the relationship is implicit. This is

mainly because the elements of $\bar{A}_1$ contain the K values, but could also be

because of variations in the liquid and vapor rates which also enter into

the $\bar{A}_1$. An iterative procedure, which takes each $\bar{A}_1$ constant over a time

interval of integration, is accurate only if the errors generated cancel

rather than accumulate with each succeeding iteration. For stable physical

systems, which follow this first-order equation, it is not uncommon for $\frac{d\bar{X}}{dt}$ to be quite sensitive to $\bar{X}$, and an iterative procedure to lead to quite different end points, depending upon the variation in $\bar{X}$ over the interval. Furthermore, these errors can (and for distillation problems do) accumulate very rapidly. Fig. 4 shows how a solution would behave if $\frac{d\bar{X}}{dt}$ were computed from conditions only at the initial point of each interval of integration. In this case the error in the slope increases as the error in $\bar{X}$ increases.

Sargent ⁽²⁶⁾ has investigated a variety of methods of integration. Among those tried are Runge-Kutta, Euler's, and various predictor-corrector types. The method he found to be superior is an iterative scheme which accounts for a linear variation in the coefficient matrices over each time interval of integration. Sargent's formulae and method are presented below. For a formal mathematical derivation the reader is referred to Ref. (26).

For the sets of matrix equations represented by

$$\frac{d\bar{X}}{dt} = \bar{A}_1 \bar{X}_1 + \bar{F}_1 \quad i=1,2..I \quad (3.15)$$

assume the coefficient matrices $\bar{A}_1$ may be represented as linear functions of time over an interval of integration. Then $\bar{A}_1 = \bar{B}_1 + \bar{C}_1 t$ where $\bar{B}_1$ and $\bar{C}_1$ are matrices of constant coefficients. Similarly, each feed vector is approximated as a linear function of time over a small interval as $\bar{F}_1 = \bar{R}_1 + \bar{S}_1 t$ where $\bar{R}_1$ and $\bar{S}_1$ are constant vectors. Substituting the linear expressions for $\bar{A}_1$ and $\bar{F}_1$, Eq. (3.15) becomes

$$\frac{d\bar{X}}{dt} = (\bar{B}_1 + \bar{C}_1 t) \bar{X}_1 + \bar{R}_1 + \bar{S}_1 t \quad i=2,3..I \quad (3.16)$$

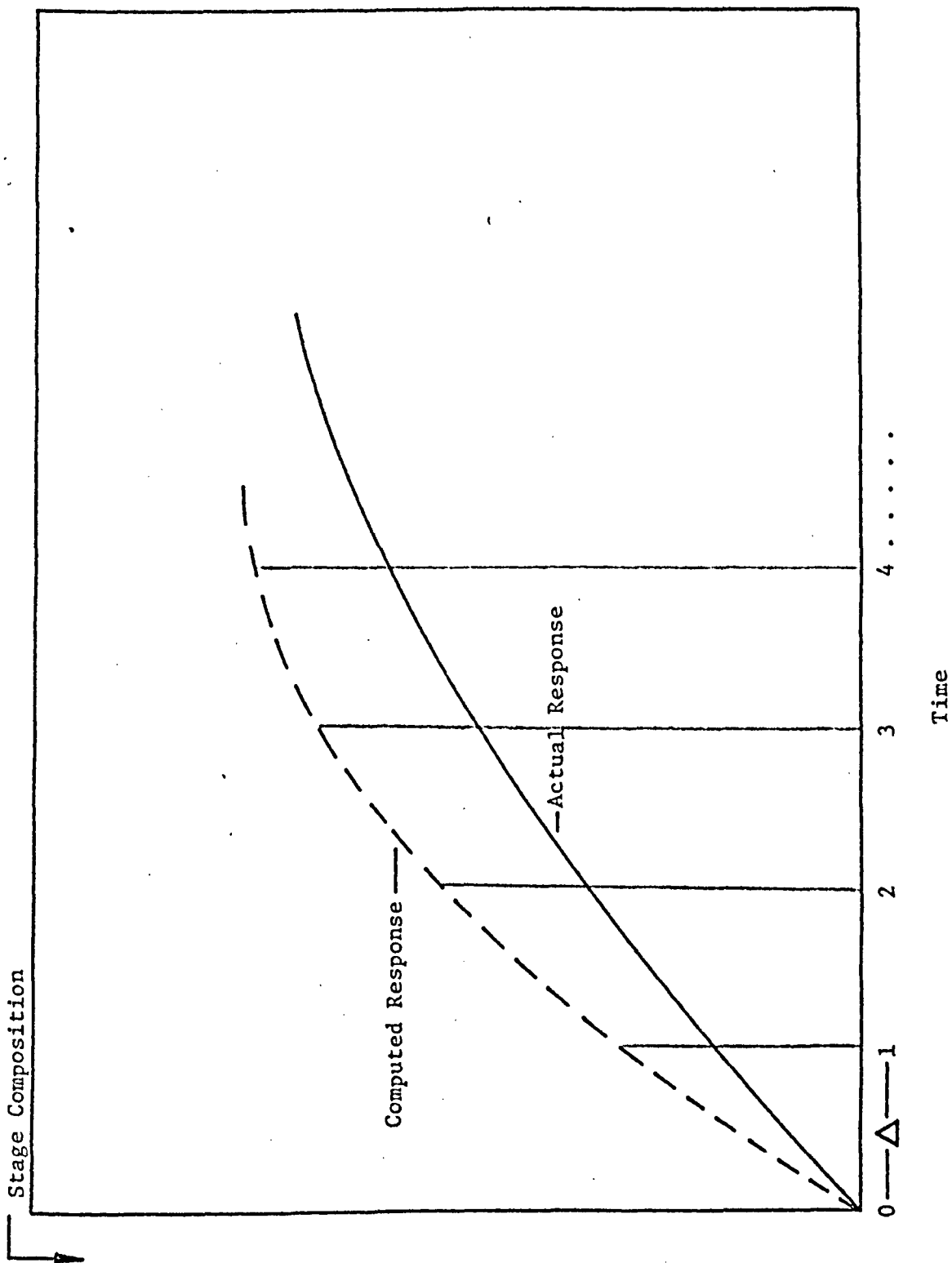


FIGURE 4 Accumulation of error in an iterative procedure.

Sargent has solved this equation for constant $\bar{B}_1, \bar{C}_1, \bar{R}_1$, and $\bar{S}_1$, and after truncation of terms in t^3 and higher, his solution is

$$\bar{X}_1(t) = \exp(\bar{B}_1 t) \left\{ (\bar{I} + 1/2 \bar{C}_1 t) \bar{X}_1(0) + \bar{B}_1^{-1} \bar{F}_1 \right\} - (\bar{B}_1^{-1} \bar{F}_1 + 1/2 \bar{S}_1 t) \quad (3.17)$$

where:

$$\bar{X}(t) = \bar{X}(0) \quad \text{at } t=0,$$

$\bar{I}$ = the identity matrix,

$\bar{B}_1^{-1}$ = the inverse matrix of $\bar{B}_1$.

In solving this equation the initial conditions are always known and the $\bar{B}_1$ are readily computed from $\bar{B}_1 = \bar{A}_1(0)$. As a first approximation $\bar{C}_1$ may be taken as zero and Eq. (3.17) solved for $\bar{X}_1(t)$, which at the end of the time interval is $\bar{X}_1(\Delta t)$. Having the approximate conditions at the end of the interval the $\bar{C}_1$ may now be computed according to $\bar{C}_1 = (\bar{A}_1(\Delta t) - \bar{A}_1(0)) / \Delta t$. Eq. (3.17) may be solved again, this time including the $\bar{C}_1$ in the solution, which produces refined estimates of $\bar{X}_1(\Delta t)$ and hence a refined $\bar{C}_1$. The sequence is repeated until the $\bar{X}_1(\Delta t)$ as computed from two successive iterations are sufficiently unchanged. Note that Eq. (3.17) must be solved for each component present since it is a component balance. While the component balances are not strictly independent since their sum is the total mass balance, all equations must be solved to maintain corresponding orders of accuracy for each component. More will be said about this in the following section.

For a step-change in feed composition, $\bar{S}_1$ in Eq. (3.17) equals the zero vector and after replacing $\exp(\bar{B}_1 t)$ with its equivalent diagonalized form Eq. (3.17) becomes

$$\bar{X}_1(t) = \bar{E}_1^{-1} \exp(\bar{\Lambda}_1 t) \bar{E}_1 \left\{ (\bar{I} + 1/2 \bar{C}_1 t^2) \bar{X}_1(0) + \bar{B}_1^{-1} \bar{F}_1 \right\} - \bar{B}_1^{-1} \bar{F}_1 \quad (3.18)$$

where:

Λ_1 is the diagonal matrix or eigen values,

$\bar{E}_1$ is the NxN matrix of eigen vectors,

and E_1^{-1} is the inverse of E_1 .

It is the computation of the eigen values and eigen vectors of the $\bar{B}_1$ matrices which represents the major computational effort involved in the numerical solution of Eq. (3.17). A good point concerning Sargent's method is that this need be done only once for each interval of integration, in that each $\bar{B}_1$ is computed from conditions at the beginning of the interval only.

As shown in Sec. II, when ideal trays are assumed the coefficient matrices are tridiagonal. For the tridiagonal matrix where, as for distillation, the elements along the central diagonal are negative and those along the two adjacent diagonals are positive, the eigen values are negative real numbers. ⁽¹⁴⁾ Methods of computing the eigen values and eigen vectors of tridiagonal matrices have been well developed and will not be dealt with here. For a complete discussion of these methods see Refs. 2 and 33.

For the supertriangular matrix Hyman ⁽³³⁾ has devised a method for finding the eigen values and vectors. His method is easily programmed and results in a great savings of time and effort, and is described below.

Hyman's Method ⁽³³⁾

Written in the left-handed system, the eigen value problem is as follows:

For the NxN matrix $\bar{B}_1$ find the diagonal matrix Λ_1 ; and the NxN matrix $\bar{E}_1$ such that

$$\bar{E}_1 \bar{B}_1 = \Lambda_1 \bar{E}_1 \quad (3.19)$$

Eq. (3.19) may be written for each individual element of the diagonal matrix, say λ_{1j} , and each row of the matrix $\bar{E}_1$ as

$$\bar{E}_{1j} \bar{B}_1 = \lambda_{1j} \bar{E}_{1j} \quad (3.20)$$

where $\bar{E}_{1j}$ is a row of $\bar{E}_1$ and is an eigen vector. Similarly λ_{1j} is a scalar element of the diagonal matrix Λ_1 . In order to satisfy Eq. (3.20) λ_{1j} must satisfy the relation $\det(\bar{B}_1 - \lambda \bar{I}) = 0$. Hyman's method consists of constructing a simplified function having the same roots as $\det(\bar{B}_1 - \lambda \bar{I})$, however, which is much easier to evaluate.

Elementary row transformations may be applied to a matrix without changing its determinant. If multiples of rows 2 to N are added to row 1 of $(\bar{B}_1 - \lambda \bar{I})$ its determinant remains unchanged. Accordingly $k_1, k_2, \dots, k_N$ are defined such that, if we replace the first row of $\det(\bar{B}_1 - \lambda \bar{I})$ by $\bar{I} + \sum_{i=2}^N (k_i \cdot \text{row}_i)$, the first N-1 elements vanish. Then

$$\det(\bar{B}_1 - \lambda \bar{I}) = (-1)^{N+1} b_{21} b_{32} b_{43} \dots b_{N,N-1} (b_{1,N} k_1 + b_{2,N} k_2 \dots$$

$$\dots (b_{N,N} - \lambda) k_N)$$

where the simplified function having the same zeros is $f(\lambda)$ defined as

$$f(\lambda) = (b_{1,N} k_1 + b_{2,N} k_2 \dots (b_{N,N} - \lambda) k_N)$$

The relevant algorithm for the k_1 is:

$$k_1 = 1$$

$$k_{i+1} = (b_{1,1} k_1 + b_{1,2} k_2 \dots (b_{1,i} - \lambda)) / b_{1,i-1}$$

where $i = 1, 2, \dots, N-1$

An important aspect of Hyman's method is that as λ approaches a true eigen value λ_{ij} the k_i approach the elements of the row eigen vector for λ_{ij} . That is, the k_i become the elements of each $\bar{E}_{ij}$.

IV NUMERICAL METHODS

Introduction

In this section the numerical methods which were used to generate solutions to the matrix equations are described. The equations themselves have been developed in Sec. II and some of the pertinent algorithms for solution have been developed in Sec. III. The numerical methods consist mainly of iterative methods, which become necessary at various points in the problem, when a trial and error approach is needed. In the steady-state solution Admundson's method (an adaptation of Newton's iterative method) is used to adjust an assumed temperature profile for the tower until the component mass balances and heat balances are satisfied on each stage of the tower. In the dynamic solution Newton's iterative method is used with Hyman's method for evaluating the determinant of a matrix and to locate the eigen values of the matrix. Each of these techniques, and others, are described below.

Steady-State Solutions

The solution of the steady-state distillation problem begins with the assumption of constant molal overflow and the computation of liquid and vapor rates. Next, an assumed temperature profile is assigned to the tower. For lack of better estimates a linear profile is usually taken. The matrices of coefficients may then be formed for each component using the algorithm presented in Sec. II, and the linear set of equations $\bar{A}_1 \bar{X}_1 = -\bar{F}_1$ solved for the composition of each component on each tray. Solution

algorithms for these equations are presented in Sec. III. If the correct tray temperatures and flow rates had been chosen the total mole balance ($\sum x_i = 1$) and the bubble point relation ($\sum K_i x_i = 1$) would be satisfied on each and every stage of the tower and the flow rates, as computed from the compositions and enthalpies, would not change from one iteration to the next.

In general, these relations will not be satisfied and corrections must be made to the liquid and vapor rates and to the tray temperatures. Using normalized liquid compositions and normalized equilibrium vapor compositions ($y_i^* = K_i x_i$) the efficiency definition Eq. (2.9) may be used to compute the actual vapor composition leaving each tray. The tray temperatures are then adjusted according to Amundson's iterative formula

$$T_n = T_n^* + \left(\sum x_i - \sum K_i x_i \right) \left(\sum \frac{\partial K_i}{\partial T_i} x_i \right) \quad (4.1)$$

where the star refers to the old value and the x_i s are the unnormalized liquid mole fractions.

After computing the new compositions and temperatures the enthalpies are recomputed and the liquid and vapor rates adjusted by the heat balance. A new matrix of coefficients is then computed and the entire process repeated until $\sum x_i = 1$ and $\sum K_i x_i = 1$ for each tray.

Dynamic Solution

If the component matrix equations were indeed linear, including the variation in K values, then only I-1 of the equations for I components need be solved. The Ith component could be computed by difference since

the sum of the mole fractions on each tray must equal 1. We know, however, that the equations are highly nonlinear and widely different magnitudes of mole fractions may occur on the same tray. For instance, a tray in the stripping section may contain a light component in 10^{-6} mole per cent and heavier components on the order of 30 to 50 mole per cent. If the concentration of light component were computed by difference it would be folly since proportional accuracy due to significant figures could not be maintained. Solving each component matrix over a time interval and normalizing the mole fractions allows for the same percentage error in each composition; moreover, trace components may be followed as well as the major components.

In matching the linear variation of the component matrices at the beginning and end of an interval regular iteration is used. For $\bar{A}_1 = \bar{B}_1 + \bar{C}_1 t$, $\bar{C}_1$ is assumed to be zero in the first iteration and Eq. (3.17) used to compute the $\bar{X}_1 (\Delta t)$ at the end of the time interval. Using conditions at the end of the interval of time and knowing $\bar{B}_1$, the matrix $\bar{C}_1$ may be computed and the solution repeated and $\bar{C}_1$ further refined until the $\bar{X}_1 (\Delta t)$ cease to change.

Root Search in Hyman's Method

As shown in Sec. III Hyman's method provides a simplified function $f(\lambda)$ having the same zeros as the function $\det(\bar{B} - \lambda \bar{I})$. Moreover the function $f(\lambda)$ is term by term differentiable and $f'(\lambda)$ may be computed by differentiating the algorithm for $f(\lambda)$. Newton's iteration formula with $\lambda_{p+1} = \lambda_p - f(\lambda_p)/f'(\lambda_p)$ provides an excellent search

technique for locating the roots of $f(\lambda)$. Here the subscript p refers to the iteration and λ_{p+1} is the new value and λ_p the old. Once a particular eigen value, say λ_1 , has been found, steps must be taken to insure that the search does not converge to the previously found value again. Synthetic division by the previously found factors of the function prevents this.

In evaluating the i -th eigen value, with $i-1$ eigen values having been found, let $g(\lambda) = (\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3) \dots (\lambda - \lambda_{i-1})$. The new function for search is then $h(\lambda) = f(\lambda)/g(\lambda)$ having the same zeros as $f(\lambda)$. Newton's iterative formula, applied to this new function, becomes

$$\lambda_{p+1} = \lambda_p - f(\lambda_p) / (f'(\lambda_p) - f(\lambda_p) \sum_{i=1}^{i-1} 1/(\lambda_p - \lambda_i)) \quad (4.2)$$

where, as before, $p+1$ refers to the new and p to the old value of .

Eq. (4.2) provides the basic iterative formula for determining the eigen values. In Eq. (4.2) $f(\lambda)$ remains exactly as given in Hyman's method. The derivative of $f(\lambda)$ may be computed from the following algorithm.

$$\text{Define } d_1 = 0 \text{ and } d_2 = 1/b_{2,1} \quad (4.3)$$

$$\text{then } d_{i+1} = \sum_{p=1}^{i-1} b_{p,i} d_p + (b_{i,i} - \lambda) d_{i-k_i} / b_{i+1,i} \quad i=2,3..N-1 \quad (4.4)$$

$$\text{and } f'(\lambda) = \sum_{p=1}^{N-1} b_{p,N} d_p + (b_{N,N} - \lambda) d_N \quad (4.5)$$

(33) .

The eigen values of $\bar{B}$ are bounded by the maximum row modulus of $\bar{B}$.

This provides a convenient starting point for the search for the eigen

$$\text{values. That is, } |\lambda|_{\max} = \max \sum |b_k| \quad (4.6)$$

From experience, the value is negative and nearly always a pure real number. It is generally a good idea to assume that the eigen values are all real numbers until convergence problems are encountered and then switch to a complex search. It may be shown from the Cauchy-Riemann conditions that, as long as $f(\lambda)$ is an analytic function, Newton's iterative formula and Eq. (4.2) apply equally well to complex or real numbers. (Even though the variables are labeled as COMPLEX in the machine program, computation is more rapid if the complex part equals 0.0)

Inversion of the Matrix of Eigen Values (39)

With ideal trays the eigen values must be real numbers and so must the elements of the matrixes of row eigen-vectors. With non-ideal trays no such assumption may be made, and allowance must be made for complex elements in the matrix of eigen vectors and its inverse. The inversion method must also handle complex quantities.

Elimination with pivoting on column elements written in COMPLEX programming notation is easily programmed and provides a good general inversion routine. Newman's method (39) may be used to save computer storage space by performing all of the row transformations on the $(N+1)$ by N matrix $(\overline{B}, i)$ where i is a column vector of length N with zeros in all positions except the position in the row being used for elimination. This element is unity. After each stage of elimination the columns of $(\overline{B}, i)$ are shifted one place to the left, column 1 being discarded and a new unit vector entered in column $N+1$. Upon completion of the elimination $\overline{B}^{-1}$ is in the space previously occupied by $\overline{B}$.

V PRELIMINARY NUMERICAL RESULTS

Introduction

In this section preliminary tests conducted with the mathematical model are presented. These include the testing of the numerical methods and using the model in a simplified form to access the effects of efficiencies upon tower dynamic response. Criteria of convergence and the average number of iterations needed for convergence are presented in tabular form for all of the iterative loops in the steady-state and dynamic calculations in Table A of Appendix A.

Verification of the Numerical Method

In problems of this size and completely accurate mathematical method is no guarantee that a numerical solution can be realized. Parts of the problem may be so sensitive to round-off errors that, unless an interminable number of significant figures is carried in the computations, the final answers are meaningless. For the methods used in this thesis the most sensitive are the calculation of eigen values and vectors, and the inversion of the matrix of eigen vectors. It is frequently suggested that once the eigen values have been found, back substitution into the equation $\bar{E}_1 \bar{B}_1 = \bar{E}_1$ may be used to solve for the eigen vector elements. ⁽¹⁴⁾ Wilkinson ⁽¹⁴⁾ has shown that even if the eigen values are accurate to 1 part in 10^9 the elements of the eigen vectors computed in this manner maybe, "hopelessly inaccurate". To check the method used, after computing the eigen values and vectors according to Hyman's method, each side of the equation; $\bar{E}_1 \bar{B}_1 = \bar{E}_1$ was computed separately and the worst agreement on any element was 1 part in

10^3 . This occurred in the last element of the eigen vectors of the largest and least significant eigen values. The eigen values were computed to 1 part in 10^6 .

The matrix inversion method was tested by computing the inverse matrix $\bar{E}^{-1}$ and multiplying it by the original matrix $\bar{E}$ to form $\bar{C} = \bar{E}\bar{E}^{-1}$. If there were no roundoff error $\bar{C}$ should equal the identity matrix, $\bar{I}$. As computed for the matrix of eigen vectors the elements along the main diagonal were within 1 part in 10^6 of unity and the "zero elements" were all less than 3×10^{-5} .

Check solutions for eigen values and vectors are readily obtained from several texts and can be used to check numerical methods. (33,40) A simple working method, which can be computed with little extra effort, is a trace check of the matrix before and after diagonalization. If the eigen values are correct the sum of the eigen values should equal the sum of the diagonal elements of the original matrix. While this does not guarantee that cancelling errors have not been made, it is a quick and easy method which can be used on every matrix solved. Agreement to 1 part in 10^6 was obtained for matrices with and without complex eigen values.

General Effects of Efficiencies

Using a simplified model, which assumes a constant matrix of coefficients for each component, the response for a hypothetical distillation tower distilling a mixture of normal hexane, heptane, and octane was simulated with various tray efficiencies. Using equal component and tray efficiencies of 100%, 75%, and 20%, response to a step change in feed composition was computed for each efficiency. The feed change was identical in all cases

as were the feed rate, product rates, reflux rate, etc. The selected efficiency was the same for all components on all trays and the initial and final steady states were taken as the true steady states computed on the basis of each respective efficiency.

Figure 5 shows the percent complete response vs. time for each case as seen at the distillate stream for the component N-octane. This is representative of the response of all of the components on any of the trays of the tower. On all of the trays the response, as measured either by the initial rate of change or the time for 90% response, increased with separation efficiency. For separation efficiencies of 20% the response was an order of magnitude slower than for ideal trays.

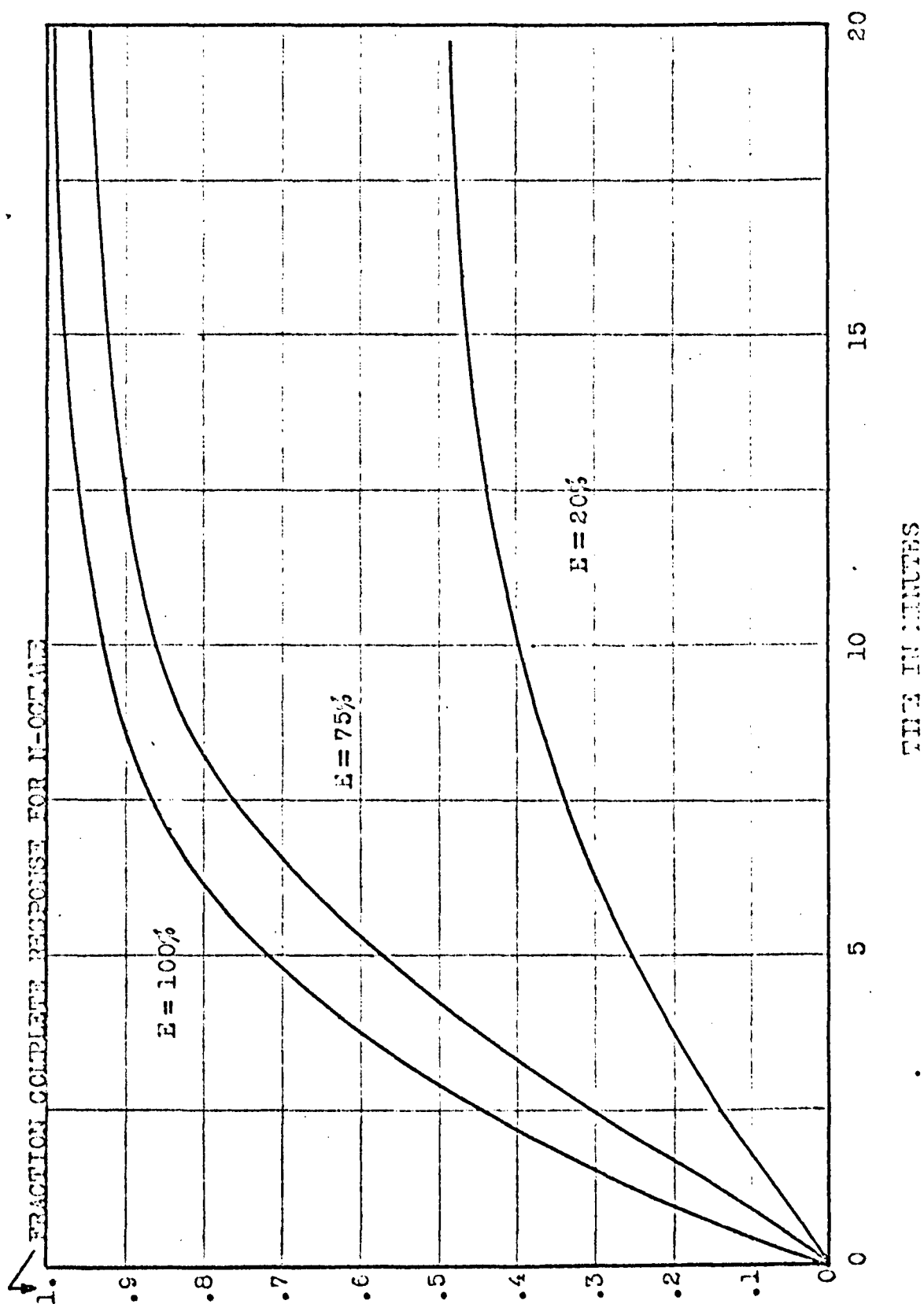


FIGURE 5

VI EQUIPMENT

Introduction

Since the matrix method of solving distillation tower dynamic problems has received little numerical and no experimental verification it was decided that this study should be complete and that some experimental work be performed. The intent of the experimental work was to show that the concept of using a Murphree efficiency for each component on each tray was a workable one and that the numerical methods used in the calculations were stable and gave results consistent with observation. In order to best demonstrate the mass transfer effects the dynamic studies were confined to determinations of tray response for step changes in feed composition at constant feed flow rate and constant tower conditions. This, in effect, kept the flow rates constant and therefore the tray hold-ups constant and limited changes to composition.

In selecting an experimental system the qualities desired were: well known physical properties, simple vapor-liquid equilibrium relations, easy to analyze, and distillable under atmospheric pressure with steam as a heating medium and tap water as a coolant. The system of benzene, toluene, p-xylene satisfied all of the above requirements and was chosen. This system had some other advantages in that it was non-corrosive, cheap and readily available, and was quite stable. The only drawbacks were the systems toxic attributes and its flammability.

The distillation equipment used in this study was designed and built by the author expressly for studying tower dynamics. The unit is

a small pilot model with a 4-inch diameter, 8-tray tower; partial reboiler and total condenser. A photograph of the tower and associated equipment is presented in Figure 6 and a diagram in Figure 7. This particular size of tower was chosen on the basis that; it provided a rate of response measurable by ordinary sampling methods, was economical as to the tower, heat exchangers, and flow meters, reached steady state in a reasonable period of time, and could operate with an economical and safe amount of chemicals. By combining the product streams in an agitated sump and recycling the combined products as feed, the unit had the capability of being operated continuously on as little as 5 gallons of liquid.

Feed to the tower was from two sources, either from the product sump via a constant head tank, or from a separate feed tank. The feed entered the tower on the fourth tray from the top and the products were drawn from the reboiler and condenser. The feed, bottoms, distillate, and combined distillate and reflux were metered with rotameters.

The calibration charts for the flow meters, component hold-ups, and tower pressure drop are in Appendix D. A more detailed description of the major components of the experimental unit follows.

Distillation Tower

The tower was constructed of nine 8-inch nipples of 4-inch, Sch. 40, steel pipe. Each nipple was screw fitted to a standard set of companion

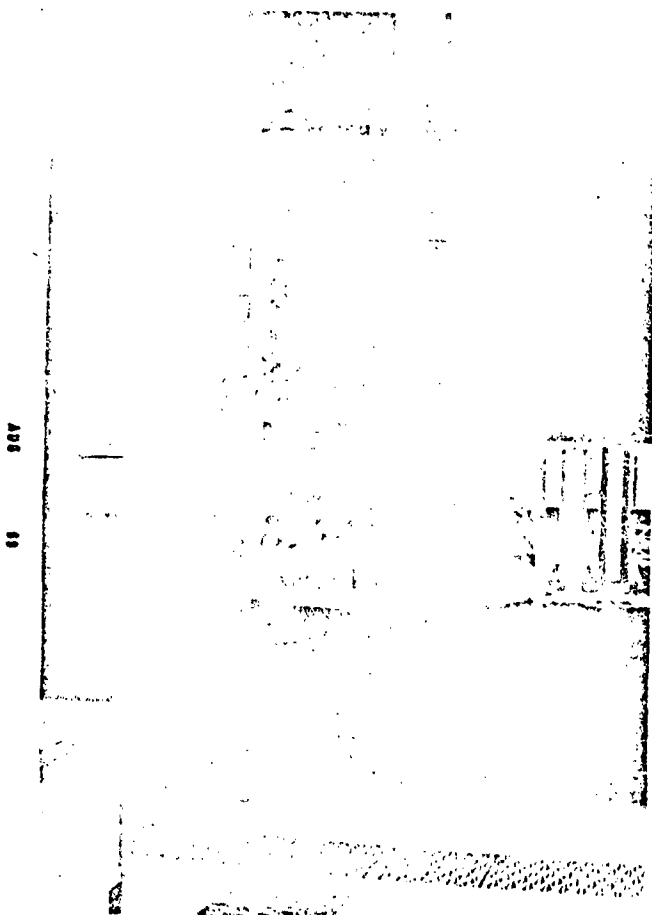
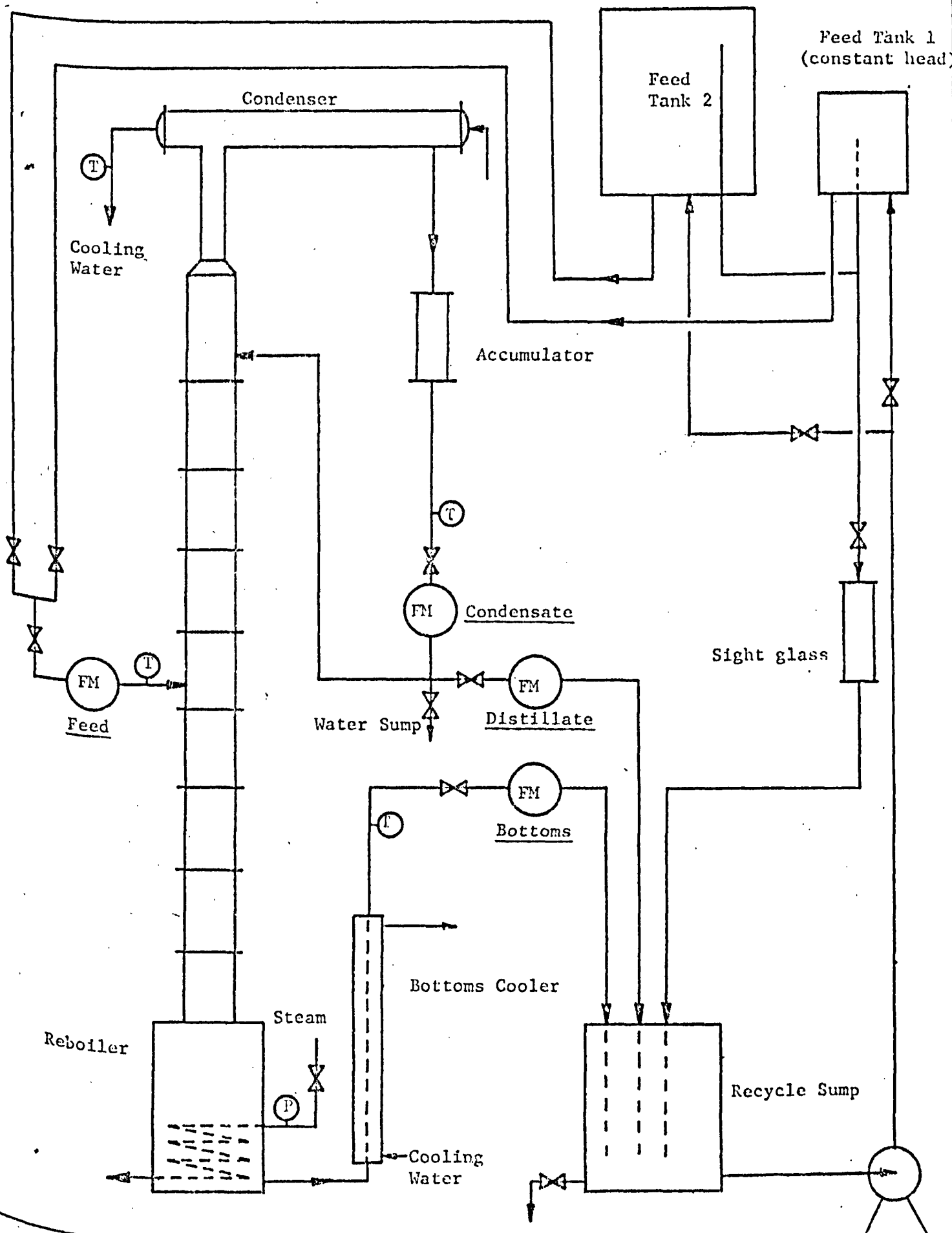


Figure 6 . Photograph of the experimental unit showing the tower, reboiler condenser, sump tank and panel board. The feed tanks are above the condenser and are not shown.

FIGURE 7



flanges to form thimbles, with nine stacked thimbles forming the tower. Six-inch-diameter aluminum trays were set between the connecting flanges and held in place by the compression of the flange bolts. Tray details are presented in Figure 8 .

Each tray section was equipped with liquid and vapor sample taps. Made of 1/8-inch copper tubing, the sample taps were extended through the tower wall with bulkhead adaptors to select samples directly from the liquid and vapor streams. This prevented the samples from being contaminated by selectively condensed liquid on the tower wall. The liquid sample was drawn from a point 1/2-inch below the lip of the outlet weir and the vapor sample was taken one inch inside the tower wall and 6 inches above the tray floor. Design data for the tower and trays is presented in Table 1.

Reboiler

The reboiler was constructed of a 16-inch length of 10-inch, Sch. 40, steel pipe with welded, flat heads of 3/8-inch steel plate. The bottom flange on the distillation tower bolted directly to the top head of the reboiler and there was no tray at this junction.

A helical copper coil, 1/2-inch O.D. and 20 ft. in length, formed an outside heat transfer surface of approximately 2.0 sq. ft. The volumetric calibration for the reboiler is presented in Appendix D .

Condenser

Manufactured by the Vulcan Copper and Supply Co. of Cincinnati, Ohio, the condenser was constructed entirely of copper. The unit was horizontal, single pass, counter-current with cooling water in the tubes, condensing vapor in shell. The shell was 3 inches in diameter and 31 inches long. It

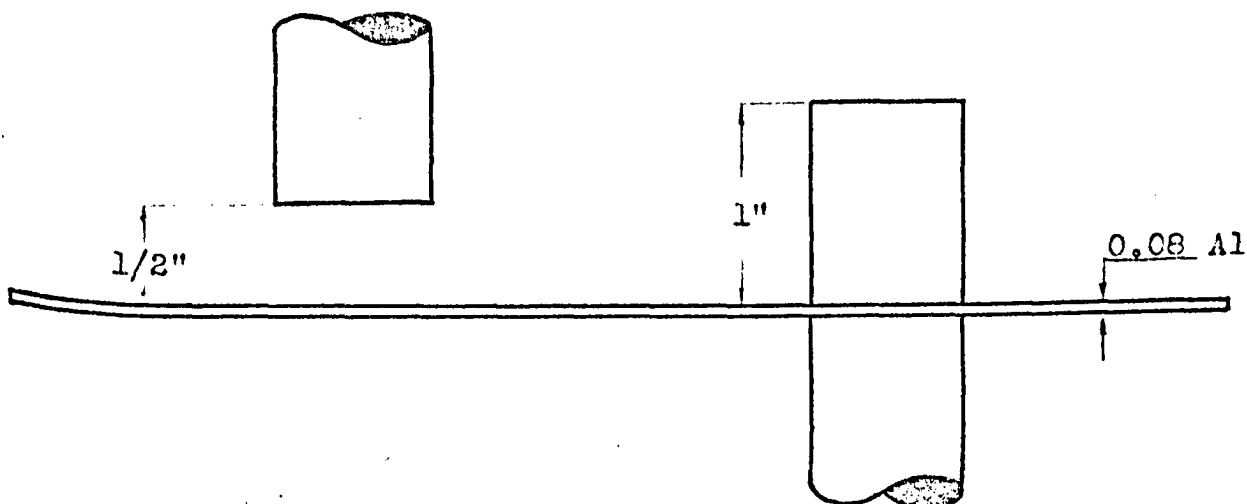
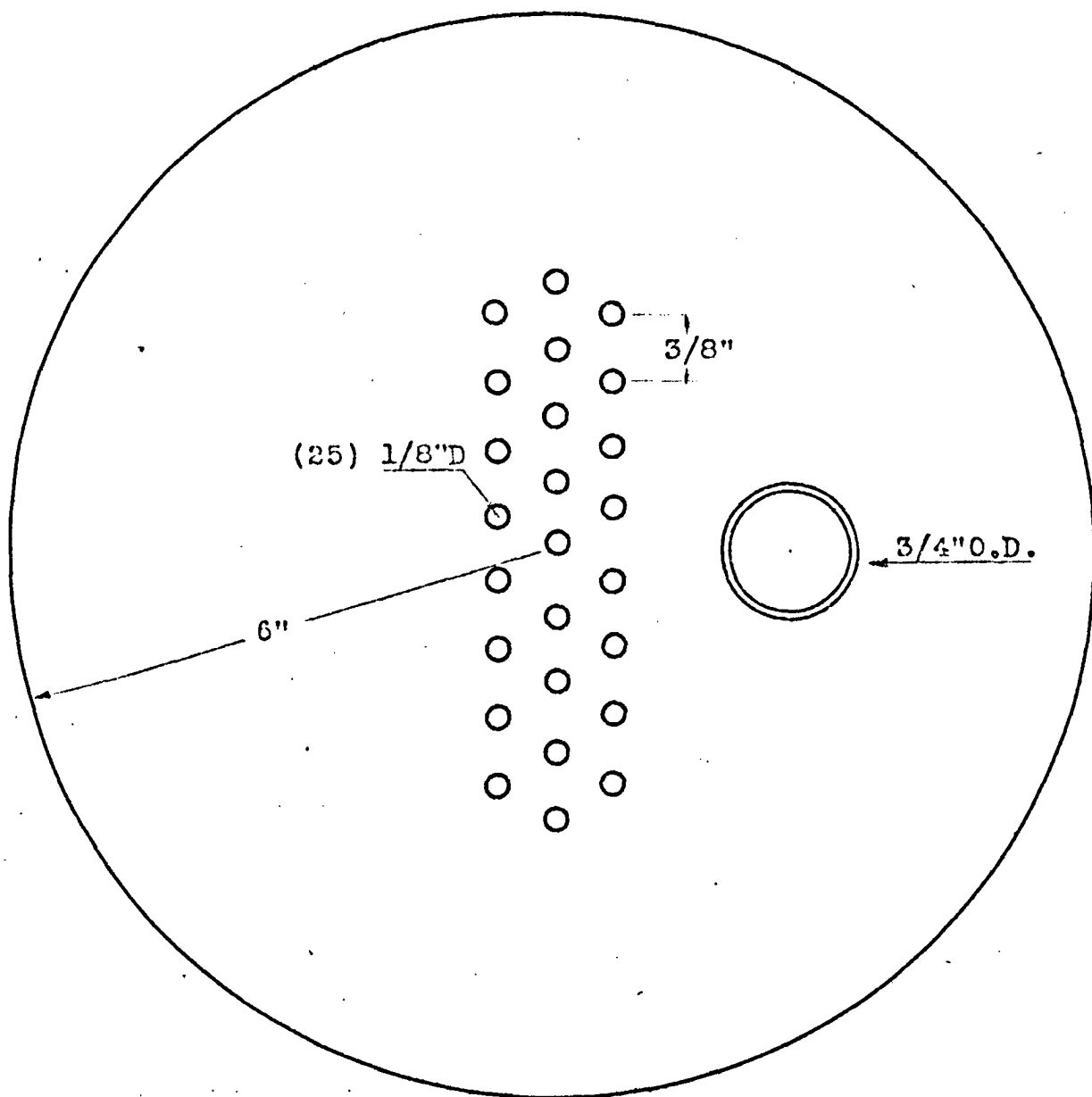


Figure 8
Tray Layout
Scale 1:1

TABLE I

Tower design data

Vapor rate	0.126 cu. ft./sec. (1.0 moles/hr.)
Liquid rate	0.460 g.p.m. (2.0 moles/hr.)
Vapor density	0.210 lb./cu. ft.
Liquid density	50. lb./cu. ft.
Tower diameter	4.0 in.
Tray spacing	8.0 in.
Trays	8 cross flow, perforated
Superficial vapor velocity	1.45 ft./sec.
Total tray area	12.5 sq. in.
Weir length	2.36 in.
Weir height	1.0 in.
Downcomer area	0.65 sq. in.
% Free area	3.3%
Perforations	34 per tray (1/8" on 3/8" pitch)
Perforation velocity	43.6 ft./sec.
Perforation factor	20.6 ft./sec. (lb./cu. ft.) ^{1/2}
Head over weir	0.18 in. <u>C.T.L.</u>
Downcomer velocity	0.33 ft./sec.
Pressure drop per tray	4.6 in. C.T.L.
Downcomer buildup	5.8 in. C.T.L.

Reboiler

Minimum heat duty	13,000 Btu/hr. (Δh_v for 1.0 mole/hr.)
Design duty	20,000 Btu/hr.
Required area	2.0 sq. ft. (based on 150 Btu/hr. sq. ft. °F.H.T.C.)

contained seven 1/4-inch ID tubes on a 3/4-inch triangular pitch for an inside heat transfer area of 1.14 sq. ft. To facilitate condensate removal the unit was mounted approximately 5° from true horizontal.

Special Design Considerations

Since the purpose of this thesis is the investigation of factors affecting mass-transfer it was desired to keep heat and holdup effects minimal. This was done by designing the trays to operate at very low liquid loads with a long outlet weir. This low liquid loading per inch of outlet weir (0.15 gpm/inch) maintained an extremely low liquid crest over the weir and consequently very little change of tray liquid level with liquid throughput. For the maximum expected change of loading of 200 to 500 cc/min. the total liquid height increased from 1.015 to 1.03 inches.

Operating at atmospheric pressure with an eight-inch tray spacing and a one-inch weir height provided a volumetric holdup of liquid to vapor of 1:7 versus a liquid to vapor density ratio of approximately 170:1. This put about 95% of the tray holdup in the liquid phase which is in line with the assumptions made when deriving the dynamic equations in Section II.

To minimize heat losses to the atmosphere the entire unit was insulated with 2 inches of fiberglass and covered with aluminum -paper laminate.

Bottoms Cooler

To keep the bottom product temperature within the calibration range of the flow meter and for the sake of safety, the bottoms product was withdrawn through a double-pipe heat exchanger. Constructed of 1/2-inch and 1/4-inch Sch. 40 pipe mounted concentrically, the 3-foot long unit afforded about

0.32 sq. ft. of external surface for heat transfer. Cooling water was used as a coolant and the flow of both fluids was upward for venting purposes.

Water Coalescer

Since small quantities of water tended to accumulate in the unit over long periods of time some method of collecting the water was needed. Any water present was taken overhead when the unit was in operation and was gradually concentrated in the condensing section. To collect the water as it was driven to the condenser a coalescer was provided at the lowest point of the reflux return line. This little sump made of a 9-inch section of 1/2-inch pipe hung vertically down from the 1/4-inch return line and performed in an admirable manner. It was connected to the return line with a "T" and had a drain cock at the bottom.

Instrumentation

Every stream in and out of the unit was flow metered. Rotameters were used throughout and they were calibrated under actual operating conditions with pure benzene at 82°F. The streams measured were: the feed, combined reflux and top product, and bottom product. In-line thermometers were installed ahead of each rotameter.

Tower pressure was measured both in the reboiler with a bourdon gage and in the condenser with a mercury manometer. The manometer was the prime indicator of tower pressure and the reboiler gage was a safety feature. Steam pressure to the reboiler was measured with a bourdon gage, which had been dead-weight calibrated to ± 0.3 psi.

The reboiler and trays 1,3,5, and 7 were equipped with iron-constantan

thermocouples which were connected to an L&N multi-point recorder. The thermocouple beads were wired to the trays (external to the tower) and did not contact the liquid or vapor. They were used for monitoring the tower during heatup and were invaluable in determining the state of the unit.

VII EXPERIMENTAL PROCEDURE

General Comments

Three types of distillation runs were made; determination of tray efficiencies at total reflux, determination of tray efficiencies with continuous feed, and dynamic response from steady-state conditions caused by a step change in feed composition. Trial runs for each of the above types were made with a binary mixture of benzene and toluene. This was done mainly to get some idea of the speed of response of the column and a feel for the manual control and analysis.

All distillations were conducted at one atmosphere pressure as measured at the condenser and with 50°F to 70°F subcooling of the reflux. This brought the reflux and distillate streams down to 120°F for metering. A bottoms cooler was placed before the rotameter at the bottom draw off to keep this stream below 100°F. With the effluent streams cooled to these temperatures they could be combined in an agitated sump and recycled as feed within 5°F of room temperature. Also the stream metering could be conducted reasonably close to calibration conditions (pure benzene at 82°F).

Total Reflux

Total reflux provides a quick and comparatively easy method of determining tray efficiencies using tray liquid compositions only since $y_{n+1} = x_n$. The liquid samples are generally more reliable than vapor samples since they are less sensitive to flash and can be obtained more quickly. After approximately two hours of refluxing, steady state was reached and samples of the eight trays plus the reboiler vapor were taken. These samples could

be taken in about 10 minutes.

Continuous Distillation

To achieve a continuous steady-state distillation, the bottoms and distillate were combined in the agitated sump and recycled as feed until steady state was obtained. This normally took about three hours after refluxing started. The volume of liquid in the sump during the recycle operation was about 4000cc, and for the feed rates used, this gave a tank turnaround time of 20 minutes. A multi-point recorder was used to monitor the temperature at trays 1, 3, 5, 7 and the reboiler and gave a reliable indication of when steady state had been reached.

Step Changes in Feed

All of the dynamic changes introduced were step changes in the feed composition at constant feed rates, product rates, and reflux ratio. After reaching steady state with recycle feed from the sump, two quick closing valves were switched just above the feed rotameter. This switched the feed supply from the sump to a separate 5 gallon supply tank. Control of the tower during the period of transition was done manually, and after a little practice, could be done to within 5% of the desired values.

Sample Taking

To prevent selective flash-off all liquid and vapor samples were taken through cold traps constructed of about 5 inches of 1/8-inch OD tubing immersed in a container of ice water. The sample emerged from the cold traps into covered 10-cc sample vials filled with 3 mm glass beads to provide a large, cold surface for condensation and cooling. The sample

vials were also cooled in ice. After clearing the line, samples of 1 to 3 cc of liquid were taken and tightly capped.

Time Delays

Since approximately 86 inches of 1/4-inch pipe runs from the quick closing valves where the feed change is made to the tower feed inlet, the step change as seen by the tray is not instantaneous. Computed on a plug-flow basis this amounts to a time delay of approximately 20 seconds. Monitor of the feed tray temperature indicated about 30 to 40 seconds which gave a reasonable check. An additional measurement delay exists in the sample cocks and sample lines which run inside the tower to the outlet weir lip of approximately 20 seconds. Since the dynamic measurements were made over time periods of 40 to 90 minutes the total error introduced by these time delays is slight beyond the first two or three minutes. To account for these delays a minute was subtracted from each real time reading after the step change.

Tower Holdups

The reboiler was equipped with a calibrated sight glass, and volumetric holdup could be determined whenever desired in the course of experiments. Special calibration runs were necessary to determine the holdups of the condenser and trays.

Condenser holdup was determined by allowing the tower to reach steady state at a specified throughput and quickly cutting off the vapor supply by shutting off steam to the reboiler. The condensate was then drained into a graduated cylinder. This operation was performed with a vented condenser to prevent column vapor from being pulled into the condenser after the

steam was shut off.

Tray holdup was determined by allowing the tower to reach a specified steady-state and quickly closing off both the steam to the reboiler and the condensate return from the condenser. Average holdup per tray was then computed from the change in level of the reboiler after drainage. In light of the low liquid loadings used in all of the determinations it was reasonable that the main variable affecting tray volumetric holdup should be vapor rate rather than liquid rate. Thus these determinations were made at total reflux with varying vapor rates. This kept the column in a very stable situation which facilitated accurate measurement and kept all trays under as equal a vapor loading as possible.

Rotameter Calibration

All of the rotameters were calibrated by volume collection of pure benzene at 82°F. Calibration charts for the rotameters are included in Appendix D.

Analysis and Handling of Data

The experimental work required a large amount of data even for the 10-stage, three-component system. Computer processing of the analytic data greatly simplified the process. The samples were analyzed chromatographically and the area of each elution peak approximated with two triangular areas. Thus the complete chromatogram for a single sample is described in terms of heights and widths of six triangles. A sample chromatogram is given in Appendix E. The peak dimensions were punched on cards and processed to obtain component composition.

For the determination of component separation efficiencies a complete set of tray liquid and vapor data were processed to determine liquid and vapor compositions. An equilibrium vapor composition was computed for each liquid composition by a bubble point calculation and component efficiencies computed according to the Murphree definition.

The original and processed data is in Appendix F.

VIII PRELIMINARY EXPERIMENTS

Introduction

The preliminary experiments were done with the purpose of obtaining basic data on the experimental unit, which are needed for a dynamic description of the unit. In this section all of the experimental results except those for the full dynamic tests are presented. These include: the determination of component tray efficiencies, tray and condenser holdups, and tower heat losses.

All determinations were made with U. S. P. benzene, industrial grade toluene, and practical grade p-xylene distilled at atmospheric pressure. Gas phase chromatography was used for analysis and details of the analysis are presented in Appendix F. The original chromatographic data are given in Appendix E.

Component Separation Efficiencies

Tray efficiencies for the three components were determined at total reflux and with continuous feed through a range of superficial vapor velocities of 0.99 to 1.25 ft./sec. (vapor loading factors of 0.42 to 0.52 ft./sec. $(\text{lb}_m/\text{ft.}^3)^{1/2}$)*. In each run all trays of the tower were sampled and a Murphree efficiency computed for each tray and each component. The data is presented in tabular form in Tables 1F to 5F, and a summary of the average efficiency per run is presented in the following Table II. Tables 1F through 5F are in Appendix F.

* The vapor load is defined as the superficial vapor velocity times the square root of vapor density.

TABLE II

<u>Run</u>	<u>Vapor Vel.</u> <u>ft./sec.</u>	<u>Loading</u> <u>Factor</u>	<u>Average Efficiency</u>		
			<u>Benzene</u>	<u>Toluene</u>	<u>p-Xylene</u>
14A	0.99	0.42	65.2	65.0	72.8
12A	1.04	0.44	61.5	64.5	60.6
12B	1.12	0.47	61.4	56.3	61.6
13	1.15	0.48	62.2	59.4	64.2
14B	1.25	0.52	<u>65.0</u>	<u>65.0</u>	<u>69.6</u>
Overall Average			62.6	62.1	65.9

Since no appreciable difference was obtained between component efficiencies the efficiencies of all components were taken as 62.3% for modeling. This is the average of the benzene and toluene efficiencies which are more reliable since they are computed from a range of compositions which can be more accurately analyzed. Many of the xylene efficiencies are computed from compositions in the range of 2.0 to 0.05% where impurities may affect the accuracy of analysis.

Note that component efficiencies may not be computed independently since they are related through the total mole balance or $\sum y_i = 1$. For an I component system, if I-1 component efficiencies are specified, then the Ith is specified by the mole balance. Furthermore, if the I-1 component efficiencies are specified as being equal, the Ith must also be equal.

Steady-State Model

The relative accuracy of the steady state model with ideal and non-ideal trays may be seen in Table III where the experimental liquid and vapor compositions are given along with the computed values. While the total separation is not greatly different for the two cases, the concentration

Mole fractions of benzene, toluene, and p-xylene

Tray	Experimental			Computed Ei,n = .623			Computed Ei,n = 1.00		
	x_B	x_T	x_X	x_B	x_T	x_X	x_B	x_T	x_X
D	0.7742	0.2249	0.0009	0.7727	0.2255	0.0017	0.7947	0.2053	0.0001
1	0.6342	0.3632	0.0025	0.6625	0.3340	0.0035	0.6015	0.3943	0.0006
2	0.5172	0.4780	0.0047	0.5433	0.4502	0.0065	0.4187	0.5794	0.0019
3	0.3870	0.6038	0.0092	0.4272	0.5615	0.0113	0.2792	0.7155	0.0052
* 4	0.2978	0.6853	0.0169	0.3259	0.6555	0.0186	0.1930	0.7943	0.0127
5	0.2619	0.7039	0.0342	0.2653	0.7007	0.0359	0.1443	0.8271	0.0287
6	0.1644	0.8107	+0.0430	0.1817	0.7742	0.0440	0.0736	0.8923	0.0341
7	0.1038	0.8444	0.0518	0.1180	0.8254	0.0566	0.0353	0.9172	0.0476
8	0.0552	0.8687	0.0760	0.0726	0.8518	0.0756	0.0161	0.9049	0.0790
B	0.0289	0.8239	0.1472	0.0317	0.8228	0.1455	0.0068	0.8459	0.1473

* Feed Tray +Smoothed data point.

TABLE III Actual and computed stage compositions for Run 13.
 Feed: 42.6% ben., 50.5% Tol., 6.90% Xyl., 0.261 moles/hr.
 Reflux Ratio 3.39, Distillate 0.139 moles/hr. Bottoms 0.122 moles/hr.

profiles differ by as much as 14% in the trays just above the feed where most of the separation occurs. Average deviation for the model with efficiencies is .0048 mole fraction and for the ideal model is .0137 mole fraction.

Holdups and Heat Losses

As determined by volumetric collection from the trays and condenser, after closing the steam valve to the reboiler, the average condenser holdup was 558 ml $\pm$ 10 % over the range of condensate rates of 380 to 450 ml./min.

Tray holdup was determined to be 121 ml. $\pm$ 10% for each tray over the range of liquid and vapor rates of 0.5 to 1.2 moles/hr. This compares to a geometric volume of 199 ml. up to the tip of the outlet weir, which would mean the liquid pool was 40% aerated.

Total heat losses for the tower were determined by enthalpy balance to be 5040 btu/hr. for ambient conditions of 80 to 85°F. Divided equally over the nine sections of the tower this becomes 560 Btu/hr. per tray section.

IX DYNAMIC RESULTS AND COMPARISONS

Introduction

In this section the predicted response to step change in feed composition is compared to actual response for a variety of operating conditions around the design load conditions of the tower. Predicted solutions with and without component separation efficiencies are included. In all cases the predicted response is based upon a predicted initial steady state for the feed, operating conditions, and efficiencies appropriate for the simulation. Thus, when ideal trays are assumed in the dynamic model, the original steady state is computed on the basis of ideal trays.

Ten response curves are presented in Figs. 9 to 18, of which, three are for the binary mixture of benzene-toluene, and seven are for the ternary mixture of benzene, toluene, p-xylene. The response of stages above and below the feed was measured since propagation occurs primarily through the vapor phase above the feed and through the liquid below. Individual stages were selected for sampling on the basis of their position in the tower and the expected magnitude of the composition changes. Random errors associated with the sampling of the turbulent pool of tray liquid and the analysis made a high density of samples necessary. With the sampling and manual control of the tower flow rates only one or two stages could be followed effectively on any given run. One tray, however, characterizes the tower response since the response of each stage is dependent upon the response of every stage. This is

true for the model as well as for the real tower.

In most cases the response is shown as mole per cent benzene versus time; for changes to lower concentrations of benzene the scale is inverted. This provides a better picture for comparing the different runs and better reveals the shape of the response curves and their non-linear nature.

In all of the predictions the holdups, heat losses, and component efficiencies are as given in Section VII.

Discussion of Results

The response of the distillate was examined since it is usually the controlled stream and is the furthest tray from the point of the disturbance. Fig. 9 and 10 show the computed and experimental response to approximately equal changes in feed composition. The only difference in the two is the direction of the change Fig. 9 showing a change to a lighter boiling feed and Fig. 10 to a higher boiling. While a better fit was obtained in the former, both show good accuracy in predicting the character of response as indicated by the shape of the response curves. If the system were linear the curves would be nearly identical. This confirms the nonlinear nature of the response and indicates that the model is capable of accounting for it.

Figs. 11 and 12 show the response of the top tray to a change to a lighter and heavier feed, respectively. Again, the fit is reasonably good and the character of curves well matched. A poor match on the initial steady-state in Fig. 12 causes the curve to be high throughout the response.

Over the range of feed compositions used the trays which underwent the most violent changes in composition were those just above the feed,

trays 3 and 4. These would be good candidates for temperature control of the tower since they respond rapidly and greatly to changes in feed composition. Figs. 13 , 14 , and 15 show the response of these trays.

Trays below the feed initially respond by virtue of liquid propagation down the tower. The changes in composition are smaller in the stripping section and the bulk of the change occurs faster and more abruptly than in the enriching section. Following the initial change, the slow rate of response reflects the dependence of the lower trays upon the reboiler response which is very slow. Figs. 16 and 17 show the response of tray 6 which is just below the feed and Fig. 18 the response of tray 8.

Comparing Ideal and Non-ideal Predictions

Comparing the predicted response for the ideal and non-ideal models may be like comparing apples to oranges if the initial and final steady states as computed with ideal and non-ideal trays are widely different. With the ternary mixture it is even possible for individual trays to respond in opposite directions to a given feed change when computed with and without efficiencies.

When used as a pure model the inclusion of component efficiencies must increase the accuracy since the non-ideal model contains everything that the ideal model contains and becomes the ideal model when the efficiencies are set equal to 1.0. If the ideal predicts better than the non-ideal the input data must be in error.

Figs. 10 and 11 represent the extremes in agreement and disagreement of the models. In Fig. 10 the steady states are similar and response is

nearly identical. In Fig. 11 the response curves are quite different to the point of having nearly twice the speed of response for the ideal prediction as compared to the non-ideal. In general, the non-ideal model gives a better prediction and matches the shape of the response more accurately. In the figures the dotted line is the ideal prediction and the solid line the non-ideal.

Figure 9

Data Set 19

Response of distillate to a step
change in feed composition.

Feed rate: 0.202 lb. moles/hr.

Distillate rate: 0.118 lb.moles/hr.

Bottoms rate: 0.084 lb. moles/hr.

Reflux Ratio: 4.36

Initial Feed: 30%, 64.4%, 5.6%

Final Feed: 51%, 43.3%, 5.4%

% Benzene, Tolu ene, p-Xylene

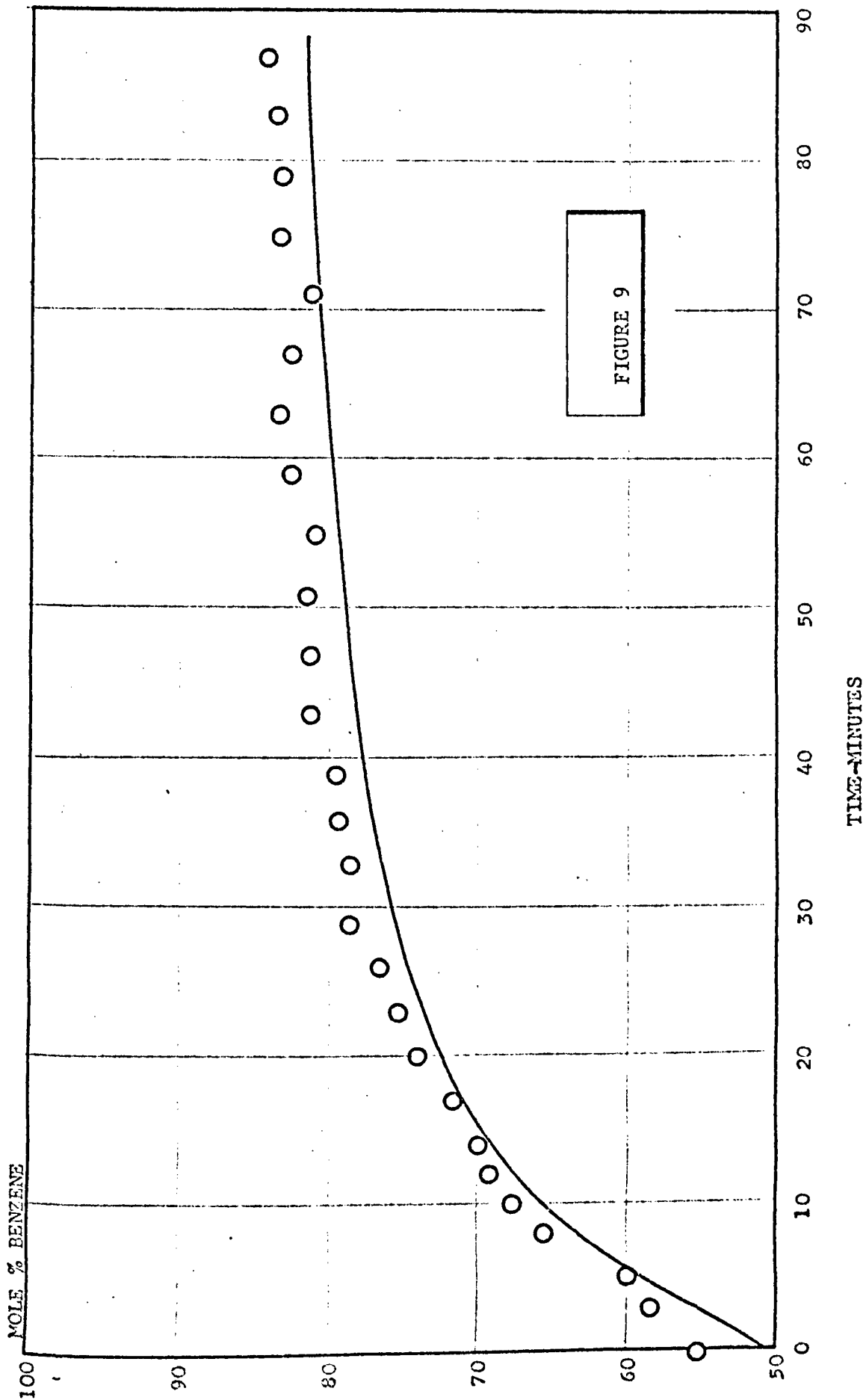


Figure 10

Data Set 20

Response of distillate to a step
change in feed composition.

Feed rate: 0.202 lb. moles/hr.

Distillate rate: 0.113 lb.moles/hr.

Bottoms rate: 0.089 lb. moles/hr.

Reflux Ratio: 3.06

Initial Feed: 55.8%, 39.3%, 5.9%

Final Feed: 31.8%, 61.0%, 7.2%

% Benzene, Toluene, p-Xylene

- - - - - Ideal prediction

————— Non-ideal, $E_{n,i} = 0.623$

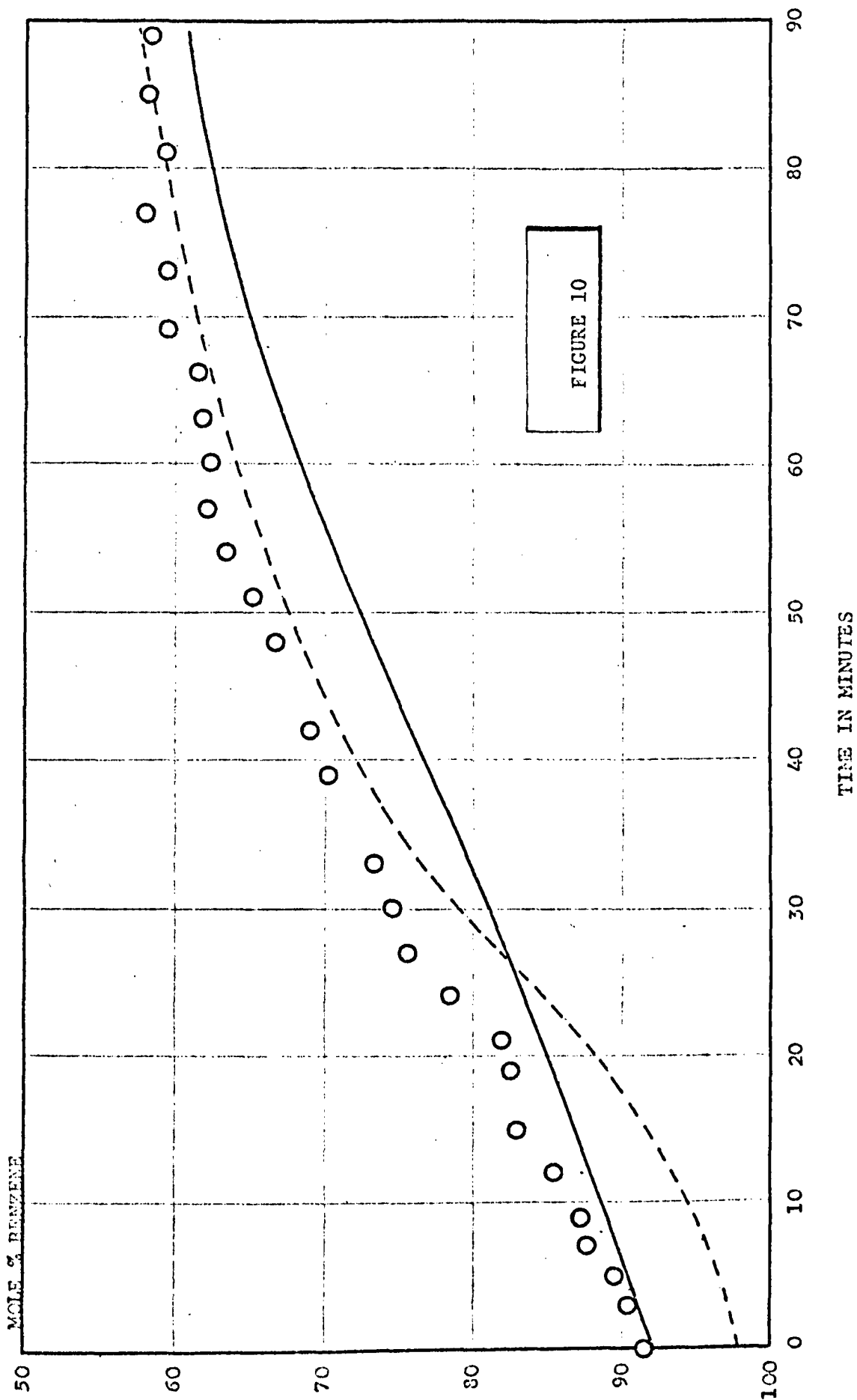


FIGURE 10

Figure 11

Data Set 17

Response of tray 1 (top) to a step
change in feed composition.

Feed rate: 0.276 lb.moles/hr.

Distillate rate: 0.149 lb.moles/hr.

Bottoms rate: 0.127 lb.moles/hr.

Reflux Ratio: 3.06:1

Initial Feed: 50.1%, 44.1%, 5.8%

Final Feed: 31.5%, 60.2%, 8.3%

% Benzene, Toluene, p-Xylene

- - - - - Ideal prediction

————— Non-ideal, $E_{n,i} = 0.623$

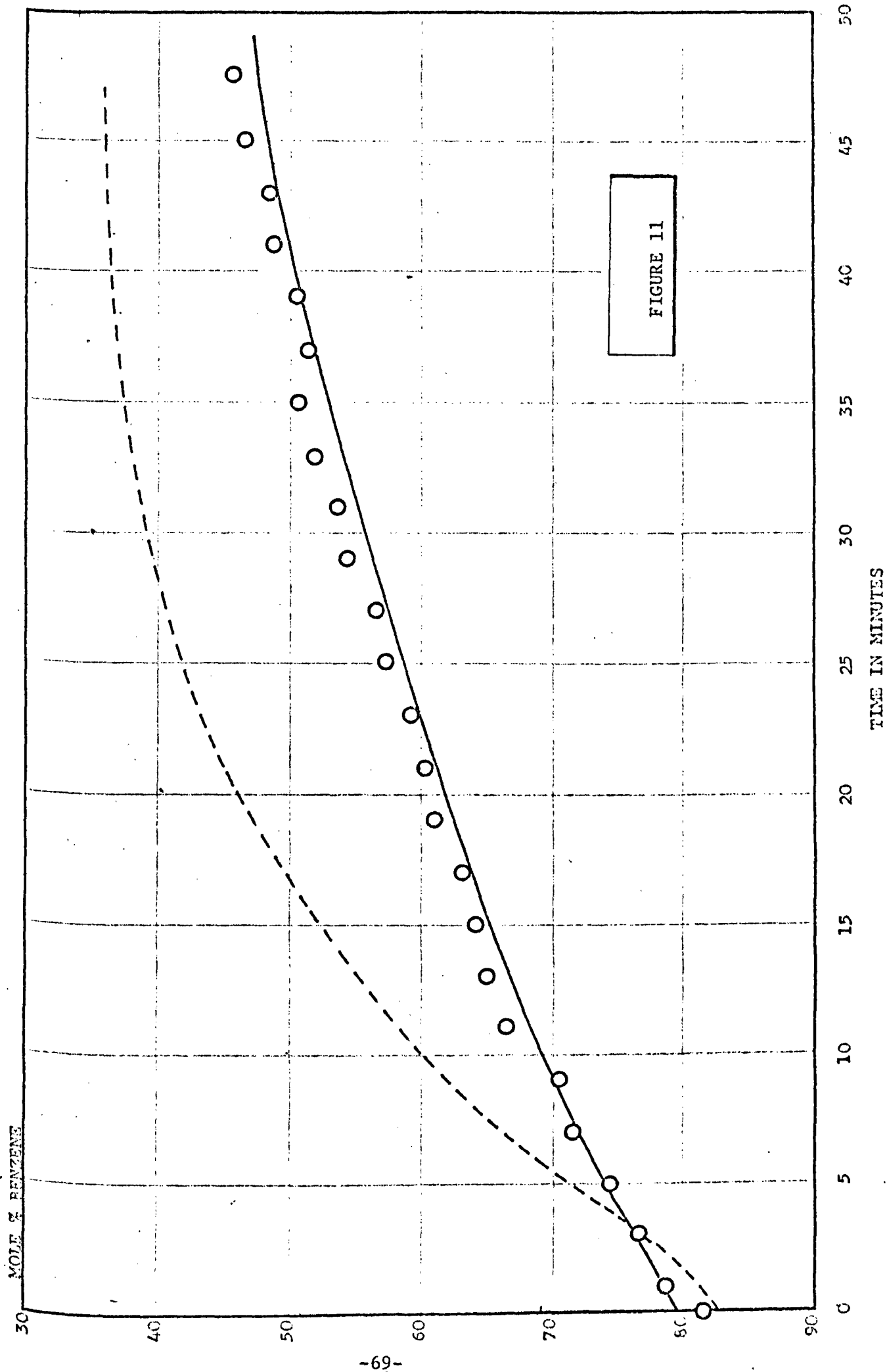


Figure 12

Data Set 9

Response of tray 1 to step
change in feed composition.

Feed rate: 0.250 moles/hr

Distillate rate: 0.138 moles/hr

Bottoms rate: 0.112 moles/hr

Reflux ratio: 3.14

Initial feed: 44.9%, 55.1%, 0.0%

Final feed: 58.7%, 41.3%, 0.0%

% Benzene, toluene, p-xylene

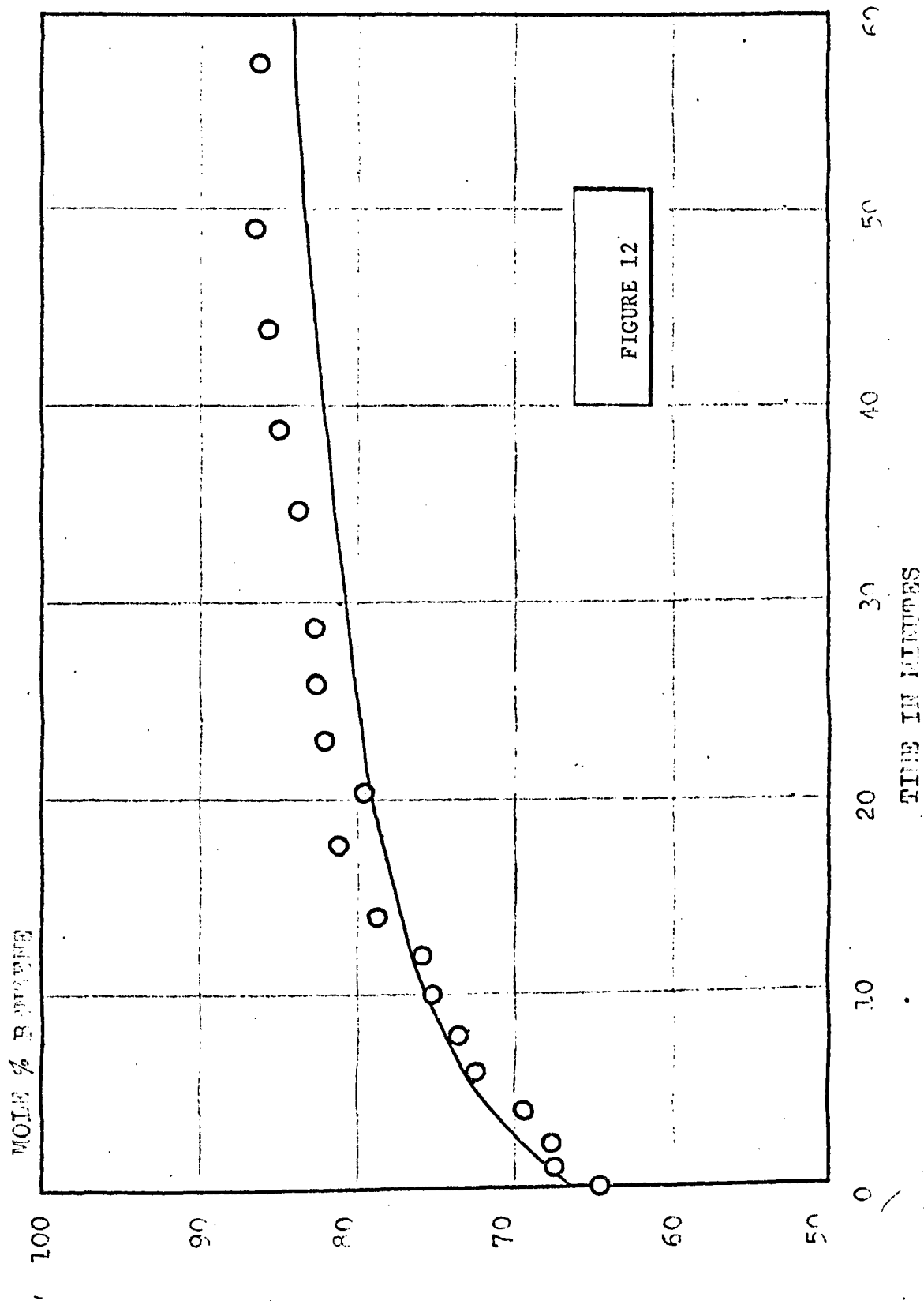


Figure 13

Data Set 15

Response of tray 1 to a step change
in feed composition.

Feed rate: 0.266 lb. moles/hr.

Distillate rate: 0.157 lb.moles/hr.

Bottoms rate: 0.109 lb. moles/hr.

Reflux Ratio: 3.16

Initial Feed: 38.5%, 54.6%, 6.9%

Final Feed: 47.7%, 45.9%, 6.4%

% Benzene, Tolu ene, p-Xylene

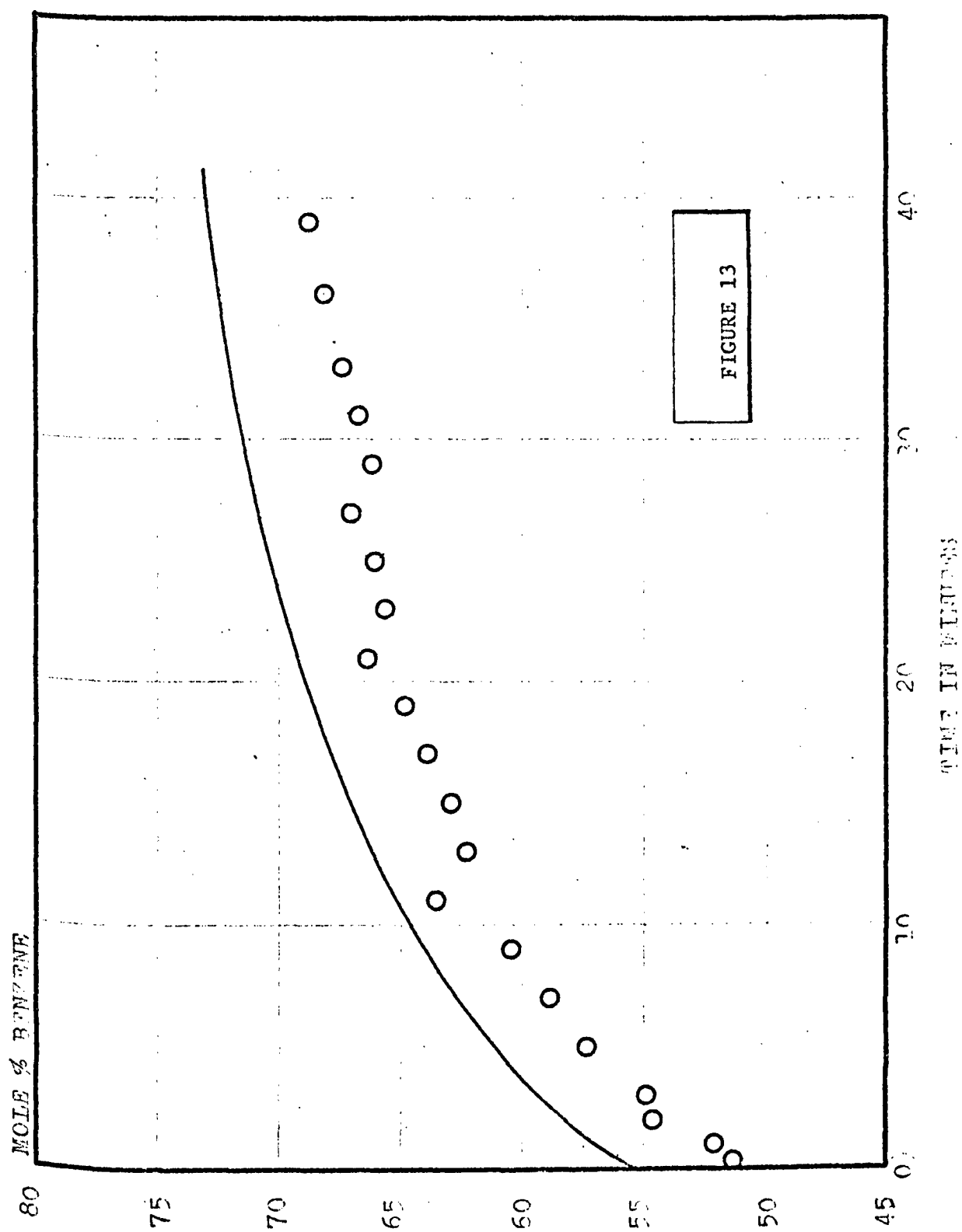


Figure 14

Data Set 18

Response of tray 4 to a step change
in feed composition.

Feed rate: 0.276 lb.moles/hr.

Distillate rate: 0.149 lb.moles/hr.

Bottoms rate: 0.127 lb.moles/hr.

Reflux Ratio: 3.16

Initial Feed: 55.3%, 39.3%, 5.4%

Final Feed: 28.4%, 63.2%, 8.4%

% Benzene, Toluene, p-Xylene

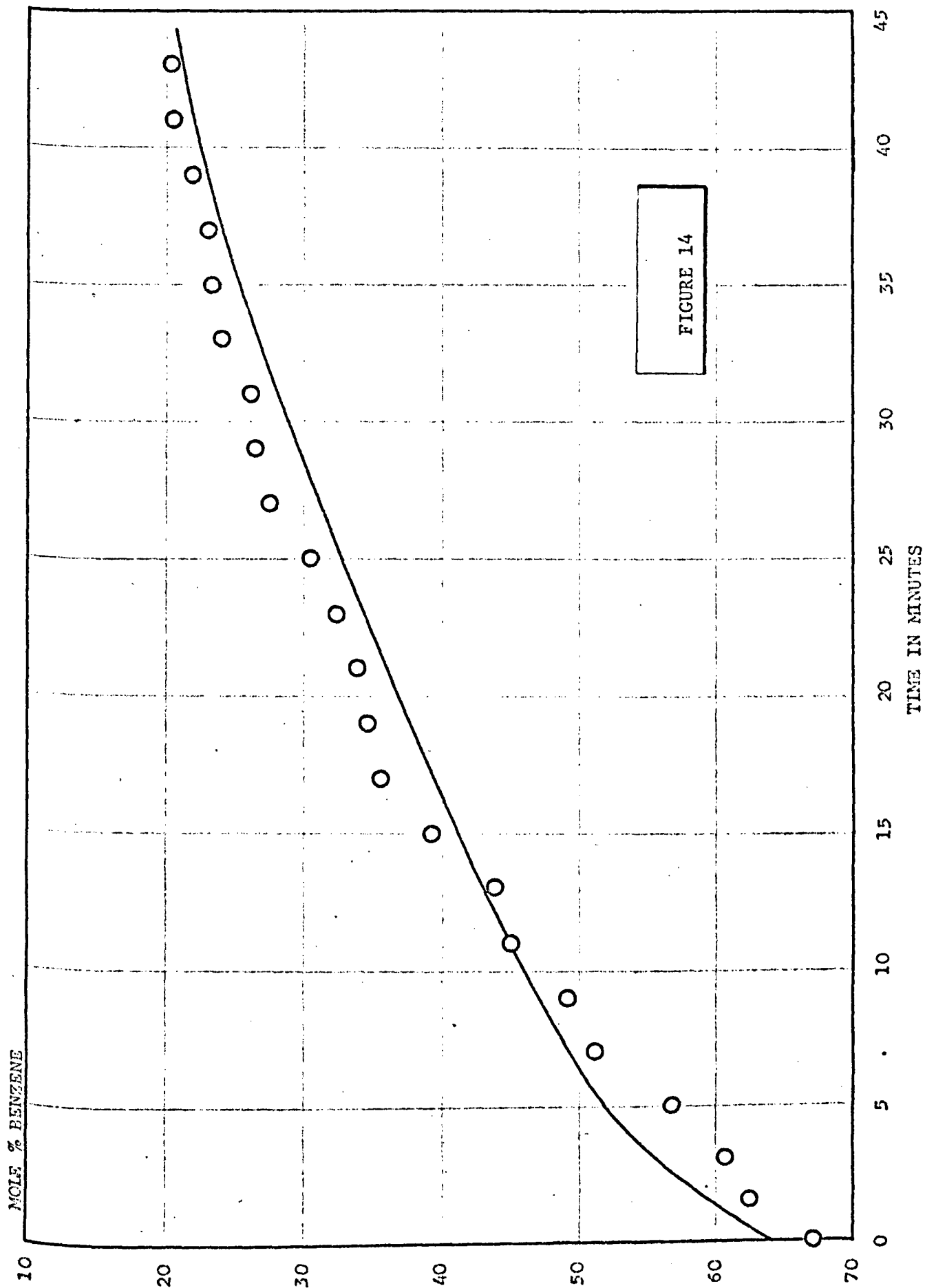


Figure 15

Data Set 10

Response of Tray 3 to a step change
in feed composition.

Feed rate: 0.250 moles/hr.

Distillate rate: 0.133 moles/hr.

Bottoms rate: 0.117 moles/hr.

Reflux ratio: 3.0:1

Initial Feed: 44.6, 55.4, 0.0

Final Feed: 58.6, 41.4, 0.0

Mole % Benzene, Toluene, p-Xylene

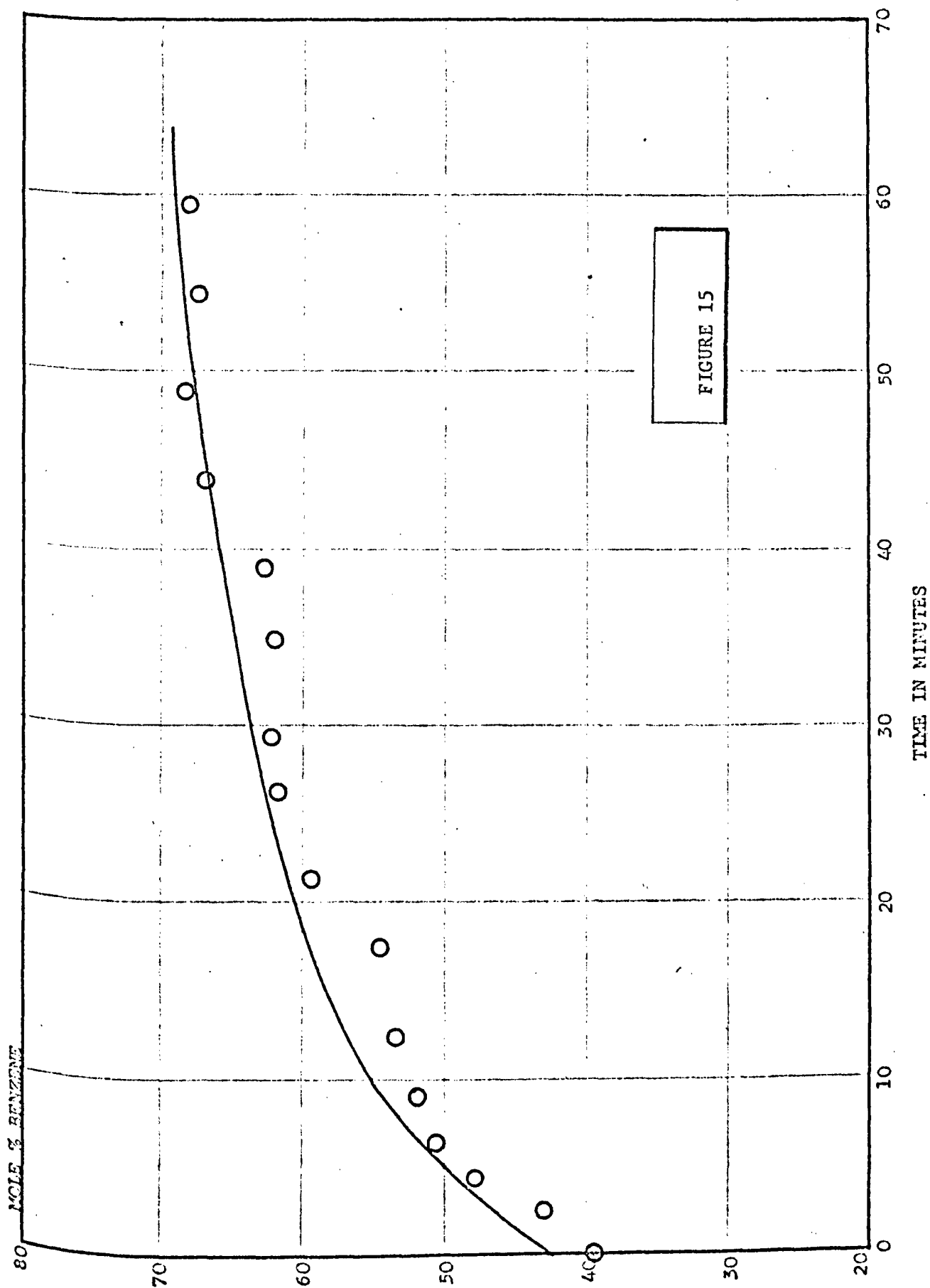


Figure 16

Data Set 22

Response of Tray 6 to a step change
in feed composition.

Feed rate: 0.202 lb. moles/hr.

Distillate rate: 0.109 lb. moles/hr.

Bottoms rate: 0.093 lb. moles/hr.

Reflux Ratio: 4.22

Initial Feed: 31.2%, 61.4%, 7.4%

Final Feed: 47.7%, 49.6%, 2.7%

% Benzene, Toluene, p-Xylene

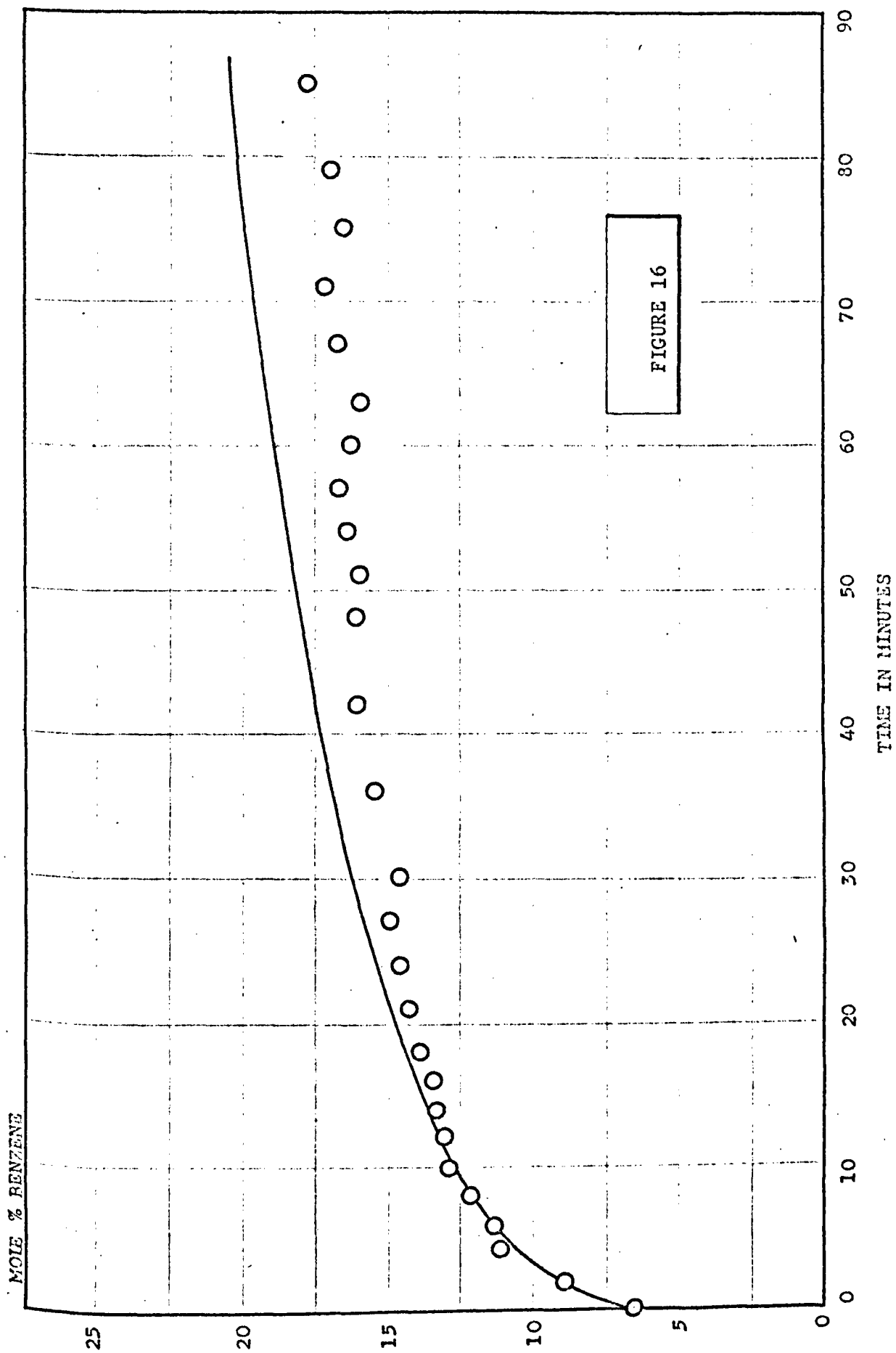


FIGURE 16

Figure 17

Data Set 10

Response of Tray 8 to a step change
in feed composition.

Feed rate: 0.250 moles/hr.

Distillate rate: 0.133 moles/hr.

Bottoms rate: 0.117 moles/hr.

Reflux ratio: 3.0:1

Initial Feed: 44.6, 55.4, 0.0

Final Feed: 58.6, 41.4, 0.0

Mole % Benzene, Toluene, p-Xylene

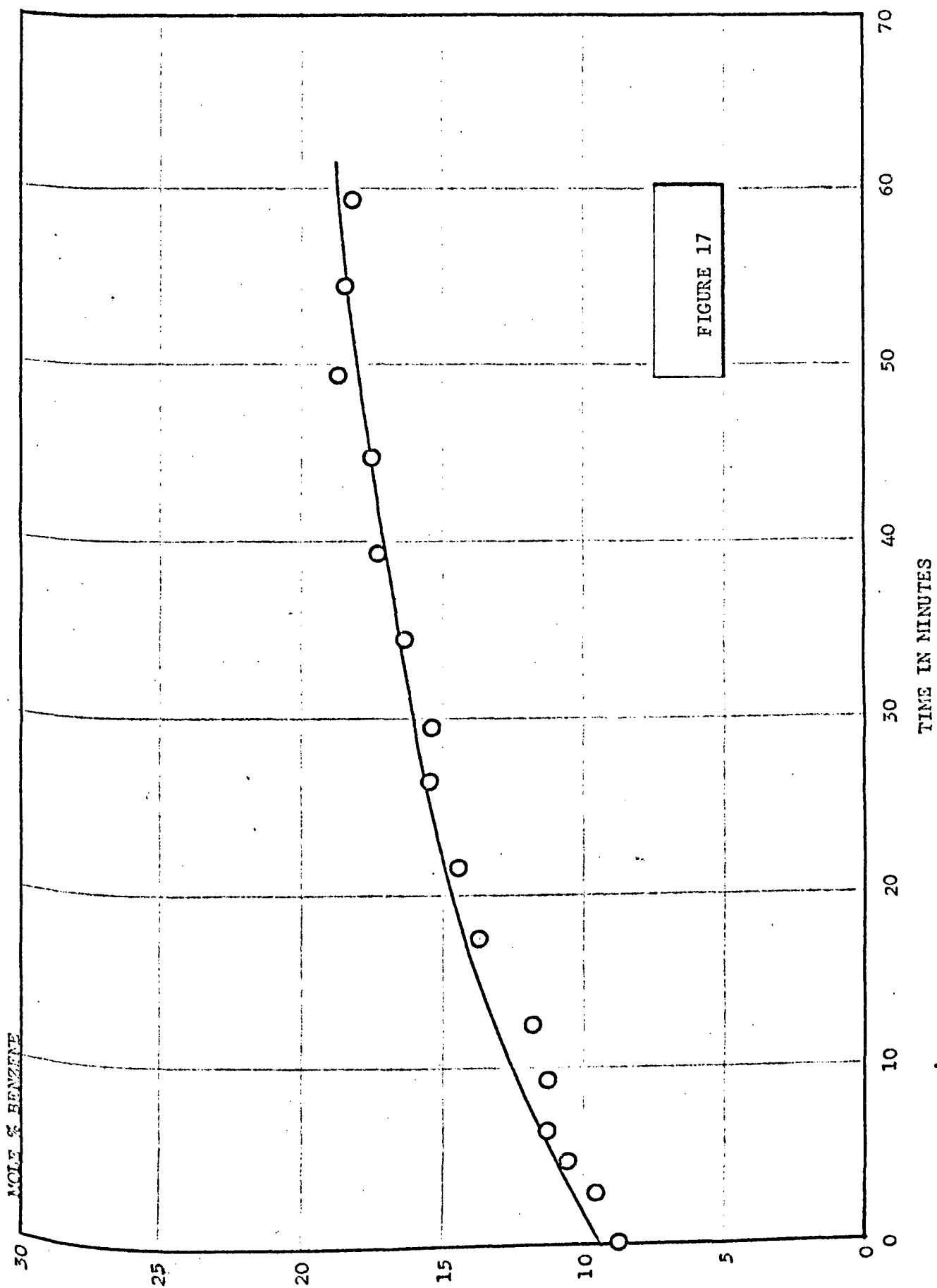


Figure 18

Data Set 16

Response of tray 8 to a step change
in feed composition.

Feed rate: 0.266 lb. moles/hr.

Distillate rate: 0.142 lb.moles/hr.

Bottoms rate: 0.124 lb. moles/hr.

Reflux Ratio: 3.06

Initial Feed: 46.6%, 46.6%, 6.8%

Final Feed: 38.3%, 54.4%, 7.3%

% Benzene, Tolu ene, p-Xylene

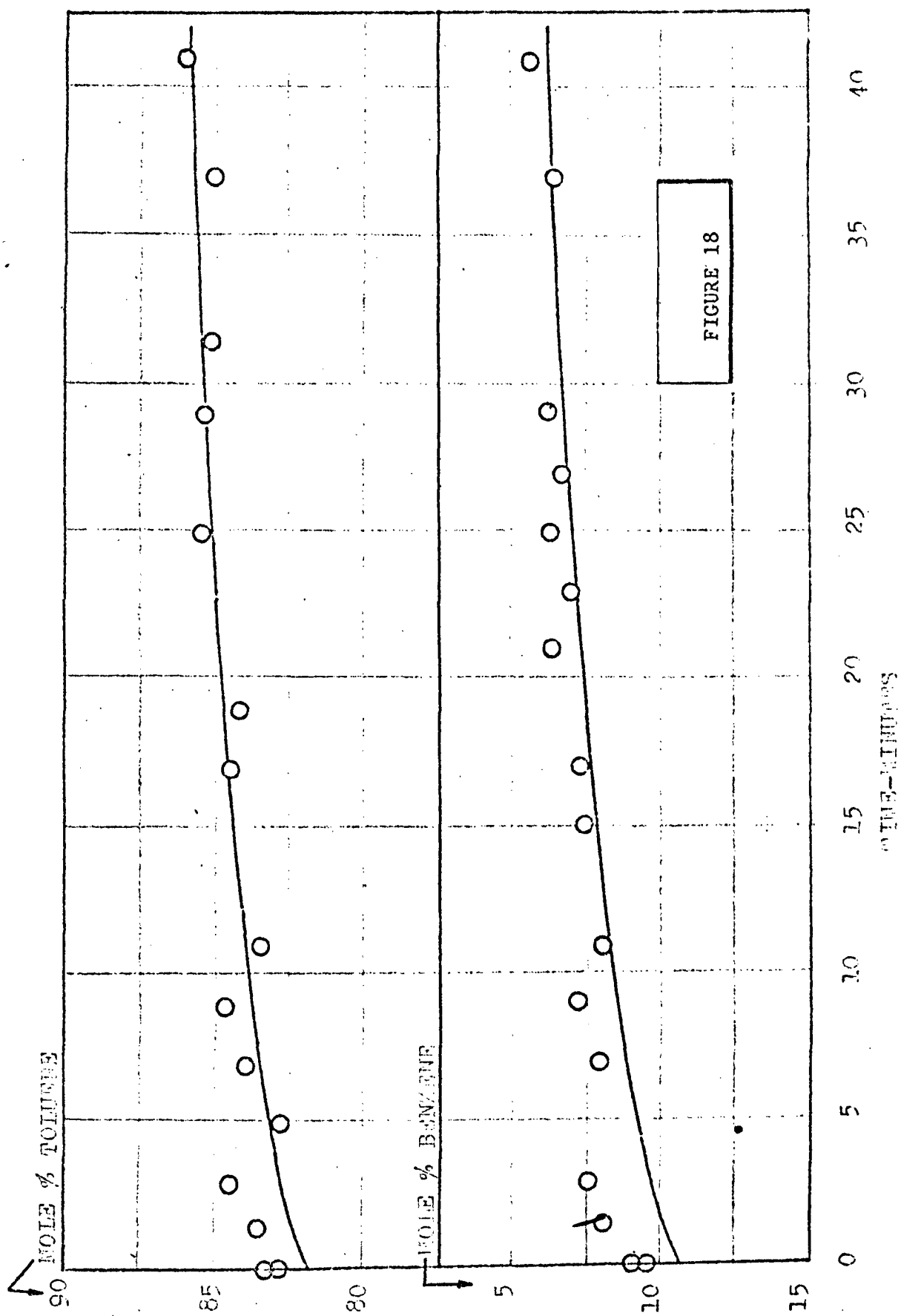


FIGURE 18

X CONCLUSIONS

Concerning the Numerical Method

The numerical and mathematical methods used to solve the non-linear matrix equations are stable and reliable. They provide a practical method for solving a more general form of matrix problem than has previously been applied to staged chemical engineering problems. This method should be applicable to a variety of chemical engineering problems involving either staged processes with by-pass or staged processes with recycle.

General Effects of Component Efficiencies

The general effect of efficiencies may be surmised from the Murphree definition when in the form, $y_n = E_n K_n x_n + (1 - E_n) y_{n+1}$. Each stage becomes more dependent upon the stage below as the efficiency decreases. In the limiting case of $E_n = 0$ all trays become completely dependent upon the response of the reboiler. Since the reboiler contains the largest quantity of liquid of any single stage it responds comparatively slowly. Thus, for distillation towers where the reboiler contains a relatively large amount of liquid decreased efficiency means greater dependence upon the reboiler and slower overall response for the tower in general.

Practicability of Including Efficiencies

The experimental comparisons gave a solid indication that component efficiencies may be included in the model to increase the accuracy of the predictions. More importantly, under normal operating conditions, they are a significant factor in determining response and when the efficiency

of a component or components becomes small any prediction of true response is impaired if they are not included.

Complex Eigen Values

The discovery of complex eigen values in the characteristic roots of the matrix equations was indeed surprising. This implies that under certain circumstances the effect of efficiencies cannot be accounted for by adjusting the K values and using the tridiagonal matrix solution since the roots of the tridiagonal matrix must be real. While in this application the complex roots all had comparatively large negative, real components and therefore decayed rapidly this may not be the case with staged reactors or other systems which are definable with the supertriangular matrix.

Reducing Problem Complexity

Since the tridiagonal matrix contains $3N-2$ elements for an N stage problem whereas the supertriangular matrix contains $N^2/2+N/2+N-1$ elements for the same number of stages, including efficiencies greatly enlarges the problem for a large number of stages. This, however, is for the two extremes. Any degree of approximation between the two types of matrix methods is also possible. Thus, for say a 100 stage problem the direct effect of stage 1 on stage 100 for anything but infinitesimal efficiency is surely negligible. Table IV shows the elements of the 10x10 supertriangular matrix which is typical of the matrices generated for this experimental comparison. Proceeding from left to right across a row of the matrix one can judge from the comparative order of magnitude of the elements the effects that each stage further down the tower has on the tray described

1	2	3	4	5	6	7	8	9	10	
-0.7032	0.4954	0.2005	0.0821	0.0339	0.0138	0.0058	0.0024	0.0010	0.0007	1
2.4318	-5.4047	2.0224	0.8288	0.3425	0.1392	0.0583	0.0244	0.0101	0.0067	2
0.0	3.1574	-6.4019	2.2022	0.9100	0.3699	0.1549	0.0648	0.0268	0.0179	3
0.0	0.0	3.4638	-7.2168	2.5805	1.0489	0.4393	0.1838	0.0759	0.0506	4
0.0	0.0	0.0	3.7904	-8.1790	2.9852	1.2503	0.5231	0.2160	0.1441	5
0.0	0.0	0.0	0.0	4.1275	-11.310	4.0523	1.6955	0.7000	0.4672	6
0.0	0.0	0.0	0.0	0.0	6.7238	-13.186	4.5445	1.8763	1.2522	7
0.0	0.0	0.0	0.0	0.0	0.0	7.1613	-14.744	5.2800	3.5238	8
0.0	0.0	0.0	0.0	0.0	0.0	0.0	7.5941	-16.322	9.8314	9
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0898	-0.1848	10

Table IV Typical orders of magnitude for the elements of the supertriangular matrix in distillation problems.

by the row of the matrix. Element ten of row one, for example, indicates the direct effect of the reboiler (stage 10) upon the condenser (stage 1). If the effects of stages more than two or three removed from the one in question were neglected, elements above the second or third upper diagonal are zero in the component matrices. While this makes little difference for the 10-stage problem it reduces the matrix elements for the 100-stage problem from 5149 for the full supertriangular matrix to 493 when the effects of stages more than three below each stage are neglected. This compares with 298 elements for the tridiagonal matrix. Thus it is possible to reduce the numerical complexity of problems without reducing the accuracy of the solution. At this time no criteria can be given for choosing the order of approximation consistent the desired accuracy.

Significance of Equal Component Efficiencies

With the system selected for the experimental portion of the thesis equal Murphree Efficiencies were obtained for each of the three components. While unequal efficiencies would have shown the full flexibility of the model more vividly no compromises were made because of this condition. In modeling the experimental unit, the individual efficiencies of every component were equal, however, the method used was independent of this particular condition.

Experimental

The size and configuration of the experimental unit was found to be generally excellent for the purposes of this study. The mixing of products and their recycle as feed was very effective in simulating continuous distillation. The constant head feed tank was invaluable during the three or four hours when the unit heated up to steady-state condition.

The chief shortcoming of the unit was the lack of flow control on the steam supply to the reboiler which necessitated constant manual adjustment during periods of dynamic change in order to keep the vapor rate constant throughout the run. Adjustment of three rotameters and the reboiler steam pressure plus the sample taking every few minutes made the dynamic runs rather hectic operations.

Chromatographic analysis was found to be generally adequate for this type of study, however, with the number of samples which were necessary an electronic integrator would have been a great help. Measuring peak heights and widths with a micrometer and magnifying glass became a laborious chore.

Sufficient cooling of the liquid and vapor samples withdrawn from the tower was found to be axiomatic for obtaining accurate composition data. The sampling line itself should be cooled in ice if possible and the sample vials should be filled with a large in inert surface such as glass beads which have been well cooled. At no point in the sampling operation should the sample contact the atmosphere for selective vaporization of the light component will surely occur.

Major Sources of Error

All other sources of experimental error are insignificant compared to

the error caused by fluctuations in the vapor rate during dynamic runs. This error was estimated to be on the order of 5% for most conditions.

The error in analysis was probably small when compared to the error involved in obtaining a representative sample from the trays. For compositions greater than 0.10 mole fraction the error was approximately 1-2% and for lower concentrations about 5%. This was due to the presence of impurities and became more discernible at the higher sensitivities required for the lower concentrations.

XI SUGGESTIONS FOR FURTHER WORK

Since experimental verification of all of the methods for predicting distillation response is scarce, almost any investigation which includes experimental comparisons is needed in this area of research. This is particularly true for the matrix methods.

While dynamic data on industrial scale units is difficult to come by, it would be most interesting to apply this method to a larger scale tower containing twenty to thirty trays. Simulating the entire unit together with the control mechanism would allow the response to be computed for different controller settings. The use of temperature rather than composition as a measure of response would probably be more convenient if a large number of response determinations were made.

Application to systems involving a small number of stages is "a natural" for the matrix methods developed here. Series chemical reactors with bypass or recycle seldom contain more than ten stages and could be modeled with these methods without modification. The rate equations would be taken as pseudo-first order over a time interval of integration.

In order to model large units with this method some simplification is probably necessary. This could be done by neglecting components of the matrix which are so small that they have little affect upon the solution. Criteria for neglecting all elements beyond a given order of magnitude might be developed to allow great savings in computation time and core storage.

NOMENCLATURE

1. Matrices and Vectors (size given is for on N stage system)

$\overline{A}_i$ = coefficient matrix for component i, N x N

$\overline{B}_i$ = coefficient matrix for component i, N x N

$\overline{C}_i$ = coefficient matrix for component i, N x N

$\overline{E}_i$ = matrix of row eigen vectors, N x N

$\overline{F}_i$ = column vector of feed rates for component i, N

$\overline{I}$ = identity matrix, N x N

$\overline{R}_i$ = column vector of feed rates for component i, N

$\overline{S}_i$ = column vector of feed rates for component i, N

$\overline{\Delta}_i$ = diagonal matrix of eigen values for component i

2. Scalars

$E_{i,n}$ = Murphree Efficiency of component i on stage n,

g_n = vapor holdup of stage n,

G_n = liquid holdup of stage n,

h_n = vapor enthalpy of vapor leaving stage n,

H_n = liquid enthalpy of liquid leaving stage n,

i = component index

I = number of components

$K_{i,n}$ = equilibrium constant for component i on stage n

L_n = liquid rate leaving stage n

n = stage number (condenser = 1)

N = total number of stages

P_n = liquid product from stage n

Q_n = heat added to stage n

T_n^1 = heat content of stage n

T_n = temperature of stage n

V_n = vapor rate leaving stage n

$x_{i,n}$ = liquid mole fraction of component i on stage n

$y_{i,n}$ = vapor mole fraction of component i in vapor leaving stage n

λ_{ij} = the jth eigen value of component matrix i

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APPENDICES

- A. Sample solutions for steady-state and dynamic problems.
Table of iterative loops and criteria of convergence.
- B. Program listings for steady-state and dynamic programs.
- C. Physical properties of benzene, toluene, and p-xylene.
- D. Equipment calibration charts.
- E. Analysis details for benzene, toluene, p-xylene.
- F. Basic and processed experimental data.

APPENDIX A

Sample Solutions for Steady-State and Dynamic Problems

1. A steady-state solution showing the printout of stage temperatures, compositions and flow rates for each iteration. The vapor rates for stages nine and ten have been clipped off for binding. The iterations are numbered in the left-hand column.
2. The dynamic solution for data set 17 is shown in detail for the first two time intervals--2 minutes and 4 minutes. The eigen values and coefficient matrices are given for these times, and iterations within each time interval are shown. In these iterations the linearized variation in the coefficient matrices is revised until the end conditions predicted are with sufficient accuracy. Only compositions and temperatures are shown for times of 8 minutes thru 42 minutes. At time 48, however, the detailed print is included so the reader may compare the eigen values and coefficient matrices at the beginning and end of the problem. The computed and experimental compositions are shown in Fig. 11.

ITERATION

START → 1 2 3 4 5 6 7 8 9 10

INITIAL VAPOR RATES

0.0 0.576520 0.615321 0.655122 0.694424 0.733725
0.866135 0.905436 0.944738 0.984039

TEMPS	182.00	185.00	190.00	194.00	200.00	205.00	210.00	216.00	220.00	225.00
X COMP	0.8689	0.7392	0.6940	0.5339	0.4813	0.3966	0.2992	0.2094	0.1367	0.0629
X COMP	0.1362	0.2088	0.3020	0.4037	0.5051	0.5741	0.6556	0.7456	0.8030	0.8169
X COMP	0.0009	0.0020	0.0040	0.0074	0.0131	0.0293	0.0352	0.0450	0.0603	0.1292
Y COMP	0.9449	0.9060	0.8528	0.7845	0.7012	0.6249	0.5176	0.3980	0.2832	0.1467
Y COMP	0.0549	0.0936	0.1464	0.2138	0.2955	0.3671	0.4716	0.5366	0.6940	0.8012
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0080	0.0107	0.0154	0.0228	0.0521
Z COMP	0.0	0.8684	0.8070	0.7322	0.6467	0.5577	0.4681	0.3347	0.2213	0.1467
Z COMP	0.0	0.1307	0.1913	0.2645	0.3472	0.4216	0.5367	0.6429	0.7347	0.8012
Z COMP	0.0	0.0009	0.0018	0.0033	0.0061	0.0107	0.0152	0.0225	0.0340	0.0521

1

TEMPS	181.00	184.24	188.40	193.36	198.94	204.03	210.08	216.33	222.10	230.10
X COMP	0.8689	0.7892	0.6940	0.5839	0.4818	0.3966	0.2992	0.2094	0.1367	0.0629
X COMP	0.1302	0.2088	0.3020	0.4037	0.5051	0.5741	0.6655	0.7456	0.8030	0.8169
X COMP	0.0009	0.0020	0.0040	0.0074	0.0131	0.0293	0.0352	0.0450	0.0603	0.1292
Y COMP	0.9450	0.9062	0.8532	0.7848	0.7016	0.6253	0.5176	0.3978	0.2824	0.1455
Y COMP	0.0548	0.0935	0.1460	0.2136	0.2951	0.3667	0.4717	0.5967	0.6946	0.8018
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0080	0.0107	0.0154	0.0230	0.0526
Z COMP	0.0	0.8686	0.8073	0.7324	0.6470	0.5579	0.4473	0.3342	0.2304	0.1455
Z COMP	0.0	0.1305	0.1909	0.2642	0.3469	0.4314	0.5369	0.6432	0.7354	0.8013
Z COMP	0.0	0.0009	0.0018	0.0033	0.0061	0.0107	0.0152	0.0226	0.0342	0.0526

2

TEMPS	180.99	184.24	188.39	193.36	198.93	204.05	210.08	216.33	222.07	229.94
X COMP	0.8659	0.7852	0.6895	0.5834	0.4757	0.3908	0.2924	0.2028	0.1307	0.0601
X COMP	0.1332	0.2128	0.3065	0.4092	0.5113	0.5805	0.6728	0.7524	0.8094	0.8188
X COMP	0.0009	0.0020	0.0040	0.0074	0.0130	0.0297	0.0348	0.0448	0.0609	0.1211
Y COMP	0.9436	0.9041	0.8505	0.7809	0.6964	0.6124	0.5092	0.3880	0.2722	0.1397
Y COMP	0.0562	0.0956	0.1487	0.2175	0.3004	0.3727	0.4801	0.5355	0.7045	0.8071
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0079	0.0107	0.0155	0.0233	0.0532
Z COMP	0.0	0.8660	0.8039	0.7273	0.6411	0.5509	0.4392	0.3249	0.2218	0.1397
Z COMP	0.0	0.1331	0.1944	0.2639	0.3528	0.4384	0.5455	0.6523	0.7434	0.8071
Z COMP	0.0	0.0009	0.0018	0.0033	0.0061	0.0107	0.0153	0.0228	0.0347	0.0532

3

---V RATES 0.0 0.577 0.655 0.693 0.732 0.770 0.962

Order of components; 1 Benzene, 2 Toluene, 3 m-Xylene
X=liquid mole fraction, Y=XX=equilibrium vapor mole fraction, Z=actual vapor mole fraction including efficiency

TEMPS	181.11	184.41	188.59	193.63	199.26	204.35	210.51	215.79	222.54	230.21
X COMP	0.8678	0.7886	0.6934	0.5866	0.4773	0.3899	0.2906	0.2008	0.1290	0.0591
X COMP	0.1313	0.2094	0.3027	0.4062	0.5100	0.5819	0.6750	0.7547	0.8103	0.8199
X COMP	0.0009	0.0020	0.0039	0.0072	0.0128	0.0232	0.0344	0.0445	0.0606	0.1209
Y COMP	0.9445	0.9058	0.8523	0.7830	0.6976	0.6182	0.5068	0.3343	0.2690	0.1375
Y COMP	0.0554	0.0936	0.1464	0.2154	0.2993	0.3740	0.4826	0.5997	0.7077	0.8092
Y COMP	0.0002	0.0004	0.0003	0.0016	0.0032	0.0077	0.0106	0.0154	0.0233	0.0533
Z COMP	0.0	0.3678	0.8058	0.7291	0.6412	0.5492	0.4265	0.3218	0.2190	0.1375
Z COMP	0.0	0.1313	0.1925	0.2676	0.3529	0.4403	0.5483	0.6554	0.7463	0.8092
Z COMP	0.0	0.0009	0.0017	0.0033	0.0060	0.0106	0.0152	0.0227	0.0347	0.0533
V RATES	0.0	0.577	0.577	0.674	0.712	0.750	0.788	0.820	0.852	0.884
TEMPS	181.03	184.26	188.41	193.47	199.17	204.39	210.61	216.92	222.57	230.29
X COMP	0.9664	0.7867	0.6907	0.5829	0.4727	0.3852	0.2856	0.1963	0.1256	0.0574
X COMP	0.1328	0.2113	0.3055	0.4099	0.5145	0.5867	0.6801	0.7591	0.8135	0.8212
X COMP	0.0009	0.0020	0.0039	0.0072	0.0128	0.0231	0.0344	0.0446	0.0609	0.1214
Y COMP	0.9438	0.9049	0.8512	0.7804	0.6937	0.6134	0.5006	0.3781	0.2629	0.1338
Y COMP	0.0560	0.0948	0.1480	0.2180	0.3031	0.3788	0.4888	0.6064	0.7136	0.8126
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0077	0.0106	0.0155	0.0235	0.0536
Z COMP	0.0	0.3664	0.8036	0.7259	0.6368	0.5438	0.4303	0.3157	0.2138	0.1338
Z COMP	0.0	0.1327	0.1947	0.2709	0.3572	0.4455	0.5544	0.6514	0.7512	0.8126
Z COMP	0.0	0.0009	0.0017	0.0033	0.0060	0.0106	0.0153	0.0229	0.0350	0.0536
V RATES	0.0	0.577	0.577	0.684	0.722	0.759	0.797	0.829	0.861	0.893
TEMPS	181.09	184.34	188.53	193.65	199.41	204.67	210.93	217.24	222.94	230.46
X COMP	0.8668	0.7876	0.6917	0.5837	0.4732	0.3848	0.2849	0.1956	0.1250	0.0571
X COMP	0.1323	0.2105	0.3045	0.4071	0.5141	0.5872	0.6803	0.7599	0.8142	0.8215
X COMP	0.0009	0.0019	0.0038	0.0072	0.0127	0.0279	0.0342	0.0445	0.0609	0.1214
Y COMP	0.9440	0.9053	0.8518	0.7810	0.6949	0.6129	0.4996	0.3769	0.2617	0.1330
Y COMP	0.0558	0.0944	0.1475	0.2174	0.3029	0.3794	0.4898	0.6076	0.7147	0.8133
Y COMP	0.0001	0.0004	0.0008	0.0016	0.0032	0.0077	0.0106	0.0155	0.0236	0.0537
Z COMP	0.0	0.8668	0.8040	0.7261	0.6367	0.5431	0.4293	0.3145	0.2128	0.1330
Z COMP	0.0	0.1323	0.1942	0.2706	0.3574	0.4463	0.5554	0.6625	0.7522	0.8133
Z COMP	0.0	0.0009	0.0017	0.0033	0.0060	0.0106	0.0153	0.0229	0.0350	0.0537
V RATES	0.0	0.577	0.577	0.689	0.727	0.764	0.797	0.829	0.861	0.893

4

5

6

TEMPS	181.07	184.30	188.49	193.61	199.39	204.68	210.97	217.29	222.99	230.49
X CUMP	0.8654	0.7356	0.6891	0.5806	0.4693	0.3818	0.2819	0.1930	0.1230	0.0561
X COMP	0.1337	0.2124	0.3070	0.4122	0.5174	0.5902	0.6838	0.7523	0.8158	0.8221
X CUMP	0.0009	0.0019	0.0039	0.0072	0.0127	0.0280	0.0343	0.0447	0.0611	0.1218
Y COMP	0.9434	0.9043	0.8503	0.7788	0.6911	0.6099	0.4958	0.3730	0.2583	0.1310
Y CUMP	0.0565	0.0954	0.1490	0.2195	0.3057	0.3824	0.4935	0.6114	0.7130	0.8151
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0077	0.0107	0.0156	0.0277	0.0539
Z COMP	0.0	0.8655	0.8021	0.7237	0.6336	0.5399	0.4256	0.3110	0.2099	0.1310
Z COMP	0.0	0.1336	0.1961	0.2731	0.3603	0.4495	0.5590	0.6659	0.7549	0.8151
Z COMP	0.0	0.0009	0.0017	0.0033	0.0060	0.0106	0.0154	0.0231	0.0352	0.0539
V RATES	0.0	0.577	0.691	0.691	0.729	0.766	0.804	0.836	0.864	0.896
TEMPS	181.13	184.39	188.60	193.76	199.57	204.86	211.17	217.48	223.14	230.58
X CUMP	0.8655	0.7858	0.6893	0.5808	0.4693	0.3817	0.2817	0.1928	0.1228	0.0560
X COMP	0.1336	0.2123	0.3069	0.4120	0.5174	0.5904	0.6840	0.7626	0.8160	0.8222
X CUMP	0.0009	0.0019	0.0039	0.0072	0.0127	0.0279	0.0343	0.0447	0.0611	0.1218
Y COMP	0.9434	0.9044	0.8503	0.7789	0.6911	0.6096	0.4955	0.3726	0.2579	0.1307
Y CUMP	0.0564	0.0953	0.1489	0.2195	0.3058	0.3826	0.4939	0.6118	0.7184	0.8153
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0077	0.0107	0.0156	0.0237	0.0539
Z COMP	0.0	0.8655	0.8022	0.7236	0.6335	0.5396	0.4252	0.3106	0.2096	0.1307
Z COMP	0.0	0.1336	0.1961	0.2731	0.3605	0.4498	0.5594	0.6663	0.7552	0.8153
Z COMP	0.0	0.0009	0.0017	0.0033	0.0060	0.0106	0.0154	0.0231	0.0352	0.0539
V RATES	0.0	0.577	0.693	0.693	0.730	0.767	0.805	0.837	0.865	0.897
TEMPS	181.12	184.38	188.59	193.75	199.57	204.87	211.18	217.49	223.16	230.59
X CUMP	0.8645	0.7843	0.6874	0.5785	0.4675	0.3797	0.2798	0.1912	0.1217	0.0554
X COMP	0.1346	0.2137	0.3088	0.4143	0.5197	0.5923	0.6858	0.7640	0.8170	0.8225
X CUMP	0.0009	0.0020	0.0039	0.0072	0.0128	0.0280	0.0344	0.0448	0.0613	0.1220
Y COMP	0.9429	0.9036	0.8492	0.7773	0.6891	0.6077	0.4931	0.3702	0.2559	0.1295
Y CUMP	0.0569	0.0960	0.1500	0.2211	0.3077	0.3846	0.4962	0.6141	0.7203	0.8164
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0077	0.0107	0.0157	0.0238	0.0541
Z COMP	0.0	0.8645	0.8008	0.7219	0.6315	0.5375	0.4230	0.3085	0.2078	0.1295
Z COMP	0.0	0.1346	0.1975	0.2749	0.3625	0.4519	0.5516	0.6533	0.7558	0.8164
Z COMP	0.0	0.0009	0.0017	0.0033	0.0060	0.0107	0.0155	0.0232	0.0353	0.0541
V RATES	0.0	0.577	0.693	0.693	0.730	0.767	0.805	0.837	0.865	0.897

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TEMPS	181.16	184.44	188.68	193.86	199.69	204.98	211.31	217.61	223.25	230.65
X COMP	0.8645	0.7843	0.6874	0.5785	0.4675	0.3796	0.2797	0.1911	0.1216	0.0554
X COMP	0.1346	0.2137	0.3083	0.4143	0.5193	0.5924	0.6259	0.7641	0.8171	0.8226
X COMP	0.0009	0.0020	0.0039	0.0072	0.0128	0.0280	0.0343	0.0448	0.0613	0.1220
Y COMP	0.9429	0.9036	0.8492	0.7772	0.6890	0.6075	0.4929	0.3700	0.2557	0.1294
10 Y COMP	0.0569	0.0961	0.1501	0.2212	0.3078	0.3847	0.4363	0.4143	0.7295	0.8155
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0077	0.0107	0.0157	0.0238	0.0541
Z COMP	0.0	0.8645	0.8008	0.7218	0.6313	0.5373	0.4223	0.3083	0.2077	0.1294
Z COMP	0.0	0.1346	0.1975	0.2749	0.3626	0.4520	0.5618	0.6585	0.7539	0.8165
Z COMP	0.0	0.0009	0.0017	0.0033	0.0060	0.0107	0.0155	0.0232	0.0353	0.0541
V RATES	0.0	0.577	0.577	0.694	0.694	0.731	0.768	0.805	0.837	0.937
TEMPS	181.16	184.44	188.68	193.86	199.70	204.98	211.31	217.61	223.26	230.65
X COMP	0.8639	0.7833	0.6860	0.5770	0.4659	0.3784	0.2735	0.1901	0.1209	0.0550
X COMP	0.1353	0.2148	0.3101	0.4153	0.5213	0.5936	0.6871	0.7650	0.8177	0.8228
X COMP	0.0009	0.0020	0.0039	0.0072	0.0128	0.0280	0.0344	0.0449	0.0614	0.1222
Y COMP	0.9426	0.9031	0.8484	0.7761	0.6876	0.6062	0.4914	0.3635	0.2544	0.1287
11 Y COMP	0.0572	0.0966	0.1509	0.2223	0.3092	0.3860	0.4978	0.6157	0.7217	0.8171
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0078	0.0108	0.0158	0.0239	0.0542
Z COMP	0.0	0.8638	0.7998	0.7206	0.6300	0.5360	0.4213	0.3070	0.2065	0.1287
Z COMP	0.0	0.1353	0.1985	0.2761	0.3639	0.4533	0.5632	0.6598	0.7530	0.8171
Z COMP	0.0	0.0009	0.0017	0.0033	0.0061	0.0107	0.0155	0.0232	0.0354	0.0542
V RATES	0.0	0.577	0.577	0.694	0.694	0.731	0.768	0.806	0.838	0.938
TEMPS	181.19	184.48	188.74	193.94	199.78	205.06	211.39	217.69	223.32	230.69
X COMP	0.8638	0.7833	0.6860	0.5769	0.4659	0.3783	0.2785	0.1901	0.1209	0.0550
X COMP	0.1353	0.2148	0.3101	0.4159	0.5213	0.5937	0.6871	0.7651	0.8177	0.8228
X COMP	0.0009	0.0020	0.0039	0.0072	0.0128	0.0280	0.0344	0.0449	0.0614	0.1222
Y COMP	0.9426	0.9030	0.8493	0.7761	0.6876	0.6062	0.4913	0.3634	0.2543	0.1286
12 Y COMP	0.0572	0.0966	0.1509	0.2223	0.3092	0.3861	0.4979	0.6158	0.7218	0.8172
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0078	0.0108	0.0158	0.0239	0.0542
Z COMP	0.0	0.8638	0.7998	0.7203	0.6299	0.5359	0.4212	0.3069	0.2066	0.1286
Z COMP	0.0	0.1353	0.1985	0.2762	0.3640	0.4534	0.5632	0.6599	0.7530	0.8172
Z COMP	0.0	0.0009	0.0017	0.0033	0.0061	0.0107	0.0155	0.0232	0.0354	0.0542
V RATES	0.0	0.577	0.577	0.694	0.694	0.731	0.768	0.806	0.838	0.938

TEMPS	181.19	184.48	188.74	193.94	199.79	205.06	211.40	217.69	223.32	230.69
X COMP	0.8633	0.7826	0.6851	0.5759	0.4648	0.3775	0.2777	0.1394	0.1204	0.0548
X COMP	0.1358	0.2155	0.3110	0.4169	0.5223	0.5945	0.6379	0.7556	0.8181	0.8229
X COMP	0.0009	0.0020	0.0039	0.0072	0.0128	0.0280	0.0345	0.0449	0.0615	0.1223
Y COMP	0.9424	0.9027	0.8473	0.7753	0.6367	0.6053	0.4904	0.3574	0.2535	0.1281
Y COMP	0.0574	0.0970	0.1514	0.2231	0.3101	0.3869	0.4499	0.6168	0.7225	0.8176
Y COMP	0.0002	0.0004	0.0003	0.0016	0.0032	0.0078	0.0103	0.0158	0.0239	0.0543
Z COMP	0.0	0.8633	0.7991	0.7197	0.6290	0.5350	0.4203	0.3060	0.2058	0.1281
Z COMP	0.0	0.1358	0.1991	0.2770	0.3649	0.4543	0.5642	0.6707	0.7587	0.8176
Z COMP	0.0	0.0009	0.0017	0.0033	0.0061	0.0107	0.0155	0.0233	0.0355	0.0543
V RATES	0.0	0.577	0.577	0.694	0.731	0.731	0.768	0.806	0.806	0.938

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TEMPS	181.21	184.51	188.73	193.99	199.84	205.11	211.45	217.74	223.35	230.71
X COMP	0.8633	0.7826	0.6851	0.5759	0.4648	0.3775	0.2776	0.1394	0.1204	0.0548
X COMP	0.1358	0.2155	0.3110	0.4169	0.5224	0.5945	0.6879	0.7557	0.8182	0.8229
X COMP	0.0009	0.0020	0.0039	0.0072	0.0128	0.0280	0.0345	0.0449	0.0615	0.1223
Y COMP	0.9424	0.9027	0.8478	0.7753	0.6866	0.6053	0.4903	0.3574	0.2535	0.1281
Y COMP	0.0575	0.0970	0.1514	0.2231	0.3102	0.3870	0.4499	0.6168	0.7226	0.8176
Y COMP	0.0002	0.0004	0.0003	0.0015	0.0032	0.0078	0.0103	0.0158	0.0239	0.0543
Z COMP	0.0	0.8633	0.7991	0.7197	0.6290	0.5350	0.4203	0.3060	0.2058	0.1281
Z COMP	0.0	0.1358	0.1992	0.2770	0.3649	0.4543	0.5642	0.6707	0.7587	0.8176
Z COMP	0.0	0.0009	0.0017	0.0033	0.0061	0.0107	0.0155	0.0233	0.0355	0.0543
V RATES	0.0	0.577	0.577	0.694	0.731	0.731	0.768	0.806	0.806	0.938

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TEMPS	181.21	184.51	188.79	193.99	199.84	205.11	211.45	217.74	223.36	230.71
X COMP	0.8630	0.7821	0.6845	0.5752	0.4641	0.3769	0.2771	0.1390	0.1201	0.0546
X COMP	0.1361	0.2159	0.3116	0.4176	0.5230	0.5950	0.6834	0.7651	0.8134	0.8230
X COMP	0.0009	0.0020	0.0039	0.0073	0.0128	0.0230	0.0345	0.0450	0.0615	0.1224
Y COMP	0.9422	0.9024	0.8474	0.7748	0.6860	0.6047	0.4897	0.3667	0.2529	0.1278
Y COMP	0.0576	0.0972	0.1513	0.2235	0.3107	0.3875	0.4495	0.6174	0.7231	0.8179
Y COMP	0.0002	0.0004	0.0003	0.0016	0.0032	0.0078	0.0103	0.0158	0.0240	0.0543
Z COMP	0.0	0.8630	0.7937	0.7192	0.6284	0.5344	0.4197	0.3054	0.2054	0.1278
Z COMP	0.0	0.1361	0.1996	0.2775	0.3655	0.4549	0.5648	0.6713	0.7591	0.8179
Z COMP	0.0	0.0009	0.0017	0.0033	0.0061	0.0107	0.0156	0.0233	0.0355	0.0543
V RATES	0.0	0.577	0.577	0.694	0.731	0.731	0.768	0.806	0.806	0.938

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TEMPS	181.22	184.53	188.81	194.03	199.88	205.15	211.48	217.77	223.38	230.73
X COMP	0.8630	0.7821	0.6845	0.5752	0.4641	0.3769	0.2771	0.1890	0.1201	0.0546
X COMP	0.1361	0.2159	0.3115	0.4176	0.5230	0.5950	0.6884	0.7661	0.8184	0.8230
X COMP	0.0009	0.0020	0.0039	0.0073	0.0129	0.0280	0.0345	0.0450	0.0615	0.1224
Y COMP	0.9422	0.9024	0.8474	0.7748	0.6860	0.6047	0.4894	0.3567	0.2529	0.1278
Y COMP	0.0576	0.0972	0.1518	0.2236	0.3108	0.3875	0.4494	0.5175	0.7231	0.8179
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0078	0.0108	0.0158	0.0240	0.0543
Z COMP	0.0	0.8630	0.7987	0.7191	0.6284	0.5344	0.4196	0.3054	0.2054	0.1278
Z COMP	0.0	0.1361	0.1996	0.2775	0.3655	0.4549	0.5648	0.6713	0.7591	0.8179
Z COMP	0.0	0.0009	0.0017	0.0033	0.0061	0.0107	0.0156	0.0233	0.0355	0.0543
V RATES	0.0	0.577	0.577	0.694	0.731	0.731	0.768	0.806	0.838	0.838
TEMPS	181.22	184.53	188.81	194.03	199.88	205.15	211.48	217.77	223.38	230.73
X COMP	0.8628	0.7818	0.6841	0.5747	0.4637	0.3756	0.2768	0.1887	0.1199	0.0545
X COMP	0.1363	0.2162	0.3120	0.4180	0.5235	0.5954	0.6837	0.7663	0.8186	0.8230
X COMP	0.0009	0.0020	0.0039	0.0073	0.0129	0.0231	0.0345	0.0450	0.0615	0.1224
Y COMP	0.9422	0.9023	0.8472	0.7745	0.6856	0.6043	0.4892	0.3563	0.2526	0.1276
Y COMP	0.0577	0.0974	0.1520	0.2239	0.3112	0.3879	0.5000	0.6179	0.7235	0.8191
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0078	0.0108	0.0158	0.0240	0.0544
Z COMP	0.0	0.8628	0.7984	0.7188	0.6280	0.5340	0.4192	0.3050	0.2051	0.1276
Z COMP	0.0	0.1363	0.1999	0.2779	0.3659	0.4553	0.5652	0.6717	0.7594	0.8191
Z COMP	0.0	0.0009	0.0017	0.0033	0.0061	0.0108	0.0156	0.0233	0.0355	0.0544
V RATES	0.0	0.577	0.577	0.694	0.731	0.731	0.768	0.806	0.838	0.838
TEMPS	181.23	184.55	188.83	194.05	199.91	205.17	211.51	217.79	223.40	230.74
X COMP	0.8628	0.7818	0.6841	0.5747	0.4637	0.3766	0.2768	0.1887	0.1199	0.0545
X COMP	0.1363	0.2162	0.3120	0.4180	0.5235	0.5954	0.6837	0.7663	0.8186	0.8230
X COMP	0.0009	0.0020	0.0039	0.0073	0.0129	0.0231	0.0345	0.0450	0.0615	0.1224
Y COMP	0.9422	0.9023	0.8472	0.7745	0.6856	0.6043	0.4892	0.3563	0.2525	0.1276
Y COMP	0.0577	0.0974	0.1520	0.2239	0.3112	0.3879	0.5000	0.6179	0.7235	0.8181
Y COMP	0.0002	0.0004	0.0008	0.0016	0.0032	0.0078	0.0108	0.0158	0.0240	0.0544
Z COMP	0.0	0.8628	0.7984	0.7188	0.6280	0.5340	0.4192	0.3050	0.2051	0.1276
Z COMP	0.0	0.1363	0.1999	0.2779	0.3659	0.4553	0.5652	0.6717	0.7594	0.8191
Z COMP	0.0	0.0009	0.0018	0.0033	0.0061	0.0108	0.0156	0.0233	0.0355	0.0544
V RATES	0.0	0.577	0.577	0.694	0.731	0.731	0.768	0.806	0.838	0.838

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FINAL CONVERGED SOLUTION

DATA 17 PP 3.06 SPLIT .142/.124
TOP DRAW 0.142 REFLUX RATIO 3.060
XBEN# 0.8628 XTOL# 0.1363 X-PX# 0.0009 X

TRAY 1

V# 0.577 L# 0.552 T# 184.55
XBEN# 0.7818 XTOL# 0.2162 X-PX# 0.0020 X
YBEN# 0.8628 YTOL# 0.1363 Y-PX# 0.0009 Y
FEED# 0.0 PRODUCT# 0.0

TRAY 2

V# 0.694 L# 0.589 T# 188.83
XBEN# 0.6841 XTOL# 0.3120 X-PX# 0.0039 X
YBEN# 0.7984 YTOL# 0.1999 Y-PX# 0.0018 Y
FEED# 0.0 PRODUCT# 0.0

TRAY 3

V# 0.731 L# 0.626 T# 194.05
XBEN# 0.5747 XTOL# 0.4180 X-PX# 0.0073 X
YBEN# 0.7188 YTOL# 0.2779 Y-PX# 0.0033 Y
FEED# 0.0 PRODUCT# 0.0

TRAY 4

V# 0.768 L# 0.664 T# 199.91
XBEN# 0.4637 XTOL# 0.5235 X-PX# 0.0129 X
YBEN# 0.6280 YTOL# 0.3659 Y-PX# 0.0061 Y
FEED# 0.0 PRODUCT# 0.0

TRAY 5

V# 0.806 L# 1.062 T# 205.17
XBEN# 0.3766 XTOL# 0.5954 X-PX# 0.0281 X
YBEN# 0.5340 YTOL# 0.4553 Y-PX# 0.0108 Y
FEED# 0.266 PRODUCT# 0.0

TRAY 6

V# 0.938 L# 1.101 T# 211.51
XBEN# 0.2768 XTOL# 0.6897 X-PX# 0.0345 X
YBEN# 0.4192 YTOL# 0.5652 Y-PX# 0.0156 Y
FEED# 0.0 PRODUCT# 0.0

TRAY 7

V# 0.977 L# 1.142 T# 217.79
XBEN# 0.1887 XTOL# 0.7663 X-PX# 0.0450 X
YBEN# 0.3050 YTOL# 0.6717 Y-PX# 0.0233 Y
FEED# 0.0 PRODUCT# 0.0

TRAY 8

V# 1.018 L# 1.177 T# 223.40
XBEN# 0.1199 XTOL# 0.8185 X-PX# 0.0615 X
YBEN# 0.2051 YTOL# 0.7594 Y-PX# 0.0355 Y
FEED# 0.0 PRODUCT# 0.0

REBOILER HEAT DUTY, 14739.27

CONDENSER DUTY 9164.4 DEGREES SUBCOOLED REFLUX 64.000

DYNAMIC SOLUTION

The solution shown is for data set 17 and shows the initial steady-state compositions and temperatures for all of the trays and the variation of all compositions and temperatures with time.

(C 1=Benzene, C 2=Toluene, C 3=p-Xylene)

TABLE 10. STAGE 1										
	1	2	3	4	5	7	8	9	10	
C1	0.3703	0.7974	0.7033	0.0066	0.4099	0.4117	0.3126	0.2207	0.1450	0.0663
C2	0.1242	0.2024	0.2015	0.3638	0.4060	0.3097	0.6321	0.7334	0.7926	0.8076
C3	0.0010	0.1022	0.0042	0.0076	0.0132	0.0237	0.0353	0.0459	0.0623	0.1256
TEMP	186.92	133.90	137.75	192.53	197.93	203.14	209.23	215.57	221.50	229.80

COEFFICIENT MATRIX 1									
	1	2	3	4	5	7	8	9	10
-0.0077	0.2309	0.0040	0.0037	0.0066	0.0153	0.0065	0.0027	0.0011	0.0003
0.0014	-0.1955	0.0453	0.0389	0.1533	0.0153	0.0173	0.0112	0.0112	0.0077
0.0	0.6156	-0.2090	0.3133	1.0340	0.4227	0.1730	0.0725	0.0298	0.0203
0.0	0.0	0.0344	-0.1734	2.9322	1.1300	0.4562	0.2037	0.0846	0.0577
0.0	0.0	0.0	4.2673	-9.2054	2.4047	1.4094	0.5944	0.2404	0.1639
0.0	0.0	0.0	0.0	4.6100	-12.7913	4.0735	1.9373	0.7972	0.5435
0.0	0.0	0.0	0.0	0.0	7.5211	-14.3015	5.1574	2.1217	1.4464
0.0	0.0	0.0	0.0	0.0	0.0	7.2533	-16.4307	5.9756	4.0737
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3913	-12.1023	11.3267
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0043	-0.2049

COEFFICIENT MATRIX 2									
	1	2	3	4	5	7	8	9	10
-0.0079	0.2239	0.0067	0.0072	0.0159	0.0027	0.0011	0.0005	0.0003	0.0000
0.0014	-0.1955	0.0113	0.2767	0.1533	0.0042	0.0163	0.0113	0.0047	0.0032
0.0	0.6156	-0.2045	0.3061	0.4142	0.1711	0.0716	0.0300	0.0125	0.0035
0.0	0.0	0.9344	-0.1050	1.1745	0.4040	0.2030	0.0351	0.0354	0.0245
0.0	0.0	0.0	4.2673	-6.3911	1.5771	0.0702	0.2413	0.1305	0.0695
0.0	0.0	0.0	0.0	4.6100	-0.5000	1.0117	0.3016	0.3333	0.2305
0.0	0.0	0.0	0.0	0.0	7.0211	-10.0793	2.1339	0.3371	0.0135
0.0	0.0	0.0	0.0	0.0	0.0	7.9533	-11.0522	2.4985	1.7279
0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.3913	-12.6302	4.8043
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0943	-0.0926

COEFFICIENT MATRIX 3									
	1	2	3	4	5	7	8	9	10
-0.0079	0.0916	0.0379	0.0195	0.0065	0.0027	0.0012	0.0005	0.0002	0.0001
0.0014	-0.1704	0.0153	0.1500	0.0059	0.0273	0.0116	0.0049	0.0021	0.0014
0.0	0.6156	-0.4000	0.4107	0.1743	0.0727	0.0353	0.0131	0.0055	0.0039
0.0	0.0	0.9344	-0.1050	0.4042	0.2030	0.0273	0.0370	0.0155	0.0109
0.0	0.0	0.0	4.2673	-5.2039	1.5000	0.2479	0.1052	0.0442	0.0310
0.0	0.0	0.0	0.0	4.6100	-0.2019	0.3219	0.3488	0.1460	0.1028
0.0	0.0	0.0	0.0	0.0	0.0	-9.0292	0.9203	0.3000	0.2737
0.0	0.0	0.0	0.0	0.0	0.0	7.2533	-9.7193	1.0965	0.7703
0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.3913	-10.3907	2.1432
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0043	-0.0463

EIGEN VALUES OF C1, C2, C3, MATRICES

1	-1.295067E 02	0.0	-0.169334E 02	0.0	-0.128954E 02	0.0
2	-1.204776E 02	0.0	-0.143937E 02	0.0	-0.112539E 02	0.0
3	-0.148374E 02	0.0	-0.107564E 02	0.0	-0.972091E 01	0.0
4	-0.119500E 02	0.0	-0.824775E 01	0.0	-0.647783E 01	0.0
5	-0.972857E 01	0.0	-0.700114E 01	0.0	-0.552163E 01	0.0
6	-0.671600E 01	0.0	-0.532509E 01	0.0	-0.519164E 01	0.0
7	-0.359003E 01	0.0	-0.307705E 01	0.0	-0.351041E 01	0.0
8	-0.102423E 01	0.0	-0.119390E 01	0.0	-0.160102E 01	0.0
9	-0.106942E 00	0.0	-0.372352E 00	0.0	-0.516423E 00	0.0
10	-0.591211E-01	0.0	-0.105037E-01	0.0	-0.983084E-02	0.0

TRACr CHECK ON C3 -0.5679947E 02 -0.5679955E 02

ITERATION 1

C1	0.5892	0.7864	0.6849	0.5591	0.4579	0.3096	0.2555	0.1847	0.1249	0.0647
C2	0.1298	0.2113	0.3105	0.4223	0.5247	0.6244	0.7001	0.7644	0.8086	0.8093
C3	0.0010	0.0023	0.0046	0.0086	0.0153	0.0300	0.0415	0.0509	0.0565	0.1260

COMPONENT MATRIX 1

-0.0000	0.5793	1.2350	0.0969	0.0404	0.0169	0.0069	0.0023	0.0011	0.0008
2.0116	-0.2305	2.3667	0.9760	0.4039	0.1725	0.0677	0.0285	0.0115	0.0077
0.0	3.6354	-7.3951	2.6017	1.0849	0.4546	0.1853	0.0758	0.0307	0.0205
0.0	0.0	3.2659	-3.2603	3.0032	1.2537	0.5285	0.2157	0.0374	0.0583
0.0	0.0	0.0	4.0137	-9.0032	3.6032	1.5056	0.6146	0.2499	0.1661
0.0	0.0	0.0	0.0	4.5870	-13.3947	5.0206	2.0494	0.8302	0.5540
0.0	0.0	0.0	0.0	0.0	7.0114	-15.4354	5.4354	2.2011	1.4687
0.0	0.0	0.0	0.0	0.0	0.0	3.9225	-16.9769	0.1751	4.1202
0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.4353	-18.5213	11.4160
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0944	-0.2055

COMPONENT MATRIX 2

-0.0000	0.2205	0.0025	0.0135	0.0133	0.0000	0.0000	0.0012	0.0005	0.0003
2.0116	-4.0034	0.0313	0.3802	0.1520	0.0000	0.0000	0.0116	0.0043	0.0033
0.0	3.0334	-0.0000	1.0000	0.4307	0.1800	0.0765	0.0315	0.0129	0.0087
0.0	0.0	3.0000	-5.0000	1.2023	0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	4.0137	-0.5542	1.5000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	4.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	0.0	0.0	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	0.0	0.0	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	0.0	0.0	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	0.0	0.0	0.0000	0.0000	0.0000	0.0000

COMPONENT MATRIX 3

-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.0116	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0000	-4.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	4.0137	-5.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	4.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	0.0	0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	0.0	0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	0.0	0.0000	0.0000	0.0000	0.0000	0.0000
0.0	0.0	0.0	0.0	0.0	0.0000	0.0000	0.0000	0.0000	0.0000

ITERATION 2

C1 0.3670 0.7006 0.6614 0.0052 0.4464 0.3371 0.2363 0.1830 0.1236 0.0640
 C2 0.1320 0.2142 0.3190 0.4201 0.5302 0.6269 0.7023 0.7661 0.8098 0.8098
 C3 0.0010 0.0023 0.0046 0.0035 0.0193 0.0360 0.0414 0.0509 0.0665 0.1262

COMPUTED MATRIX 1

9990
 -0.0000 0.5807 0.2357 0.0972 0.3405 0.6170 0.3869 0.0028 0.0011 0.0008
 2.3135 -6.2395 2.3742 0.9795 0.4084 0.1711 0.0699 0.0285 0.0115 0.0077
 0.0 3.6360 0.0 2.4115 1.0837 0.4561 0.1803 0.0769 0.0308 0.0205
 0.0 0.0 0.0 -8.3793 3.0971 1.2976 0.0370 0.2193 0.0876 0.0584
 0.0 0.0 0.0 4.3167 -9.5306 3.6961 1.5394 0.0161 0.2495 0.1664
 0.0 0.0 0.0 0.0 4.6393 -13.4147 5.0333 2.0542 0.3313 0.5547
 0.0 0.0 0.0 0.0 0.0 0.0 0.0252 -17.2094 5.4459 2.2052 1.4707
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.4375 -18.5405 6.1353 4.1254
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 11.4295
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 -0.2057

COMPUTED MATRIX 2

9990
 -0.0000 0.2205 0.0928 0.0317 0.0163 0.0069 0.0029 0.0012 0.0005 0.0003
 2.3135 -4.6044 0.9349 0.3698 0.1645 0.0694 0.0284 0.0119 0.0048 0.0033
 0.0 3.6360 0.0 1.0361 0.4365 0.1861 0.0767 0.0316 0.0129 0.0087
 0.0 0.0 0.0 -5.2606 1.2474 0.5293 0.2184 0.0399 0.0367 0.0243
 0.0 0.0 0.0 4.3167 -6.5655 1.5077 0.0219 0.2562 0.1045 0.0706
 0.0 0.0 0.0 0.0 4.6393 -9.5306 2.0733 0.3542 0.3489 0.2354
 0.0 0.0 0.0 0.0 0.0 0.0 0.0252 -11.9213 2.2645 0.6241
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.4375 -12.3153 2.5044 1.7505
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 4.8500
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 -0.0930

COMPUTED MATRIX 3

9990
 -0.0000 0.0023 0.0343 0.0162 0.0059 0.0031 0.0012 0.0005 0.0002 0.0001
 2.3135 -2.9869 0.9363 0.1629 0.0695 0.0259 0.0125 0.0052 0.0021 0.0015
 0.0 3.6360 0.0 0.4364 0.1360 0.0793 0.0332 0.0158 0.0057 0.0039
 0.0 0.0 0.0 -4.0794 0.5279 0.2269 0.0945 0.0393 0.0162 0.0111
 0.0 0.0 0.0 4.3167 -5.4124 0.8504 0.2593 0.1120 0.0462 0.0315
 0.0 0.0 0.0 0.0 4.6393 -9.5207 0.9577 0.3735 0.1539 0.1051
 0.0 0.0 0.0 0.0 0.0 0.0 -9.2409 0.9901 0.4079 0.2785
 0.0 0.0 0.0 0.0 0.0 0.0 0.0252 -9.2367 1.1443 0.7813
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.4375 -10.5044 2.1646
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 -0.0470

INTERVIEW 3

[illegible][illegible][illegible]

ITERATION 1

C1 0.8950 0.7029 0.6933 0.5520 0.4136 0.3113 0.2329 0.1652 0.1123 0.0604
 C2 0.1439 0.2345 0.3417 0.4561 0.5700 0.6513 0.7244 0.7325 0.8197 0.8126
 C3 0.0311 0.0025 0.0050 0.0093 0.0163 0.0309 0.0327 0.0524 0.0630 0.1270

COMPLEMENT MATRIX 1

-0.0100 0.0007 0.2413 0.1001 0.0410 0.0179 0.1071 0.0029 0.1012 0.0008
 2.1297 -6.3039 2.4353 1.0102 0.4222 0.1761 0.0719 0.0292 0.0113 0.0073
 0.0 3.6575 -7.9292 2.6976 1.1273 0.4733 0.1920 0.0780 0.0314 0.0203
 0.0 0.0 3.9965 -2.5906 3.2101 1.2393 0.5963 0.2221 0.0894 0.0591
 0.0 0.0 0.0 4.3472 -9.7440 3.0155 1.0570 0.6328 0.2545 0.1684
 0.0 0.0 0.0 0.0 4.7150 -13.6389 5.1057 2.1109 0.3473 0.5605
 0.0 0.0 0.0 0.0 0.0 7.0593 -19.7471 5.3325 2.2467 1.4855
 0.0 0.0 0.0 0.0 0.0 0.0 8.0504 -17.2443 0.2452 4.1622
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 8.4607 -18.7249 11.5157
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0945 -0.2069

COMPLEMENT MATRIX 2

-0.0100 0.0007 0.0932 0.0400 0.0159 0.0071 0.0029 0.0012 0.0005 0.0003
 2.0357 -4.0610 0.9610 0.4933 0.1700 0.0721 0.0237 0.0122 0.0047 0.0033
 0.0 3.6575 -0.0290 1.0769 0.4560 0.1924 0.0793 0.0325 0.0132 0.0088
 0.0 0.0 3.9965 -5.9581 1.2970 0.5400 0.2259 0.0926 0.0276 0.0251
 0.0 0.0 0.0 4.3472 -0.0702 1.5011 0.0434 0.2633 0.1070 0.0715
 0.0 0.0 0.0 0.0 4.7150 -10.0272 2.1421 0.8782 0.3561 0.2380
 0.0 0.0 0.0 0.0 0.0 7.0593 -11.1581 2.3272 0.9433 0.6397
 0.0 0.0 0.0 0.0 0.0 0.0 8.0504 -12.0517 2.0445 1.7672
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 8.4607 -12.9139 4.8893
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0945 -0.0935

COMPLEMENT MATRIX 3

-0.0100 0.0007 0.0395 0.0100 0.0072 0.0051 0.0013 0.0005 0.0002 0.0001
 2.0357 -4.0610 0.3900 0.1601 0.0725 0.0310 0.0129 0.0053 0.0022 0.0015
 0.0 3.6575 -4.4092 0.4510 0.1935 0.0828 0.0344 0.0143 0.0054 0.0039
 0.0 0.0 3.9965 -4.9980 0.3511 0.2557 0.0981 0.0406 0.0165 0.0112
 0.0 0.0 0.0 4.3472 -5.4619 0.6714 0.2794 0.1156 0.0473 0.0319
 0.0 0.0 0.0 0.0 4.7150 -8.0014 0.2003 0.2849 0.1573 0.1063
 0.0 0.0 0.0 0.0 0.0 7.0593 -9.3307 1.0200 0.4170 0.2816
 0.0 0.0 0.0 0.0 0.0 0.0 8.0504 -9.9670 1.1683 0.7692
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 8.4607 -10.0640 2.1834
 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0945 -0.0473

1000

EIGEN VALUES OF C1, C2, C3, MATRICES

1	-0.222323E 02	0.0	-0.173753E 02	0.0	-0.131287E 02	0.0
2	-0.212555E 02	0.0	-0.148769E 02	0.0	-0.116290E 02	0.0
3	-0.151545E 02	0.0	-0.110416E 02	0.0	-0.936622E 01	0.0
4	-0.122960E 02	0.0	-0.864140E 01	0.0	-0.662189E 01	0.0
5	-0.500798E 01	0.0	-0.709320E 01	0.0	-0.50024E 01	0.0
6	-0.685501E 01	0.0	-0.537925E 01	0.0	-0.520215E 01	0.0
7	-0.370223E 01	0.0	-0.310258E 01	0.0	-0.350835E 01	0.0
8	-0.136535E 01	0.0	-0.113023E 01	0.0	-0.157276E 01	0.0
9	-0.183776E 00	0.0	-0.359406E 00	0.0	-0.610048E 00	0.0
10	-0.661513E-01	0.0	-0.107919E-01	0.0	-0.904985E-02	0.0

TRACE CHECK IN C3 -0.5775925E 02 -0.57759277 02

ITERATION 2

C1 0.8534 0.7609 C.6509 0.5301 C.4115 0.3099 0.2317 0.1643 C.1117 0.0601
C2 0.1455 0.2366 0.3441 0.4606 0.5722 0.6932 0.7256 0.7834 0.8203 0.8128
C3 0.0011 0.0025 0.0060 0.0093 0.0113 0.0369 0.0427 0.0524 0.0680 0.1271

COEFFICIENT MATRIX 1

-0.0007	0.0017	0.0014	0.1003	0.0419	0.0176	0.0071	0.0029	0.0012	0.0008
2.0206	-6.3124	2.6420	1.0127	0.4232	0.1765	0.0720	0.0293	0.0118	0.0078
0.0	3.6593	-7.5353	2.7043	1.1327	0.4712	0.1923	0.0761	0.0314	0.0208
0.0	0.0	3.9938	-3.5035	3.2174	1.3419	0.0477	0.2225	0.0895	0.0592
0.0	0.0	0.0	4.3491	-0.7002	3.0225	1.3532	0.0333	0.2550	0.1635
0.0	0.0	0.0	0.0	4.7171	-13.6824	5.1937	2.1097	0.3487	0.5610
0.0	0.0	0.0	0.0	0.0	7.6613	-15.7907	5.5905	2.2490	1.4865
0.0	0.0	0.0	0.0	0.0	0.0	8.0595	-17.2561	6.3009	4.1647
0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.4615	-18.7344	11.5221
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0945	-0.2070

COEFFICIENT MATRIX 2

-0.0009	0.2313	0.0054	0.0401	0.0169	0.0072	0.0029	0.0012	0.0005	0.0003
2.3268	-4.6452	0.9633	0.4043	0.1711	0.0722	0.0293	0.0122	0.0049	0.0033
0.0	3.6593	-5.3344	1.0798	0.4503	0.1923	0.0795	0.0325	0.0132	0.0086
0.0	0.0	3.9938	-5.9369	1.3009	0.5491	0.2263	0.0927	0.0376	0.0251
0.0	0.0	0.0	4.3491	-0.6356	1.3042	0.0446	0.2642	0.1071	0.0715
0.0	0.0	0.0	0.0	4.7171	-10.0339	2.1657	0.8794	0.3505	0.2382
0.0	0.0	0.0	0.0	0.0	7.6613	-11.1652	2.3302	0.9443	0.6311
0.0	0.0	0.0	0.0	0.0	0.0	8.0595	-12.0573	2.6470	1.7683
0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.4615	-12.9124	4.9921
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0945	-0.0936

COEFFICIENT MATRIX 3

-0.0007	0.0045	0.0350	0.0168	0.0072	0.0061	0.0013	0.0005	0.0002	0.0001
2.0206	-4.0149	0.3383	0.1090	0.0727	0.0411	0.0129	0.0053	0.0022	0.0015
0.0	3.6593	-4.4027	0.4525	0.1941	0.0829	0.0345	0.0143	0.0058	0.0039
0.0	0.0	3.9935	-4.9522	0.5527	0.2362	0.0983	0.0406	0.0165	0.0112
0.0	0.0	0.0	4.3491	-5.4365	0.6723	0.2800	0.1153	0.0473	0.0320
0.0	0.0	0.0	0.0	4.7171	-9.0057	0.3229	0.3854	0.1575	0.1064
0.0	0.0	0.0	0.0	0.0	7.6613	-9.3355	1.0213	0.4174	0.2813
0.0	0.0	0.0	0.0	0.0	0.0	8.0595	-9.9701	1.1694	0.7896
0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.4615	-10.5565	2.1346
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0945	-0.0473

FINAL

TIME MIN.	STAGE 1	2	3	4	5	6	7	8	9	10
4.0	C1 0.2533	0.7607	0.6508	0.5309	0.4112	0.3098	0.2316	0.1642	0.1116	0.0601
	C2 0.1456	0.2367	0.3442	0.4607	0.5723	0.6933	0.7257	0.7835	0.8203	0.8128
	C3 0.0011	0.0025	0.0060	0.0093	0.0113	0.0369	0.0427	0.0524	0.0680	0.1271
Temp	141.51	152.44	160.57	166.33	202.60	209.45	214.73	219.72	224.29	230.40

TIME MIN.	STAGE 1	2	3	4	5	6	7	8	9	10
8.00	C1	0.8262	0.7247	0.6083	0.4362	0.2719	0.2815	0.2065	0.1444	0.0972
	C2	0.1725	0.2725	0.3863	0.5039	0.6109	0.6809	0.7498	0.8022	0.8337
	C3	0.0013	0.0028	0.0054	0.0099	0.0171	0.0376	0.0436	0.0534	0.0691
	TEMP	182.70	187.00	192.33	198.63	205.18	211.23	216.43	221.21	225.36

TIME MIN.	STAGE 1	2	3	4	5	6	7	8	9	10
12.00	C1	0.8019	0.6913	0.5689	0.4459	0.3363	0.2550	0.1843	0.1268	0.0844
	C2	0.1967	0.3056	0.4257	0.5435	0.6457	0.7057	0.7712	0.8187	0.8451
	C3	0.0014	0.0030	0.0059	0.0106	0.0180	0.0334	0.0445	0.0545	0.0705
	TEMP	183.69	188.48	194.31	200.32	207.34	212.31	218.03	222.59	226.44

TIME MIN.	STAGE 1	2	3	4	5	6	7	8	9	10
18.00	C1	0.7689	0.6483	0.5207	0.3993	0.2966	0.2273	0.1691	0.1075	0.0700
	C2	0.2296	0.3483	0.4729	0.5894	0.6845	0.7329	0.7644	0.8367	0.8579
	C3	0.0016	0.0034	0.0064	0.0113	0.0184	0.0392	0.0455	0.0558	0.0721
	TEMP	185.08	190.45	196.75	203.46	209.83	214.89	219.93	224.11	227.65

TIME MIN.	STAGE 1	2	3	4	5	6	7	8	9	10
24.00	C1	0.7357	0.6058	0.4745	0.3562	0.2613	0.2035	0.1396	0.0918	0.0586
	C2	0.2625	0.3905	0.5185	0.6318	0.7128	0.7564	0.8138	0.8512	0.8678
	C3	0.0018	0.0037	0.0070	0.0121	0.0199	0.0401	0.0466	0.0570	0.0737
	TEMP	186.50	192.46	199.19	206.09	212.13	216.54	221.37	225.41	228.66

TIME MIN.	STAGE 1	2	3	4	5	6	7	8	9	10
30.00	C1	0.7032	0.5658	0.4331	0.3104	0.2325	0.1842	0.1238	0.0799	0.0501
	C2	0.2949	0.4301	0.5594	0.6678	0.7467	0.7750	0.8287	0.8619	0.8747
	C3	0.0019	0.0041	0.0075	0.0128	0.0208	0.0408	0.0475	0.0582	0.0752
	TEMP	187.93	194.42	201.46	208.25	214.08	217.94	222.62	226.41	229.44

TIME MIN.	STAGE 1	2	3	4	5	6	7	8	9	10
36.00	C1	0.6734	0.5307	0.3934	0.2393	0.1695	0.1121	0.0712	0.0439	0.0210
	C2	0.3245	0.4649	0.5937	0.6967	0.7390	0.8396	0.8595	0.8795	0.8400
	C3	0.0021	0.0044	0.0079	0.0134	0.0415	0.0434	0.0593	0.0766	0.1390
	TEMP	189.28	196.20	203.44	210.13	219.04	223.56	227.17	230.02	234.25

TIME MIN.	STAGE 1	2	3	4	5	6	7	8	9	10
42.00	C1	0.6479	0.5017	0.3708	0.2672	0.1836	0.1036	0.0650	0.0395	0.0185
	C2	0.3498	0.4936	0.6209	0.7183	0.7942	0.8472	0.8747	0.8826	0.8406
	C3	0.0023	0.0046	0.0084	0.0140	0.0222	0.0402	0.0604	0.0779	0.1410
	TEMP	190.45	197.70	205.05	211.54	216.76	224.25	227.72	230.45	234.56

*****FINAL*****

TIME MIN.	STAGE 1	2	3	4	5	6	7	8	9	10
48.00	C1	0.6272	0.4739	0.3497	0.2504	0.1816	0.0976	0.0606	0.0364	0.0167
	C2	0.3704	0.5162	0.6416	0.7351	0.7956	0.8525	0.8782	0.8844	0.8404
	C3	0.0024	0.0049	0.0087	0.0144	0.0226	0.0427	0.0613	0.0791	0.1429
	TEMP	191.43	193.91	205.25	212.67	217.63	224.75	228.12	230.76	234.80

EIGEN VALUES OF C1,C2,C3, MATRICES

1	-0.288947E 02	0.0	-0.189095E 02	0.0	-0.140273E 02	0.0
2	-0.236871E 02	0.0	-0.163314E 02	0.0	-0.127347E 02	0.0
3	-0.174280E 02	0.0	-0.120799E 02	0.0	-0.102221E 02	0.0
4	-0.145701E 02	0.0	-0.983693E 01	0.0	-0.756673E 01	0.0
5	-0.116396E 02	0.0	-0.816290E 01	0.0	-0.648095E 01	0.0
6	-0.795343E 01	0.0	-0.588945E 01	0.0	-0.546510E 01	0.0
7	-0.431619E 01	0.0	-0.326903E 01	0.0	-0.352403E 01	0.0
8	-0.178474E 01	0.0	-0.123895E 01	0.0	-0.153327E 01	0.0
9	-0.183734E 00	0.0	-0.209155E 00	0.0	-0.569578E 00	0.0
10	-0.929889E-01	0.0	-0.126828E-01	0.0	-0.999552E-02	0.0

COMPONENT MATRIX 1

-0.3499	0.7709	0.3260	0.1354	0.0550	0.0216	0.0087	0.0034	0.0013	0.0009
2.9980	-7.3996	3.3295	1.3932	0.5613	0.2205	0.0685	0.0350	0.0137	0.0088
0.0	3.8952	-9.1426	3.7104	1.5058	0.5914	0.2374	0.0939	0.0367	0.0235
0.0	0.0	4.2436	-10.4105	4.2719	1.6779	0.5734	0.2664	0.1043	0.0668
0.0	0.0	0.0	4.5713	-11.6165	4.7337	1.3993	0.7515	0.2641	0.1884
0.0	0.0	0.0	0.0	4.8850	-15.2683	6.2309	2.4648	0.9647	0.6178
0.0	0.0	0.0	0.0	0.0	7.8974	-17.5247	4.5012	2.5444	1.6296
0.0	0.0	0.0	0.0	0.0	0.0	3.2582	-18.8522	7.0363	4.5384
0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.6211	-20.0349	12.4851
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0957	-0.2223

COMPONENT MATRIX 2

-0.3499	0.3093	0.1326	0.0558	0.0228	0.0090	0.0036	0.0014	0.0005	0.0004
2.9980	-5.2395	1.3544	0.5693	0.2531	0.0920	0.0372	0.0148	0.0058	0.0038
0.0	3.8982	-5.1817	1.5272	0.6253	0.2468	0.0593	0.0397	0.0155	0.0101
0.0	0.0	4.2436	-6.9313	1.7740	0.7093	0.2832	0.1127	0.0443	0.0286
0.0	0.0	0.0	4.5713	-7.6515	1.9755	0.7989	0.3173	0.1250	0.0806
0.0	0.0	0.0	0.0	4.8850	-10.9142	2.6200	1.0425	0.4098	0.2643
0.0	0.0	0.0	0.0	0.0	7.8974	-12.1060	2.7496	1.0810	0.6970
0.0	0.0	0.0	0.0	0.0	0.0	8.2582	-12.9056	3.0106	1.9413
0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.6211	-13.6342	5.3404
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0957	-0.1003

COMPONENT MATRIX 3

-0.8499	0.1304	0.0567	0.0241	0.0100	0.0040	0.0015	0.0006	0.0003	0.0002
2.9980	-4.4022	0.5791	0.2453	0.1013	0.0404	0.0165	0.0066	0.0025	0.0017
0.0	3.8982	-5.0103	0.6603	0.2730	0.1033	0.0441	0.0177	0.0070	0.0045
0.0	0.0	4.2436	-5.5507	0.7746	0.3073	0.1252	0.0501	0.0198	0.0129
0.0	0.0	0.0	4.5713	-6.0651	0.8670	0.3533	0.1414	0.0558	0.0363
0.0	0.0	0.0	0.0	4.8850	-9.1642	1.1586	0.4637	0.1831	0.1189
0.0	0.0	0.0	0.0	0.0	7.8974	-9.9128	1.2230	0.4830	0.3136
0.0	0.0	0.0	0.0	0.0	0.0	8.2582	-10.4859	1.3453	0.8735
0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.6211	-10.9085	2.4028
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0957	-0.0509

TABLE A

Iterative Loops and Criteria of Convergence

1. Steady State Solutions

- a. Adjustment of vapor rates and tray temperatures simultaneously.

(2)

Method: Amundson's

Tolerances: 1% change in vapor rates and 0.1%
on $\sum x_i$ and $\sum K x_{i i}$.

Iterations: Ten to eighteen depending on complexity.

2. Dynamic Solutions

- a. Adjustment of the linear variation in the coefficient matrices to match conditions at the beginning and end of the time interval of integration.

(26)

Method: Sargent's

Tolerances: 0.2% for the computed compositions on all trays and for all components.

Iterations: Three to four for periods of rapid change and two for slowly changing periods.

- b. Iteration to locate a single eigen value of the coefficient matrix.

Method: Newton's iterative method and Hyman's method of evaluating the function $\det(B_i - \lambda I)$.

Tolerance: One part in 10^5 .

Iterations: Eight to ten for well separated, real values and up to forty for poorly separated complex values. This is based upon a 'cold start' which means the search is initiated at an arbitrary point.

- c. Bubble-point calculations.

Method: Newton's iterative method.

Tolerances: $\sum K_i x_i = 1.0 \pm .001$ for all trays.

APPENDIX B

Program Listings

1. Steady-State Program

Given the feed composition, reflux ratio and distillate flow rate, this program will compute steady-state compositions and temperatures for each stage of a distillation tower.

The main program contains nearly all of the read, write and computational statements, however, a few specialized subroutines perform the following functions:

TCORRT

Adjusts the temperature of each stage according to Amundson's method.

HLFUN

Computes liquid enthalpy from temperature and liquid composition.

HVFUN

Computes liquid enthalpy from temperature and vapor composition.

EFUN

Computes individual component tray efficiencies.

```

DIMENSION X(20,6),Z(20,6),T(20),V(20),O(20),A(6,20,20),F(6,20)
DIMENSION Q(20),Y(20),XN(20,6)
DIMENSION HL(20),HV(20),K(20,6),VN(20)
DIMENSION FR(20),HF(20),XF(20,6),S(20),ANAME(6),KA(6),KB(6)
DIMENSION KC(6),KD(6),HLA(6),HLB(6),HLC(6),HVA(6),HVB(6),HVC(6)
DIMENSION ALFA(20),BETA(20),E(20,6)
REAL K,KA,KB,KC,KD,O
COMMON N,T,E, IC,X,HVA,HVB,HVC,Z,DSC,HLA,HLB,HLC,KA,KB,KC,KD,K
COMMON KICK,ITS,A

```

5555 CONTINUE

IE=1

READ(5,700)

READ(5,1) N,IC,IFD,IS,TOP,BOT,R,IO,DSC

DC 2151 L=1,IC

DO 2151 J=1,N

Z(J,L)=0.0

DO 2151 I=1,N

2151 A(L,I,J)=0.0

1187 IOVER=1

ITS=1

IF(IE.NE.1) GO TO 1156

N1=N-1

DO 105 I=1,N

X(I,3)=0.0

Q(I)=0.0

FR(I)=0.0

S(I)=0.0

105 HF(I)=0.0

1 FORMAT(4I2,3F8.3,I2,F8.3)

C IO EQUAL ZERO FOR NON CONSTANT OVERFLOW

DO 1111 J=1,IFD

READ(5,2) M,FR(M),HF(M)

2 FORMAT(I2,F10.5,F10.2)

READ(5,1121) (XF(M,I),I=1,IC)

1121 FORMAT(5F10.5)

1111 Y(J)=Y(J)

DO 1112 J=1,IS

READ(5,3) M,S(M)

3 FORMAT(I2,F10.5)

1112 Y(J)=Y(J)

READ(5,4) (ANAME(I),KA(I),KB(I),KC(I),KD(I),I=1,IC)

4 FORMAT(1X,A3,E16.8,E16.8,E16.8,E16.8)

IF(IO.NE.0) GO TO 65

READ(5,5) (HLA(I),HLB(I),HLC(I),I=1,IC)

READ(5,6) (HVA(I),HVB(I),HVC(I),I=1,IC)

5 FORMAT(4X,E16.8,E16.8,E16.8)

6 FORMAT(4X,E16.8,E16.8,E16.8)

READ(5,71) (Q(I),I=2,N1)

71 FORMAT(5F10.4)

READ(5,51) (T(J),J=1,N)

51 FORMAT(5F10.5)

C Q%J< IS HEAT **ADDED** TO STAGE J

CALL ICORRT

```

      AIC=IC
      DO 52 I=1,IC
      X(5,I)=1./AIC
52    Z(5,I)=1./AIC
      IC1=IC-1
      HLCC=HLFUN(5)
      HVCC=HVFUN(5)
      WRITE(6,725) HLCC,HVCC,T(5)
725  FORMAT(3H HL,F10.2,2HHV,F10.2,1HT,F10.4)
      GO TO 82
      65 READ(5,7) HLCC,HVCC
      7  FORMAT(2F10.4)
      82 Y(1)=FR(1)-S(1)
      DO 10 J=2,N
      10 Y(J)=Y(J-1)+FR(J)-S(J)
      WRITE(6,726) (Y(J),J=1,N)
726  FORMAT(3H YJ,12F8.4)
      V(2)=S(1)*(R+1.)
      V(1)=0.0
      Q(1)=S(1)*R
      IF(IE.EQ.1) CALL EFUN(N,IC)
1156 IF(IE.NE.1) CALL EFID(N,IC)
      IE=IE+1
C ASSUME CONSTANT MOLAL OVERFLOW FOR FIRST TRY
      DO 15 J=2,N1
      15 Q(N)=Q(N)-FR(J)*HF(J)-Q(J)+S(J)*HLCC
      Q(N)=Q(N)+V(2)*HVCC-Q(1)*HLCC +S(N)*HLCC
      DO 111 J=2,N1
      111 V(J+1)=V(J)-(Q(J)+(HF(J)-HLCC)*FR(J))/(HVCC-HLCC)
      WRITE(6,500) (V(J),J=1,N)
500  FORMAT(20H INITIAL VAPOR RATES,/, (6F12.6))
      13 DO 18 I=1,IC
      DO 17 J=1,N
      17 F(I,J)=-FR(J)*XF(J,I)
      18 CONTINUE
      DO 123 L=1,IC
      DO 11 I=2,N
      11 A(L,I,I-1)=Y(I-1)+V(I)
      DO 120 I=1,N1
      A(L,I,I)=- (Y(I)+V(I+1)+S(I)+V(I)*K(I,L)*E(I,L))
      BASE=(V(I+1)-V(I)*(1.-E(I,L)))
      I1=I+1
      DO 121 J=I1,N
      A(L,I,J)=BASE*E(J,L)*K(J,L)
      IF(J.EQ.I1) GO TO 121
      J1=J-1
      DO 122 M=I1,J1
      122 A(L,I,J)=A(L,I,J)*(1.-E(M,L))
      121 CONTINUE
      120 CONTINUE
      A(L,N,N)=- (V(N)*K(N,L)*E(N,L)+S(N))
      IF(ICOVER.EQ.1) GO TO 800
      WRITE(6,801)((A(L,I,J),J=1,N),I=1,N)

```

```

801 FORMAT(1H ,10F12.8)
GO TO 123
800 I=N
C INVERSION OF EFFICIENCY MATRIX
I=N
99 ALFA(I)=F(L,I)/A(L,I,I)
BETA(I)=-A(L,I,I-1)/A(L,I,I)
IR=I-1
DO 92 J=1,IR
A(L,J,I-1)=A(L,J,I-1)+A(L,J,I)*BETA(I)
92 F(L,J)=F(L,J)-A(L,J,I)*ALFA(I)
IF(I.EQ.2) GO TO 93
I=I-1
GO TO 99
93 X (1,L)=F(L,1)/A(L,1,1)
DO 94 I=2,N
94 X (1,L)=ALFA(I)+BETA(I)*X (I-1,L)
123 CONTINUE
IF(IOVER.EQ.2) GO TO 802
ITS=ITS+1
CALL TCCRRT
IF(ITS.EQ.20) GO TO 34
IF(ITS.LT.4) GO TO 13
IF(IO.NE.0.AND.KICK.EQ.0) GO TO 34
DO 27 J=1,N
HL(J)=HLFUN(J)
27 HV(J)=HVFUN(J)
Q(N)=0.0
DO 271 J=2,N1
271 Q(N)=Q(N)-FR(J)*HF(J)-Q(J)+S(J)*HL(J)
Q(N)=Q(N)+V(2)*HV(2)-Q(1)*HL(1)+S(N)*HL(N)
C LIQUID RATES ARE 0
KICKV=0
VN(1)=V(1)
VN(2)=S(1)*(R+1.0)
DO 28 J=2,N1
28 VN(J+1)=(-Q(J)+Y(J-1)*(HL(J)-HL(J-1))+FR(J)*(HL(J)-HF(J))
1-VN(J)*(HL(J-1)-HV(J)))/(HV(J+1)-HL(J))
DO 321 J=2,N
RV=V(J)/VN(J)
V(J)=(VN(J)+V(J))/2.
IF(RV.LT..99.OR.RV.GT.1.01) KICKV=1
321 CONTINUE
WRITE(6,721) (V(J),J=1,N)
721 FORMAT(8H V RATES,12F10.3)
IF(KICK.EQ.0.AND.KICKV.EQ.0) GO TO 34
GO TO 13
34 CALL TCCRRT
IOVER=2
GO TO 13
802 DO 35 J=1,N1
35 O(J)=Y(J)+V(J+1)
Q(1)=V(2)*(HV(2)-HL(1))

```


IV G LEVEL 1, MOD 4

```

SUBROUTINE TCORRT
REAL K,KA,KB,KC,KD,LL
DIMENSION E(20,6),X(20,6),Y(20,6),T(20),K(20,6),KA(6),KB(6),KC(6)
DIMENSION KD(6),HLA(6),HLB(6),HLC(6),HVA(6),HVB(6),HVC(6)
DIMENSION Z(20,6),XOLD(20,6),TOLD(20)
COMMON N,T,E, IC,X,HVA,HVB,HVC,Z,DSC,HLA,HLB,HLC,KA,KB,KC,KD,K
COMMON KICK,ITS
WRITE(6,719) (T(J),J=1,N)
719 FORMAT(7H TEMPS ,10F7.2)
KICK=0
DO 1 J=1,N
SUMX=C.0
SUMY=0.0
DELK=0.0
DO 2 I=1,IC
K(J,I)=EXP(KA(I)-KB(I)/(KC(I)+T(J)))
IF(ITS.EQ.1) GO TO 2
Y(J,I)=K(J,I)*X(J,I)
SUMX=SUMX+X(J,I)
SUMY=SUMY+Y(J,I)
2 DELK=DELK+(K(J,I)*KB(I)/((KC(I)+T(J))**2))*X(J,I)
IF(ITS.EQ.1) GO TO 1
DO 3 I=1,IC
X(J,I)=X(J,I)/SUMX
3 Y(J,I)=Y(J,I)/SUMY
TESTX=ABS(ABS(SUMX)-1.00)
TESTY=ABS(ABS(SUMY)-1.00)
IF(TESTX.GT..001.OR .TESTY.GT..001) KICK =1
T(J)=T(J)+(SUMX-SUMY)/DELK
1 CONTINUE
IF(ITS.EQ.1) RETURN
N1=N-1
DO 11 I=1,IC
Z(N,I)=Y(N,I)
DO 12 J=2,N1
M=N-J+1
12 Z(M,I)=E(M,I)*Y(M,I)+(1.-E(M,I))*Z(M+1,I)
11 CONTINUE
WRITE(6,718) ((X(J,I),J=1,N),I=1,IC)
718 FORMAT(7H X COMP,10F7.4)
WRITE(6,720) ((Y(J,I),J=1,N),I=1,IC)
720 FORMAT(7H Y COMP,10F7.4)
WRITE(6,721) ((Z(J,I),J=1,N),I=1,IC)
721 FORMAT(7H Z COMP,10F7.4)
RETURN
END

```

```
FUNCTION HLFUN(J)
  DIMENSION X(20,6),HVA(6),HVB(6),HVC(6),E(20,6),Z(20,6)
  DIMENSION HLA(6),HLB(6),HLC(6),T(20)
  COMMON N,T,E, IC,X,HVA,HVB,HVC,Z,DSC,HLA,HLB,HLC
  HTOT=0.0
  IF(J.NE.1) GO TO2
  T(J)=T(J)-DSC
2 DO 1 I=1,IC
1 HTOT=HTOT+(HLA(I)+HLB(I)*T(J)+HLC(I)*T(J)**2)*X(J,I)
  HLFUN=HTOT
  IF(J.NE.1) RETURN
  T(J)=T(J)+DSC
  RETURN
END
```

```
FUNCTION HVFUN(J)
  DIMENSIONX(20,6),E(20,6),T(20),HVA(6),HVB(6),HVC(6),Z(20,6)
  COMMON N,T,E, IC,X,HVA,HVB,HVC,Z
  HTOT=0.0
  DO 1 I=1,IC
1 HTOT=HTOT+(HVA(I)+HVB(I)*T(J)+HVC(I)*T(J)**2)*Z(J,I)
  HVFUN=HTOT
  RETURN
END
```

```
SUBROUTINE EFID(N,IC)
DIMENSION E(20,6),T(20)
COMMON NK,T,E
N1=N-1
DO 2 I=1,IC
DO 1 J=1,N1
1 E(J,I)=1.00
2 E(10,J)=1.
RETURN
END
```

```
SUBROUTINE EFUN(N,IC)
DIMENSION E(20,6),T(20)
COMMON NK,T,E
N1=N-1
DO 1 J=1,N1
E(J,1)=.595
E(J,2)=.595
1 E(J,3)=.595
DO 2 I=1,IC
2 E(10,I)=1.
RETURN
END
```

2. Dynamic Program

Given the initial conditions and the new feed composition, this program computes the response of a ten stage distillation tower to a step change in feed composition. The initial conditions include the stage compositions, temperatures, liquid and vapor rates, volumetric holdups and component separation efficiencies. Flow rates and efficiencies are taken as constant and response is computed for each component on each stage. Temperatures and compositions as functions of time are the final result which are output. The program is divided into the following subprograms:

MAIN

Reads initial conditions and directs the computations by calling the other subprograms as they are needed. It also directs the output of computed response.

AFORM

Forms the coefficient matrices from the flows, K values, efficiencies and holdups.

EIGEN

Computes the eigen values and vectors of the coefficient matrices by Hyman's method.

DETERM

Computes the value of the determinant and its derivative for a given value of .

MATRX

Inverts the matrix of eigen vectors by elimination with column pivoting.

TCORRT

Computes the bubble points for the liquid compositions on every tray.

HOLDUP

Computes the molar holdup from volumetric holdup and stage composition.

SOLGEN

Computes the composition as a function of time according to Sargent's formula.

AINVER

Computes the term $B^{-1}F$ in Sargent's formula. This subroutine may be used to compute compositions from a given coefficient matrix and feed for a steady-state solution.

EFUN

Set component separation efficiencies on each stage.


```

REAL K
COMPLEX ALAM, FI, FIINV
DIMENSION FI(3,10,10), FIINV(3,10,10), ALAM(3,10)
DIMENSION XD(10,3), T(10), V(10), Y(10), S(10), F(3,10), XF(3)
DIMENSION XA(10,3), XB(10,3)
DIMENSION E(10,3), K(10,3), KA(3), KB(3), KC(3), A(3,10,10), F(3,10,10)
COMMON E, K, V, Y, S, T, F, ALAM, FI, FIINV
997 DT=2.0
   READ(5,1)
   WRITE(6,788)
788 FORMAT(19H1INITIAL CONDITIONS)
   WRITE(6,1)
   1 FORMAT(50H RUN NAME )
   READ (5,119) NNODE, TMAX, RVOL, CON, TVOL
   RVOL=RVOL*3735.
119 FORMAT(12,F10.5,F10.5,F10.5,F10.5)
   READ(5,2) (XB(J,1),XD(J,2),XD(J,3),T(J),V(J),Y(J),S(J),J=1,10)
   2 FORMAT(1X,7F10.5)
   READ(5,3) (FR,XF(1),XF(2),XF(3))
   3 FORMAT(4F10.5)
   DO 2151 I=1,3
   DO 2151 J=1,10
   XB(I,L)=0.0
   XA(I,L)=0.0
   DO 2151 J=1,10
   S(L,J,J)=0.0
2151 A(L,I,J)=0.0
   TACCUM=0.0
   WRITE(6,700) (I,I=1,10)
   WRITE(6,701) TACCUM, (XD(J,1),J=1,10)
   WRITE(6,702) (XD(J,2),J=1,10)
   WRITE(6,703) (XD(J,3),J=1,10)
   WRITE(6,705) (T(J),J=1,10)
   DO 9 J=1,10
   DO 9 I=1,3
   F(I,J)=0.0
   IF(J.EQ.6) F(I,J)=FR*XF(I)
   9 CONTINUE
   ITA=1
   ITR=0
901 CALL EFUN(XD)
   CALL TCCPRT(XD)
   F(1,6)=FR*XF(1)
   F(2,6)=FR*XF(2)
   F(3,6)=FR*XF(3)
   CALL AFORM(A,XD,PVOL,CON,TVOL)
   TACCUM=TACCUM+DT
   IF(TACCUM.GT.TMAX) GO TO 997
   CALL EIGEN(A,ITA)
   CALL SELGEN(A,B,DT,NNODE,ITD,XD,XA)
999 CALL EFUN(XA)
   CALL TCCPRT(XA)
   F(J,6)=FR*XF(1)

```

```
F(2,6)=FR*XF(2)
F(3,6)=FR*XF(3)
CALL AFORM(3,XA,PVCL,CON,TVEL)
ITB=ITB+1
CALL SOLGEN(A,B,DT,NNODE,ITB,XD,XB)
IBSTOP=0
DO 4 J=1,10
DO 4 I=1,3
TEST=ABS(XA(J,I)-XB(J,I))
IF(TEST.GT..0002) IBSTOP=1
4 CONTINUE
IF(IBSTOP.EQ.0) GO TO 5
DO 13 L=1,3
DO 13 J=1,10
13 XA(J,L)=XB(J,L)
IF(ITB.GT.10) GO TO 300
GO TO 499
5 IF(NNODE.EQ.0) GO TO 17
CALL SOLGEN(A,B,DT,NNODE,-1,XD,XA)
17 WRITE(6,711)
711 FORMAT(16H *****FINAL*****)
WRITE(6,700) (I,I=1,10)
700 FORMAT(10H0TIME MIN.,6H STAGE,12,9(6X,12))
WRITE(6,701) TACCUM,(XB(J,1),J=1,10)
WRITE(6,702)(XB(J,2),J=1,10)
WRITE(6,703)(XB(J,3),J=1,10)
WRITE(6,705) (T(J),J=1,10)
701 FORMAT(2H ,F7.2,1X,1X,4H C1 ,F7.4,9(1X,F7.4))
702 FORMAT(2H ,3X,1X,4H C2 ,F7.4,9(1X,F7.4))
703 FORMAT(2H ,3X,1X,4H C3 ,F7.4,9(1X,F7.4))
705 FORMAT(10X,1X,4HTEMP,F7.2,9(1X,F7.2))
IF(TACCUM.GT.3.) DT=4.
IF(TACCUM.GT.11.) DT=6.
IF(TACCUM.GT.46.) DT=10.
DO 8 L=1,3
DO 7 I=1,10
XC(I,L)=XB(I,L)
DO 7 J=1,10
7 A(L,I,J)=B(L,I,J)
8 CONTINUE
IF(TACCUM.GT.TMAX) GO TO 997
ITA=ITA+1
ITB=0
GO TO 901
900 CALL EXIT
END
```

```

SUBROUTINE AFORN(A,X0,RVEL,CON,TVOL)
REAL K
DIMENSION X0(10,3)
DIMENSION Y(10),T(10),HU(10),F(3,10)
DIMENSION A(3,10,10),K(10,3),S(10),V(10),E(10,3)
COMMON E,K,V,Y,S,T,F
N=10
DO 123 L=1,3
DO 11 I=2,10
11 A(L,I,I-1)=Y(I-1)+V(I)
DO 120 I=1,9
A(L,I,I)=-(Y(I)+V(I+1)+S(I)+V(I)*K(I,L)*E(I,L))
CASE=(V(I+1)-V(I)*(1.-E(I,L)))
I1=I+1
DO 121 J=1,10
A(L,I,J)=CASE*E(J,L)*K(J,L)
IF(J.EQ.11) GO TO 121
J1=J-1
DO 122 M=I1,J1
122 A(L,I,J)=A(L,I,J)*(1.-E(M,L))
121 CONTINUE
120 CONTINUE
A(L,N,N)=-(V(N)*K(N,L)*E(N,L)+S(N))
CALL HOLDUP(HU,X0,T,RVEL,CON,TVOL)
DO 12 I=1,10
DO 12 J=1,10
12 A(L,I,J)=A(L,I,J)/HU(I)
F(L,6)=F(L,6)/HU(6)
WRITE(6,706) L
706 FORMAT(17H COMPONENT MATRIX,12)
WRITE(6,707) ((A(L,I,J),J=1,10),I=1,10)
707 FORMAT(1H,10F9.4)
123 CONTINUE
RETURN
END

```

```

SUBROUTINE DETERM(LAM,I,DET,SLOPE,S,L)
COMPLEX RX,ALAM,D,X,DET,SLOPE,I,DT,LAM
DIMENSION ALAM(3,10),S(3,10,10),X(3,10,10),D(10)
DIMENSION DUM(10),P(10,3),BF(10)
DIMENSION F(10,3),V(10),Y(10),F(3,10)
COMMON F,P,V,Y,DUM,DE,F,ALAM,X
DET=CMPLX(0.0,0.0)
X(L,I,1)=CMPLX(1.0,0.0)
X(L,I,2)=(S(L,1,1)-LAM)/(-S(L,2,1))
BINT=1./S(L,2,1)
D(1)=CMPLX(0.0,0.0)
D(2)=CMPLX(BINT,0.0)
SLOPE=CMPLX(0.0,0.0)
DO 2 J=3,10
X(L,I,J)=CMPLX(0.0,0.0)
D(J)=CMPLX(0.0,0.0)
K1=J-2
DO 3 K=1,K1
X(L,I,J)=X(L,I,J)+X(L,I,K)*S(L,K,J-1)
3 D(J)=D(J)+S(L,K,J-1)*D(K)
X(L,I,J)=(X(L,I,J)+(S(L,J-1,J-1)-LAM)*X(L,I,J-1))/(-S(L,J,J-1))
D(J)=(D(J)+(S(L,J-1,J-1)-LAM)*D(J-1)-X(L,I,J-1))/(-S(L,J,J-1))
2 CONTINUE
DO 4 J=1,9
SLOPE=SLOPE+D(J)*S(L,J,10)
4 DET=DET+X(L,I,J)*S(L,J,10)
SLOPE=SLOPE+(S(L,10,10)-LAM)*D(10)-X(L,I,10)
DET=DET+(S(L,10,10)-LAM)*X(L,I,10)
IF(I.EQ.1) GO TO 9
K1=I-1
DT=CMPLX(0.0,0.0)
DO 5 J=1,K1
RX=CMPLX(1.0,0.0)
5 DT=DT+RX/(LAM-ALAM(L,J))
SLOPE=SLOPE-DET*DT
9 RETURN
END

```

```

SUBROUTINE EIGEN(A,ITA)
REAL K
COMPLEX ALAM,EI,EIINV
COMPLEX ADJ,LAM,SLOPE,DLAM,D
DIMENSION E(3,10),T(10),ALAM(3,10),A(3,10,10)
DIMENSION E1(3,10,10),EIINV(3,10,10),RMOD(10)
DIMENSION E(10,3),K(10,3),V(10),Y(10),S(10)
COMMON E,K,V,Y,S,T,E,ALAM,EI,EIINV
DO 1 L=1,3
  ITRY=1
  DO 2 I=1,10
    RMOD(I)=0.0
  DO 2 J=1,10
    IF(I.NE.J) RMOD(I)=RMOD(I)+ABS(A(L,I,J))
2 CONTINUE
  DO 5 I=1,10
    RMOD(I)=A(L,I,I)-RMOD(I)
  RMAX=0.0
  DO 57 I=1,10
    IF(RMAX.GT.RMOD(I)) RMAX=RMOD(I)
57 CONTINUE
  LAM=CMPLX(RMAX,0.0)
  IF(ITA.NE.1) LAM=ALAM(L,1)
  I=1
100 J=1
50 CALL DETERM(LAM,I,D,SLOPE,A,L)
  DLAM=-D/SLOPE
  XTEST=REAL(DLAM)
  YTEST=AIMAG(DLAM)
  XLAM=REAL(LAM)
  YLAM=AIMAG(LAM)
  XTD=ABS(XLAM)+1.0E-07
  YTD=ABS(YLAM)+1.0E-07
  IF(ABS(XTEST/XTD).LT..00001.AND.ABS(YTEST/YTD).LT..00001) GO TO
17
  IF(J.GT.30) GO TO 60
  LAM=LAM+DLAM
  J=J+1
  GO TO 50
60 IF(ITRY.EQ.2) GO TO 980
  LAM=CMPLX(RMAX,1.0)
  J=1
  ITRY=2
  GO TO 50
980 WRITE(6,909)
909 FORMAT(30H *****NO CONVERGE*****)
7 CONTINUE
8 ALAM(L,I)=LAM
  I=I+1
9 IF(I.EQ.11) GO TO 70
  J=1
  XLAM=XLAM+.01*ABS(XLAM)
  LAM=CMPLX(XLAM,-YLAM)

```

```

IF(ITA.NE.1) LAM=ALAM(L,I)
ITRY=1
GO TO 50
70 I=1
49 RT1=REAL(ALAM(L,I))
RT2=REAL(ALAM(L,I+1))
RC1=AIMAG(ALAM(L,I))
RC2=AIMAG(ALAM(L,I+1))
RT=RT1/RT2
IF(RC2.EQ.0.0) GO TO 985
RC=-RC1/RC2
IF(RT.GT..99.AND.RT.LT.1.01.AND.RC.GT..99.AND.RC.LT.1.01) GO TO 52
985 CONTINUE
ALAM(L,I)=CMPLX(RT1,0.0)
RT=RT1
IF(I.EQ.9) GO TO 51
I=I+1
GO TO 49
52 RT=(RT1+RT2)/2.
RC=(RC1-RC2)/2.
ALAM(L,I)=CMPLX(RT,RC)
ALAM(L,I+1)=CMPLX(RT,-RC)
IF(I.EQ.9) GO TO 752
I=I+2
GO TO 49
51 RT=REAL(ALAM(L,10))
ALAM(L,10)=CMPLX(RT,0.0)
752 DO 59 I=1,10
ADJ=ALAM(L,I)
58 CALL DETERM(ADJ,I,D,SLOPE,A,L)
C NORMALIZE EIGENS TO LARGEST 1.0
DO 59 I=1,10
XMAX=0.0
DO 63 J=1,10
RT=REAL(EI(L,I,J))
IF(ABS(RT).GT.XMAX) XMAX=ABS(RT)
63 CONTINUE
DO 61 J=1,10
61 EI(L,I,J)=EI(L,I,J)/XMAX
59 CONTINUE
1 CONTINUE
WRITE(6,788)
788 FORMAT(35H EIGEN VALUES OF C1,C2,C3, MATRICES)
WRITE(6,857) (I,ALAM(1,I),ALAM(2,I),ALAM(3,I),I=1,10)
887 FORMAT(1H ,I2,2X,2E14.6,2X,2E14.6,2X,2E14.6)
SUML=0.0
SUMA=0.0
DO 600 I=1,10
SUMA=SUMA+A(3,I,I)
600 SUML=SUML+REAL(ALAM(3,I))
WRITE(6,601) SUMA,SUML
601 FORMAT(2E15.7)
CALL MATRX(EI,EIINV)

```

GO TO 901
901 RETURN
END

```

SUBROUTINE SOLGEN(A,3,DT,NNODE,ITB,X0,X)
REAL K
COMPLEX FI,EIINV,ALAM,C,P,W
DIMENSION X0(10,3),XS(10,3),E(10,3),K(10,3),V(10),Y(10),S(10)
1,P(10),F(3,10),C(10),ALAM(3,10)
DIMENSION XOP(10,3),A(3,10,10),D(3,10,10),EI(3,10,10)
DIMENSION EIINV(3,10,10),R(10),X(10,3)
COMMON F,K,V,Y,S,P,F,ALAM,EI,EIINV
T=DT
IF(ITB.NE.0) GO TO 13
CALL AINVER(A,F,XS)
13 IF(ITB.NE.(-(1))) GO TO 14
ANODE=NNODE
AITS=1.
999 T=DT*AITS/(ANODE+1.)
14 DO 9 L=1,3
DO 10 I=1,10
XOP(I,L)=X0(I,L)
IF(ITB.EQ.0) GO TO 10
DO 10 J=1,10
XOP(I,L)=XOP(I,L)+(R(L,I,J)-V(L,I,J))*(T**2)*X0(J,L)/(2.*DT)
10 CONTINUE
DO 1 I=1,10
R(I)=CMPLX(0.0,0.0)
DO 1 J=1,10
1 R(I)=P(I)+EI(L,I,J)*(XOP(J,L)-XS(J,L))
6 DO 2 I=1,10
W=ALAM(L,I)*T
RTEST=CABS(W)
IF(RTEST.GT.60.) C(I)=CMPLX(0.0,0.0)
IF(RTEST.GT.60.) GO TO 2
C(I)=P(I)*CEXP(W)
2 CONTINUE
DO 3 I=1,10
X(I,L)=XS(I,L)
DO 4 J=1,10
W=EIINV(L,I,J)*C(J)
4 X(I,L)=X(I,L)+REAL(W)
3 CONTINUE
9 CONTINUE
DO 12 J=1,10
XTOL=0.0
DO 11 I=1,3
11 XTOL=XTOL+X(J,I)
DO 12 I=1,3
12 X(J,I)=X(J,I)/XTOL
C NORMALIZE X
WRITE(6,722) ITB
722 FORMAT(11H ITERATION ,I2)
WRITE(6,701) (X(J,1),J=1,10)
WRITE(6,702) (X(J,2),J=1,10)
WRITE(6,703) (X(J,3),J=1,10)
IF(ITB.NE.(-(1))) RETURN

```



```

701 FORMAT(2H ,RX,1X,4H C1 ,F7.4,9(1X,F7.4))
702 FORMAT(2H ,RX,1X,4H C2 ,F7.4,9(1X,F7.4))
703 FORMAT(2H ,RX,1X,4H C3 ,F7.4,9(1X,F7.4))
    IF(AITS.EQ.AN3DE) RETURN
    AITS=AITS+1.
    GO TO 999
988 RETURN
    END

```

```

SUBROUTINE TCORRT(X)
REAL X,KA,KB,KC
DIMENSION DUM(10),E(10,3),V(10),S(10)
DIMENSION X(10,3),K(10,3),KA(3),KB(3),KC(3),      I(10),Y(10,3)
COMMON E,K,V,DUM,S,T
KA(1)=9.2487
KA(2)=9.3774
KA(3)=9.46406
KB(1)=4998.61
KB(2)=5570.19
KB(3)=6025.67
KC(1)=364.427
KC(2)=362.879
KC(3)=355.661
DO 1 J=1,10
ITS=1
999 SUMY=0.0
DELK=0.0
DO 2 I=1,3
K(J,I)=EXP(KA(I)-KB(I)/(KC(I)+T(J)))
Y(J,I)=K(J,I)*X(J,I)
SUMY=SUMY+Y(J,I)
2 DELK=DELK+(K(J,I)*KB(I)/((KC(I)+T(J))**2 ))*X(J,I)
TESTY=ABS(ABS(SUMY)-1.00)
DO 3 I=1,3
3 K(J,I)=K(J,I)/SUMY
IF((TESTY-.001).LT.0.0) GO TO 1
T(J)=T(J)+(1.0-SUMY)/DELK
ITS=ITS+1
IF(ITS.GT.30) RETURN
GO TO 999
1 CONTINUE
RETURN
END

```

```

SUBROUTINE MATRIX(A,AI)
COMPLEX RX,A,AI,EX,N
DIMENSION IP(10),AI(3,10,10),A(3,10,10),EX(10)
DO 123 L=1,3
KEY=1
DO 1 I=1,10
1 IP(I)=0
DO 2 I=1,10
DO 2 J=1,10
2 AI(L,I,J)=A(L,I,J)
25 KI=KEY-1
BMAX=0.0
DO 3 I=1,10
IF(KEY.EQ.1) GO TO 40
DO 4 J=1,KI
IF(I.EQ.IP(J))GO TO 3
4 CONTINUE
40 CONTINUE
BC=ABS(AIMAG(AI(L,I,1)))
BR=ABS(REAL(AI(L,I,1)))
IF(BMAX.GT.BR.AND.BMAX.GE.BC) GO TO 3
IP(KEY)=I
BMAX=BR
IF(BR.LT.BC) BMAX=BC
3 CONTINUE
IPK=IP(KEY)
DO 5 J=1,10
EX(J)=CMPLX(0.0,0.0)
IF(J.EQ.IPK) EX(J)=CMPLX(1.0,0.0)
5 CONTINUE
DO 6 J=2,10
6 AI(L,IPK,J)=AI(L,IPK,J)/AI(L,IPK,1)
RX=CMPLX(1.0,0.0)
EX(IPK)=RX/AI(L,IPK,1)
DO 7 I=1,10
IF(I.EQ.IPK) GO TO 7
EX(I)=-AI(L,I,1)*EX(IPK)
DO 8 J=2,10
8 AI(L,I,J)=AI(L,I,J)-AI(L,I,1)*AI(L,IPK,J)
7 CONTINUE
DO 9 I=1,10
DO 10 J=1,2
10 AI(L,I,J)=AI(L,I,J+1)
9 AI(L,I,10)=EX(I)
IF(KEY.EQ.10) GO TO 11
KEY=KEY+1
GO TO 25
11 DO 12 I=1,10
DO 13 J=1,10
13 EX(J)=AI(L,I,J)
DO 12 J=1,10
K=IP(J)
12 AI(L,I,K)=EX(J)

```

```
      DC 14 J=1,10  
      DC 15 I=1,10  
15    EX(I)=AI(L,I,J)  
      DC 14 I=1,10  
      K=IP(I)  
14    AI(L,I,J)=EX(K)  
123   CONTINUE  
      RETURN  
      END
```

```

SUBROUTINE HOLDUP(HU,X,T,TVOL,CCN,TVOL)
DIMENSION HU(10),X(10,3),T(10)
DO 1 J=1,10
VOL=TVOL
NTAVE=X(J,1)*79.11+X(J,2)*92.12+X(J,3)*106.16
SG=0.931-.00066*T(J)
IF(J.EQ.1) VOL=CCN
IF(J.EQ.10) VOL=TVOL
HU(J)=VOL*SG/NTAVE
1 HU(J)=HU(J)*50./454.
RETURN
END

```

```
SUBROUTINE AINVER(A,F,X)
  DIMENSION FD(10), ALFA(10), BETA(10)
  DIMENSION A(3,10,10), DUM(10,10), X(10,3), F(3,10)
  DO 123 L=1,3
    DO 7 I=1,10
      FD(I)=-F(L,I)
    DO 7 J=1,10
      7 DUM(I,J)=A(L,I,J)
      I=10
  99 ALFA(I)=FD(I)/DUM(I,I)
    BETA(I)=-DUM(I,I-1)/DUM(I,I)
    IR=I-1
    DO 92 J=1,IR
      DUM(J,I-1)=DUM(J,I-1)+DUM(J,I)*BETA(I)
  92 FD(J)=FD(J)-DUM(J,I)*ALFA(I)
    IF(I.EQ.2) GO TO 93
    I=I-1
    GO TO 99
  93 X(1,L)=FD(1)/DUM(1,1)
    DO 94 I=2,10
      94 X(I,L)=ALFA(I)+BETA(I)*X(I-1,L)
  123 CONTINUE
  RETURN
  END
```

```
SUBROUTINE EFUN(XO)
  DIMENSION XO(10,3),E(10,3)
  COMMON E
```

```
  C      EFFICIENCY GENERATION * * ** ** ** ** * * * * *
```

```
  DO 1 J=1,10
```

```
    E(J,1)=.623
```

```
    E(J,2)=.623
```

```
  1  E(J,3)=.623
```

```
    E(10,3)=1.0
```

```
    E(10,1)=1.
```

```
    E(10,2)=1.
```

```
  RETURN
```

```
  END
```

APPENDIX C

Physical Properties of Benzene, Toluene, p-Xylene

1. Antoine constants for vapor pressure.
2. Curve fits for vapor and liquid enthalpy as functions of temperature.
3. Density of liquid as a function of temperature.

Physical Properties

1. Vapor Pressure (3)

$$\ln (P^0) = A - B / (C + T)$$

P^0 = Vapor Pressure, atm.

T = temperature, °F

	A	B	C
Benzene	9.2487	4998.61	364.427
Toluene	9.3774	5570.19	362.879
p-Xylene	9.46406	6025.67	355.661

2. Vapor Enthalpy (17)

$$h_v = a + bT$$

h = vapor enthalpy Btu/lb. mole

T = temperature, °F 75° T 250°

	a	b
Benzene	14240.	22.10
Toluene	15560.	26.90
p-Xylene	16260.	35.40

3. Liquid Enthalpy (17)

$$H_L = a + bT$$

H_L = liquid enthalpy Btu/lb. mole

T = temperature, °F 75° T 250°

	a	b
Benzene	-1750.	37.5
Toluene	-1780.	42.8
p-Xylene	-2700.	48.0

4. Liquid Specific Gravity (17)

SG = specific gravity relative to water 60°F

T = temperature, °F, 125 T, 250

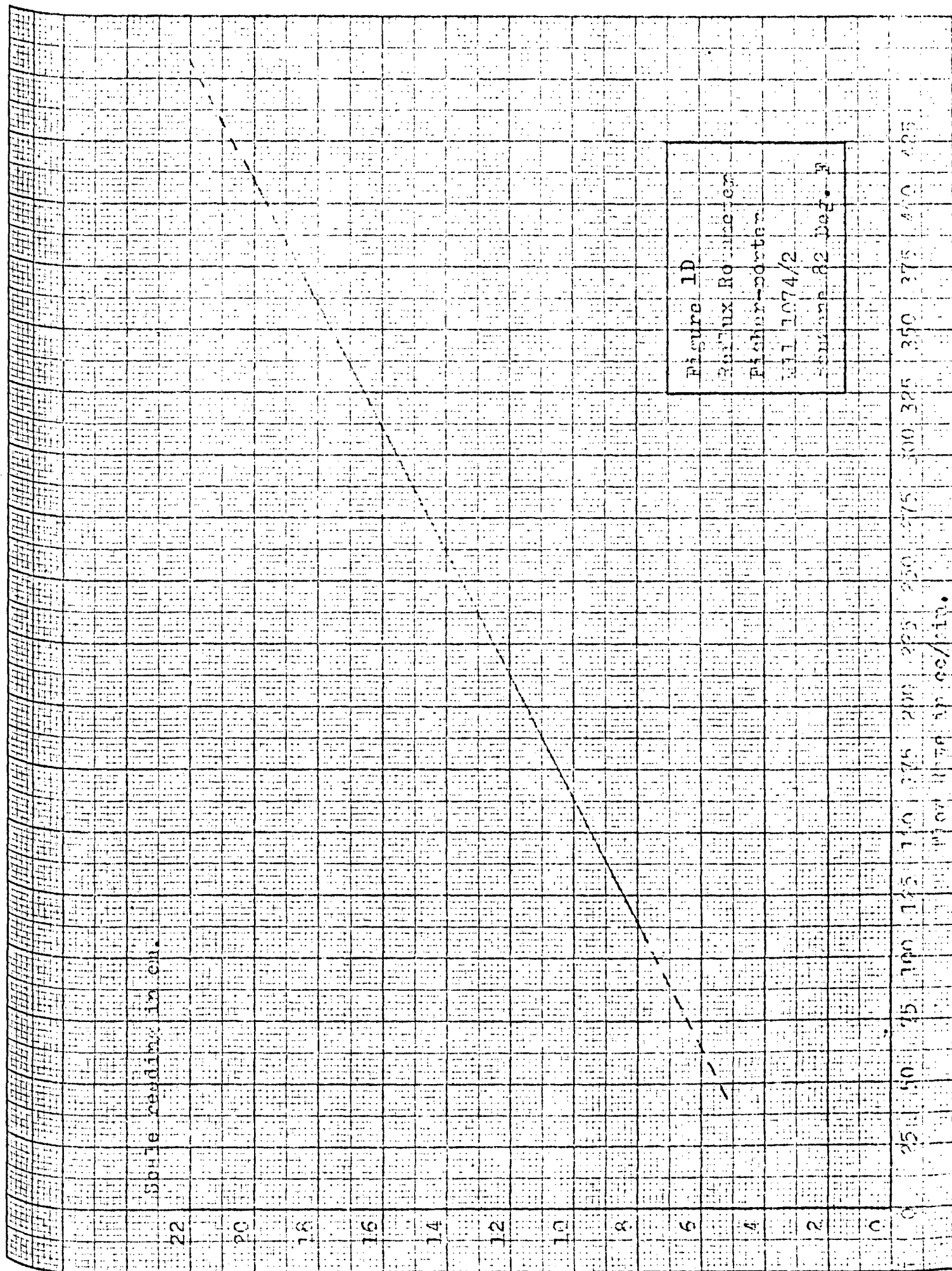
$$SG = .931 - .00066 T$$

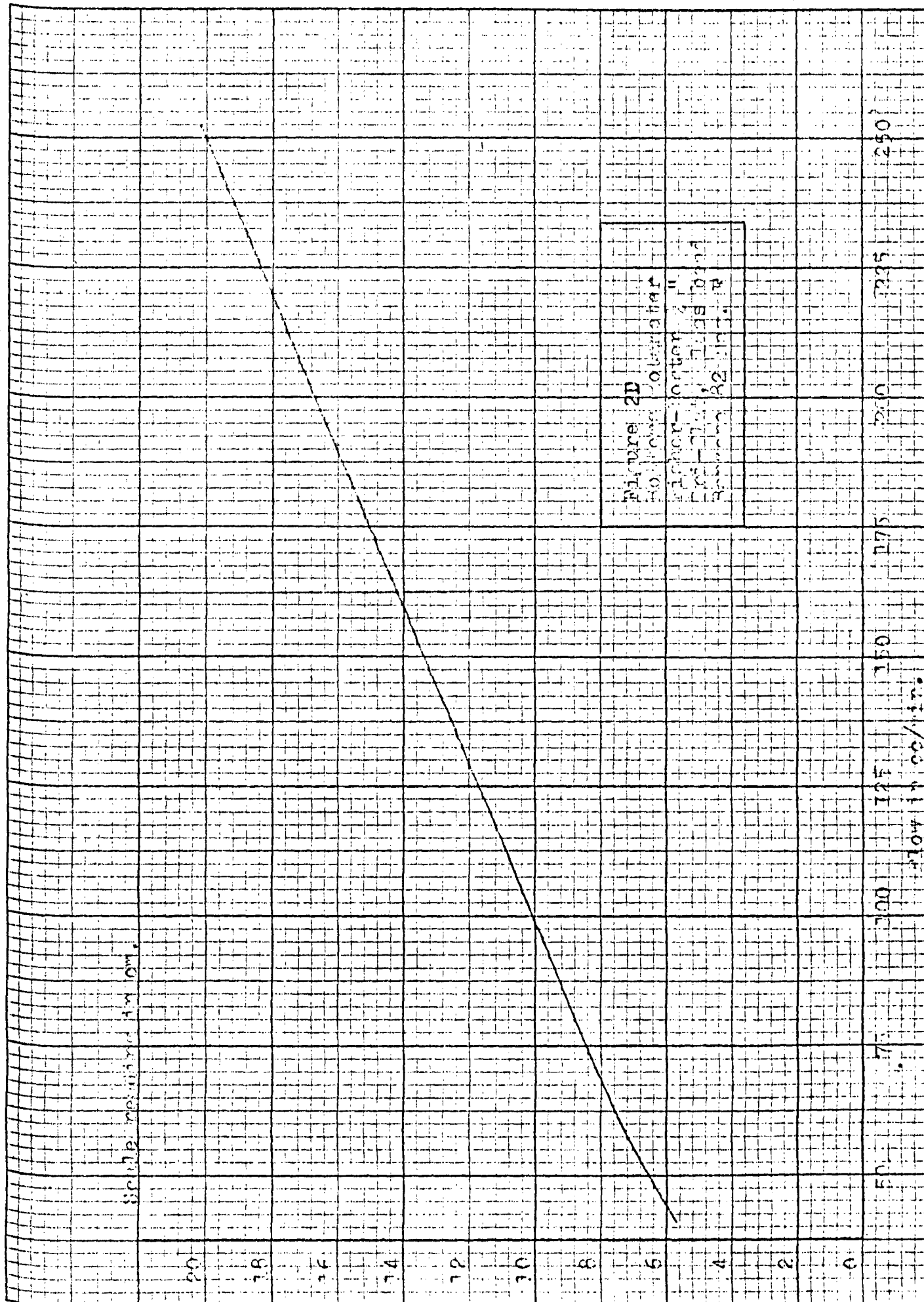
This is an average density for benzene, toluene, p-Xylene and is accurate over the temperature range to $\pm 2\%$.

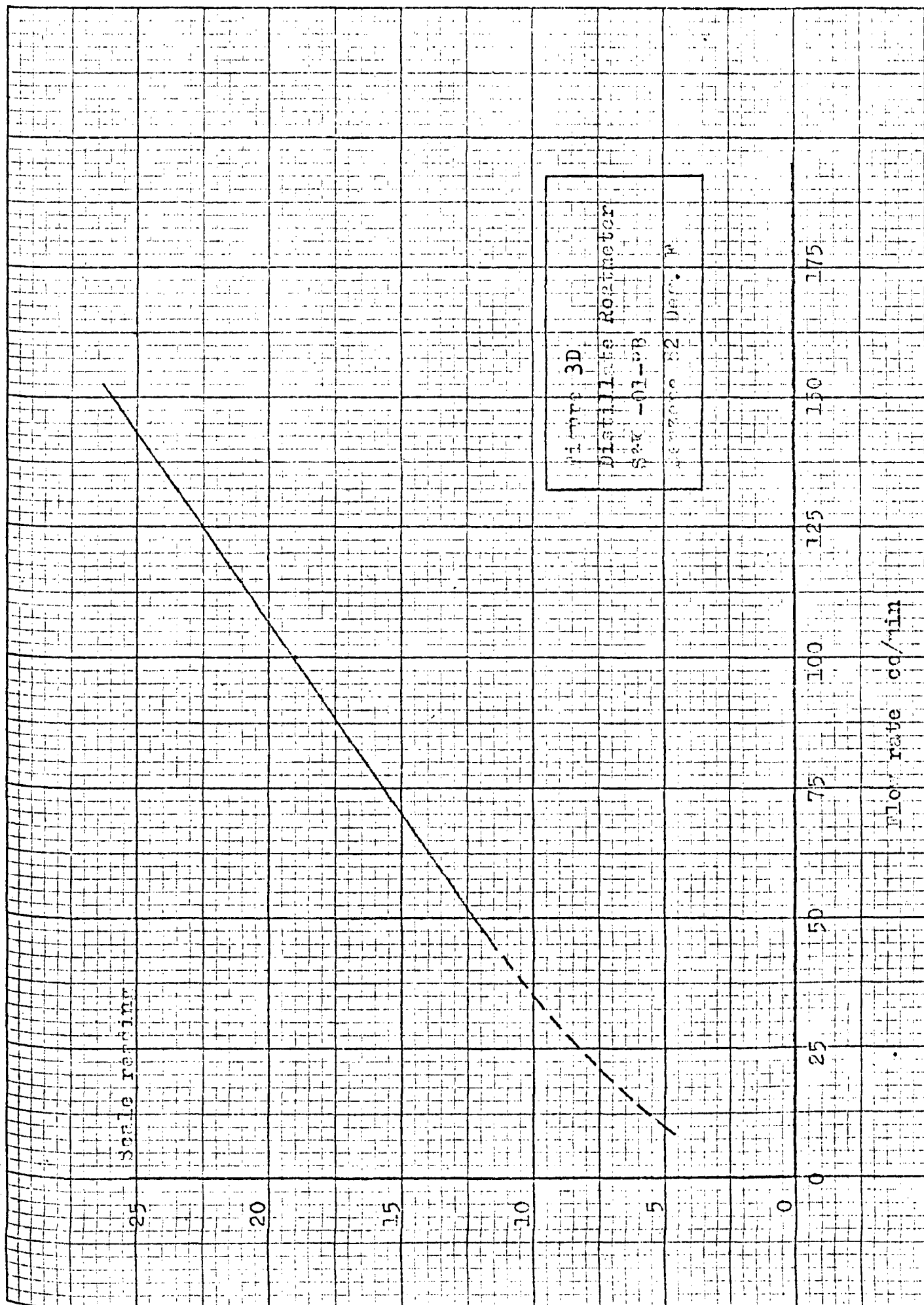
APPENDIX D

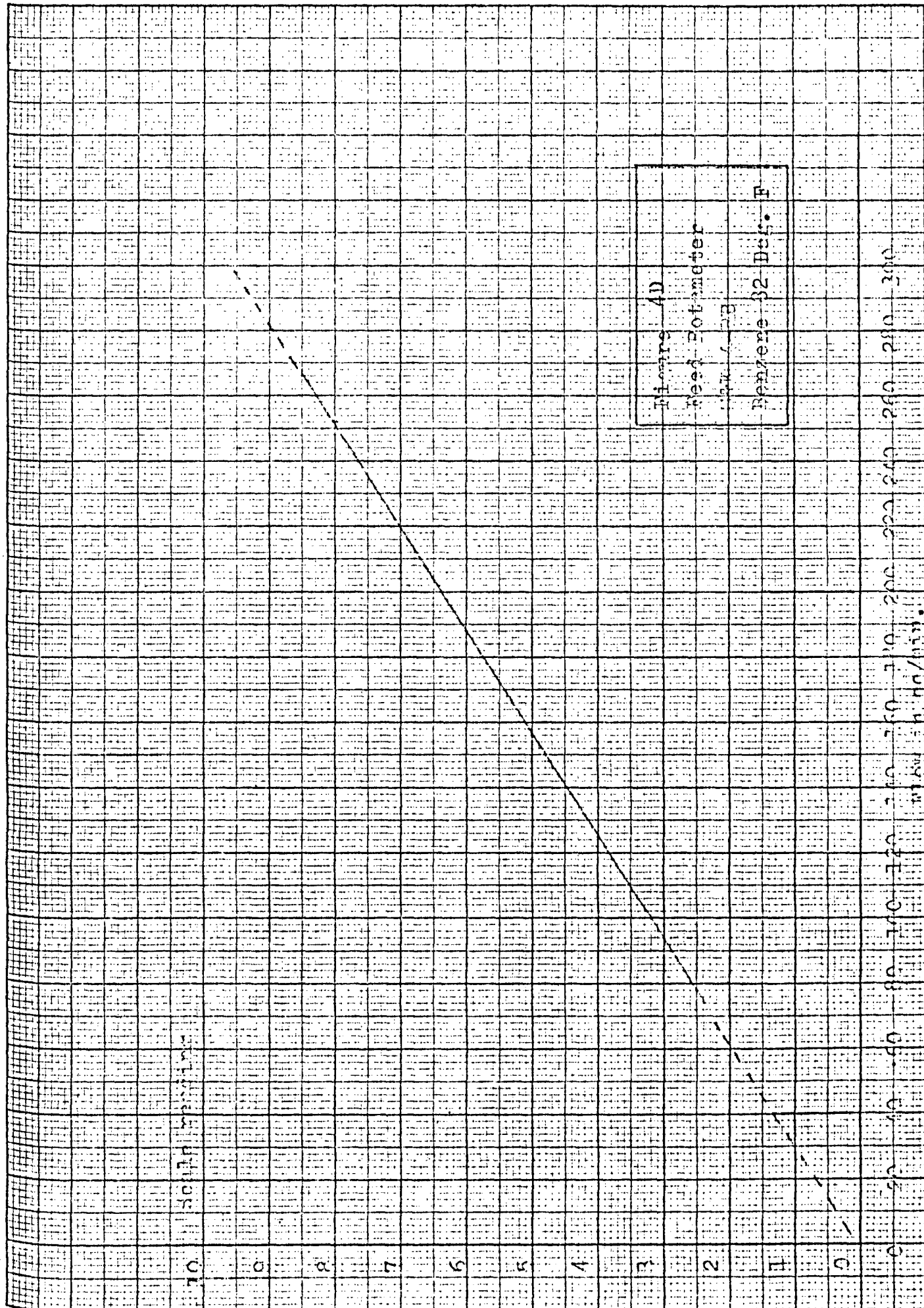
Calibration Curves

1. Calibration charts for feed, products and reflux rotameters.
2. Calibration chart for reboiler holdup.









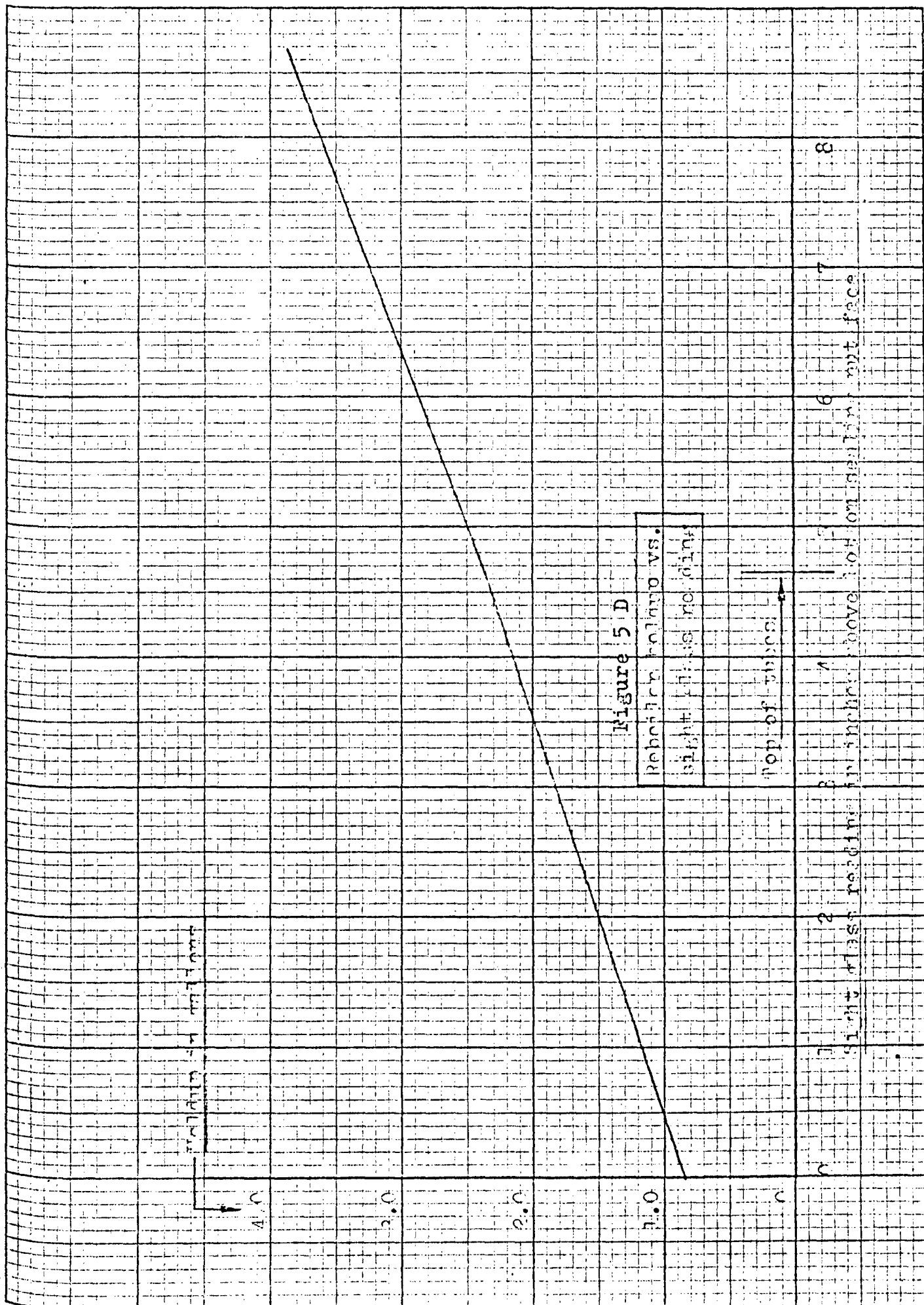
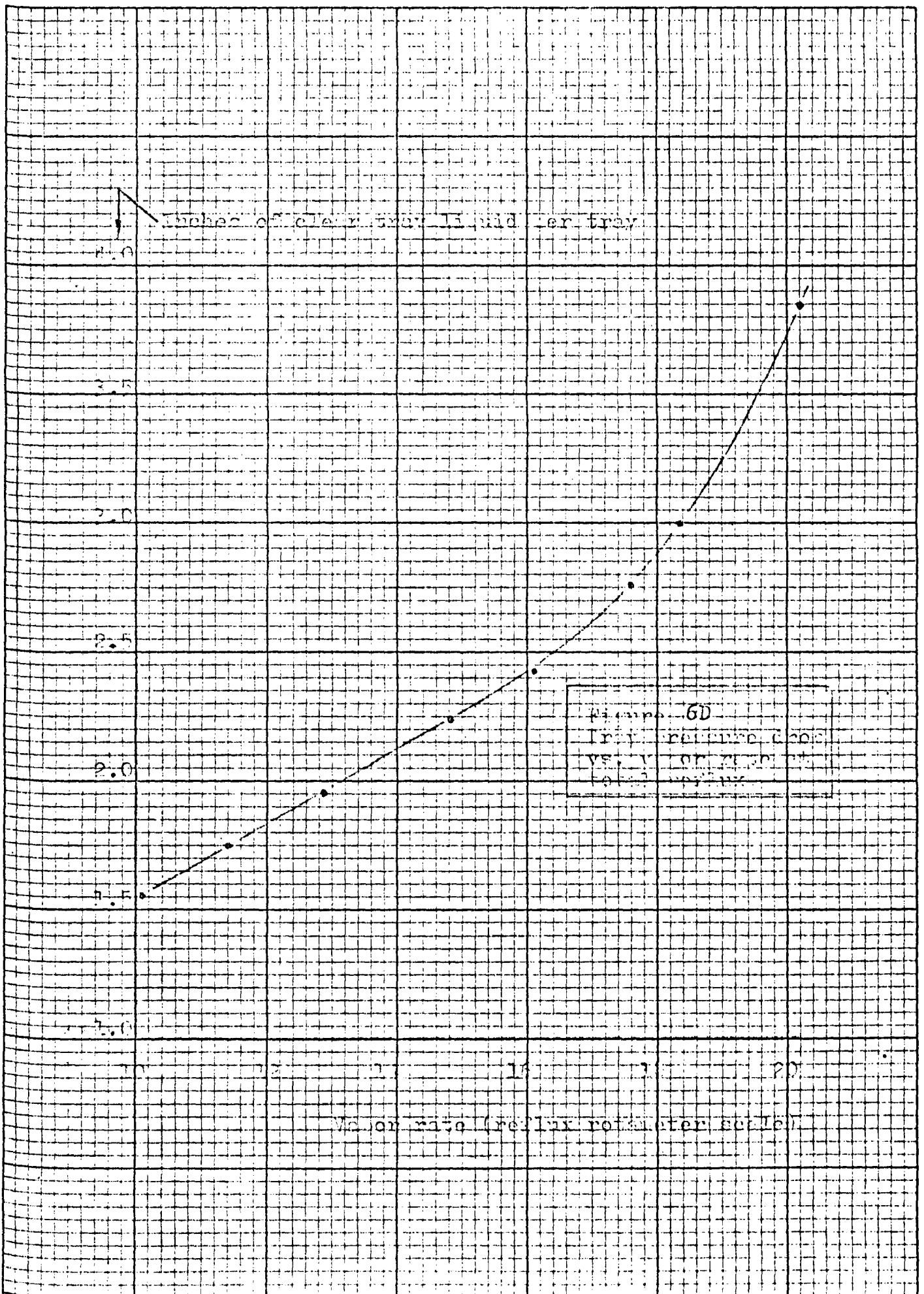


Figure 5 D

Rebottch Polymers vs.
Slightness in degrees

Top of tube



APPENDIX E

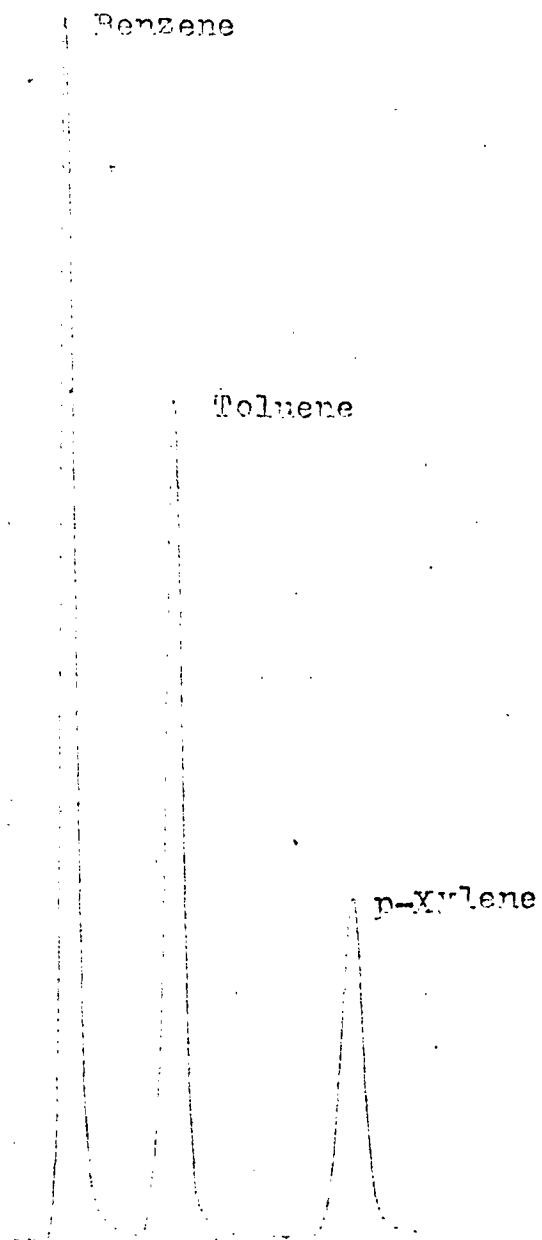
Analysis

Binary and ternary mixtures of benzene, toluene and p-xylene were analyzed using an F & M Model 700 gas chromatograph. Even though industrial and practical grade chemicals were used the elution peaks were sharp and peak areas could be approximated with two triangular segments per component. Fortunately, the relative response of the detector to equal quantities of benzene, toluene and p-xylene had been extensively studied and it was only necessary to verify the findings on the particular chromatograph used. Ten weighed samples were found to agree with Nogare's (19) values to an average accuracy of 1.0%. As with many compounds in a homologous series, the component area percentage converts directly to component weight percentage. A sample chromatogram showing the method estimating the peak area is shown in Figure 1E . Data on the chromatograph and the settings used are presented below.

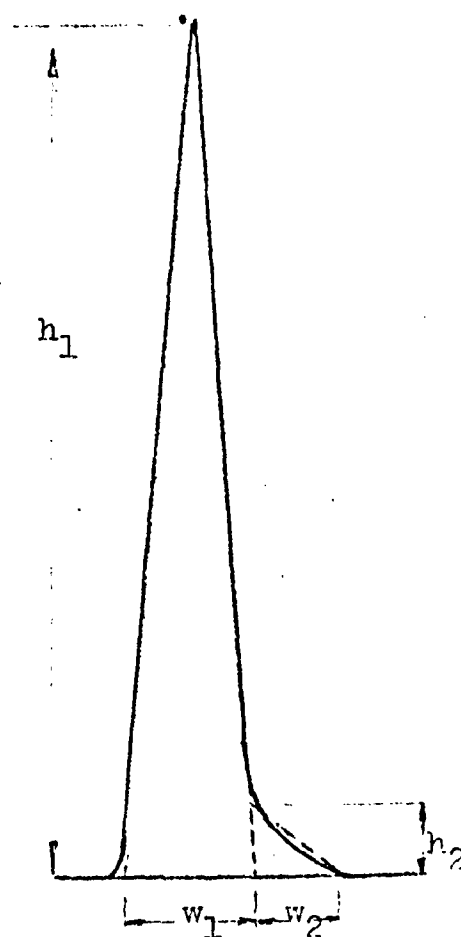
1. <u>Chromatograph</u>	F&M Scientific 700
2. <u>Column Size</u>	1/8" OD, 6 ft. long
Substrate	
3. <u>Detector type</u>	Thermal Conductivity
Detector Current	150 m.a.
4. <u>Temperature Settings</u>	
Injection Port	180° C
Oven	100° C
Detector	170° C
5. <u>Carrier Gas</u>	Helium
Flow Rate	1.0cc/sec.

6. Retention Times

Benzene	29 secs.
Toluene	45 secs.
p-Xylene	73 secs.



Actual chromatograph showing the three component peaks.



Two-triangle approximation for determining the area of a single peak.

$$\text{Area} = \frac{1}{2}h_1w_1 + \frac{1}{2}h_2w_2$$

Figure 1E

APPENDIX F

EXPERIMENTAL DATA

1. Computed and experimental data for efficiency determination runs either under total reflux or continuous distillation. Tables 1F thru 5F.
2. Processed response data for all of the dynamic runs giving run conditions and response vs. time.
3. Raw data for the dynamic runs giving the chromatographic analysis in the form of peak heights and widths for each component.

$$\text{Area of the benzene peak} = H_1 \times W_1 + H_2 \times W_2$$

$$\text{Area of the toluene peak} = H_3 \times W_3 + H_4 \times W_4$$

$$\text{Area of the xylene peak} = H_5 \times W_5 + H_6 \times W_6$$

DATA SET 12 A
DETERMINATION OF COMPONENT EFFICIENCIES
SUPERFICIAL VAPOR VELOCITY 1.04 FT/SEC

TRAY	LIQUID COMPOSITIONS			VAPOR COMPOSITIONS			EFFICIENCIES						
	MOLE PERCENT	XB	XT	XX	YB	YT	YX	LB	ET	EX	TEMP		
1	0.0070	0.9046	0.0884	0.0119	0.9364	0.0516	0.0170	0.9417	0.0413	0.496	0.858	0.781	233.68
2	0.0119	0.9364	0.0516	0.0238	0.9421	0.0341	0.0284	0.9432	0.0234	0.719	0.482	0.620	231.91
3	0.0238	0.9421	0.0341	0.0480	0.9291	0.0229	0.0553	0.9297	0.0150	0.769	1.047	0.583	230.28
4	0.0480	0.9291	0.0229	0.0655	0.9227	0.0119	0.1078	0.8825	0.0097	0.292	0.128	0.333	227.88
5	0.0655	0.9227	0.0119	0.1175	0.8755	0.0070	0.1434	0.8518	0.0049	0.668	0.665	0.655	226.10
6	0.1175	0.8755	0.0070	0.1960	0.8005	0.0036	0.2422	0.7552	0.0027	0.629	0.624	0.791	221.90
7	0.1960	0.8005	0.0036	0.2841	0.7136	0.0023	0.3711	0.6277	0.0012	0.503	0.503	0.545	216.11
8	0.2841	0.7136	0.0023	0.4617	0.5333	0.0	0.4924	0.5069	0.0007	0.852	0.848	1.441	210.22

TABLE 1F

DATA SET 12 B
DETERMINATION OF COMPONENT EFFICIENCIES
SUPERFICIAL VAPOR VELOCITY 1.12 FT/SEC

TRAY	LIQUID COMPOSITIONS			VAPOR COMPOSITIONS			EFFICIENCIES		
	MOLE PERCENT	XT	XX	YB	YT	YX	BY COMPONENT	EX	TEMP
1	0.0190	0.8948	0.0862	0.0390 0.0456	0.9084 0.9149	0.0526 0.0395	0.753	0.674	0.719 232.53
2	0.0390	0.9084	0.0526	0.0643 0.0899	0.9021 0.8872	0.0337 0.0229	0.495	0.298	0.637 229.63
3	0.0643	0.9021	0.0337	0.1090 0.1424	0.8714 0.8436	0.0196 0.0140	0.572	0.525	0.712 226.91
4	0.1090	0.8714	0.0196	0.1754 0.2281	0.8132 0.7643	0.0114 0.0076	0.553	0.544	0.681 222.93
5	0.1754	0.8132	0.0114	0.2992 0.3404	0.6951 0.6556	0.0047 0.0040	0.750	0.743	0.904 217.78
6	0.2992	0.6961	0.0047	0.4071 0.5116	0.5905 0.4870	0.0024 0.0014	0.503	0.505	0.696 209.33
7	0.4071	0.5905	0.0024	0.5512 0.6300	0.4474 0.3694	0.0014 0.0006	0.647	0.647	0.597 202.82
8	0.5512	0.4474	0.0014	0.5787 0.7554	0.4200 0.2442	0.0013 0.0003	0.134	0.135	0.042 195.11

TABLE 2F

DATA SET 13
 DETERMINATION OF COMPONENT EFFICIENCIES
 SUPERFICIAL VAPOR VELOCITY 1.15 FT/SEC

TRAY	LIQUID COMPOSITIONS			VAPOR COMPOSITIONS			EFFICIENCIES			TEMP	
	MOLE PERCENT	XB	XT	XX	YB	YT	YX	BY COMPONENT	EX		
1	0.0552	0.8687	0.0760		0.1122 0.1262	0.8406 0.8410	0.0471 0.0328	0.762	1.017	0.607	229.08
2	0.1038	0.8444	0.0518		0.1753 0.2217	0.7973 0.7578	0.0273 0.0206	0.577	0.523	0.745	224.35
3	0.1644	0.8107	0.0249		0.2666 0.3246	0.7165 0.6664	0.0169 0.0090	0.612	0.618	0.569	218.96
4	0.2619	0.7039	0.0342		0.3907 0.4677	0.5953 0.5194	0.0140 0.0109	0.611	0.615	0.483	212.48
5	0.2978	0.6853	0.0169		0.4384 0.5122	0.5528 0.4826	0.0088 0.0051	0.393	0.378	0.587	209.71
6	0.3870	0.6038	0.0092		0.5622 0.6111	0.4338 0.3864	0.0040 0.0025	0.717	0.715	0.767	204.13
7	0.5172	0.4780	0.0047		0.6566 0.7294	0.3411 0.2695	0.0023 0.0011	0.565	0.564	0.577	196.90
8	0.6342	0.3632	0.0025		0.7742 0.8150	0.2249 0.1845	0.0009 0.0005	0.742	0.742	0.796	191.10

TABLE 3F

DATA SET 14 A
DETERMINATION OF COMPONENT EFFICIENCIES
SUPERFICIAL VAPOR VELOCITY 0.99 FT/SEC

TRAY	LIQUID COMPOSITIONS			VAPOR COMPOSITIONS			EFFICIENCIES BY COMPONENT			
	MOLE PERCENT	XB	XT	XX	YB	YT	YX	FB	ET	EX
1	0.0969	0.8227	0.0804	0.1702 0.2114	0.7870 0.7559	0.0423 0.0327	0.589	0.517	0.720	225.81
2	0.1516	0.7898	0.0586	0.3462 0.3081	0.6286 0.6701	0.0252 0.0218	1.277	1.355	0.842	220.90
3	0.2305	0.7224	0.0471	0.3767 0.4238	0.6042 0.5555	0.0190 0.0157	0.370	0.334	0.643	214.93
4	0.3253	0.6328	0.0420	0.4617 0.5502	0.5253 0.4373	0.0130 0.0125	0.490	0.473	0.914	208.61
5	0.3829	0.5978	0.0192	0.5609 0.6091	0.4303 0.3856	0.0088 0.0053	0.673	0.690	0.549	204.59
6	0.4702	0.5195	0.0102	0.6217 0.6908	0.3737 0.3066	0.0047 0.0026	0.468	0.458	0.656	199.50
7	0.5642	0.4307	0.0051	0.7229 0.7661	0.2755 0.2327	0.0016 0.0012	0.701	0.696	0.885	194.53
8	0.6911	0.3065	0.0025	0.8086 0.8511	0.1905 0.1484	0.0009 0.0005	0.669	0.669	0.619	188.49

TABLE 4F

DATA SET 14 B
DETERMINATION OF COMPONENT EFFICIENCIES
SUPERFICIAL VAPOR VELOCITY 1.25 FT/SEC

TRAY	LIQUID COMPOSITIONS			VAPOR COMPOSITIONS				EFFICIENCIES			
	XB	XT	XX	YB	YT	YX		EB	ET	EX	TEMP
1	0.0906	0.3403	0.0691	0.1755 0.1980	0.7860 0.7738	0.0385 0.0282		0.779	0.801	0.743	225.95
2	0.1590	0.7893	0.0517	0.2423 0.3194	0.7287 0.6616	0.0285 0.0190		0.447	0.460	0.512	220.15
3	0.2386	0.7216	0.0398	0.3572 0.4389	0.6262 0.5430	0.0166 0.0131		0.583	0.567	0.772	214.18
4	0.3169	0.6492	0.0339	0.5006 0.5387	0.4870 0.4512	0.0124 0.0101		0.790	0.795	0.645	208.93
5	0.3945	0.5909	0.0147	0.5746 0.6200	0.4190 0.3761	0.0064 0.0040		0.620	0.613	0.718	203.82
6	0.5093	0.4821	0.0086	0.6516 0.7239	0.3448 0.2741	0.0035 0.0021		0.516	0.512	0.669	197.39
7	0.6154	0.3811	0.0035	0.7598 0.8025	0.2387 0.1967	0.0015 0.0008		0.717	0.717	0.723	192.01
8	0.7378	0.2605	0.0017	0.8468 0.8782	0.1526 0.1215	0.0006 0.0003		0.735	0.734	0.785	186.42

TABLE 5F

```

1  DIMENSION W(99,12),XB(99),XT(99),XX(99),AN(99)
2  999 WRITE(6,10)
3  10 FORMAT(1H1,/,/,/,/,/,/ )
4  READ(5,11)
5  WRITE(6,11)
6  READ(5,11)
7  WRITE(6,11)
8  READ(5,11)
9  WRITE(6,11)
10 11 FORMAT(50H
11 READ(5,7) N
12 7 FORMAT(12)
13 READ(5,444) ((W(I,J),J=1,12),AN(I),I=1,N)
14 444 FORMAT(12(F6.3),5X,A3)
15 WRITE(6,22)
16 22 FORMAT(5X,2HW1,5X,2HH1,5X,2HW2,5X,2HH2,5X,2HW3,5X,2HH3,5X,2HW4,5X,
17 12HH4,5X,2HW5,5X,2HH5,5X,2HW6,5X,2HH6,5X,2HH6,5HIDENT.)
18 WRITE(6,30) (I,(W(I,J),J=1,12),AN(I),I=1,N)
19 30 FORMAT(1H0,12,12F7.3,2X,A3)
20 GO TO 999
21 555 CALL EXIT
    END

```

Data Set 9

Tray 1 vs. time

Initial Conditions	Mole fractions			Rate
	Benzene	Toluene	Xylene	Lb.moles/hr.
Feed 1	0.449	0.551	0.0	0.250
Distillate	0.786	0.214	0.0	0.138
Bottoms	0.0341	0.966	0.0	0.112
Feed 2	0.557	0.443	0.0	0.250
Reflux Ratio	3.14			

Response

Time(minutes)	Fraction benzene
0.0	0.648
1.25	0.675
2.25	0.677
4.00	0.695
6.00	0.724
8.00	0.738
10.0	0.752
12.0	0.758
14.0	0.789
17.5	0.812
20.5	0.795
23.0	0.821
26.0	0.824
29.0	0.828
35.0	0.837
39.0	0.850
44.0	0.858
49.0	0.866
57.2	0.860

DatavSet 10 (Binary)

Trays 3 and 8 verses time.

Initial Conditions	Mole % Benzene	Flow Rate
Feed 1	44.6	0.250
Distillate	77.7	0.133
Bottoms	3.7	0.117

Reflux Ratio 3.0:1

Feed 2 58.6

<u>Tray 3</u>		<u>Tray 8</u>	
<u>Time</u>	<u>M % Benzene</u>	<u>Time</u>	<u>M % Benzene</u>
0	58.5	0	7.9
2.5	42.9	0	9.5
4.5	47.7	2.75	9.5
6.5	50.4	4.75	10.5
9.0	51.4	6.5	11.2
12.25	53.6	9.15	11.2
17.50	54.4	12.50	11.7
21.25	59.4	17.50	13.7
26.00	61.8	21.50	14.4
29.50	62.3	26.25	15.3
35.50	62.3	29.50	15.2
39.00	63.9	35.50	16.0
44.00	66.5	39.25	17.1
49.00	68.2	44.25	17.5
54.30	67.0	49.25	16.5
59.20	68.0	54.75	18.0
		59.50	18.1

DATA SET 15

TOP TRAY VS. TIME

INITIAL CONDITIONS

MOLE FRACTIONS

RATE

	BENZENE	TOLUENE	XYLENE	LS. MOLES/HR.
FEED 1	0.38445	0.54615	0.06940	0.26600
DISTILLATE	0.57935	0.31891	0.00174	0.15700
BOTTOMS	0.03454	0.79619	0.16927	0.10900
FEED 2	0.47667	0.45925	0.06414	0.26600
REFLUX RATIO	3.16			

RESPONSE

TIME (MINUTES)

BENZENE

TOLUENE

XYLENE

00.	0.52740	0.46887	0.00373
.25	0.51370	0.46283	0.00347
1	0.52111	0.47529	0.00360
2	0.54736	0.44934	0.00328
3	0.54846	0.44817	0.00337
5	0.57432	0.42257	0.00311
7	0.58938	0.40757	0.00305
9	0.60478	0.39239	0.00283
11	0.63558	0.36183	0.00259
13	0.62291	0.37464	0.00246
15	0.62899	0.36844	0.00257
17	0.63758	0.35980	0.00262
19	0.64897	0.34849	0.00254
21	0.66361	0.33383	0.00256
23	0.65674	0.34095	0.00231
25	0.66057	0.33735	0.00209
27	0.67059	0.32702	0.00239
29	0.66118	0.33656	0.00226
31	0.66728	0.33035	0.00237
33	0.67202	0.32585	0.00214
36	0.68069	0.31715	0.00216
39	0.68720	0.31065	0.00215

DATA SET 16

TRAY 8 VS. TIME

INITIAL CONDITIONS

MOLE FRACTIONS

RATE

	BENZENE	TOLUENE	XYLENE	LB. MOLES/HR.
FEED 1	0.46567	0.46626	0.06807	0.26600
DISTILLATE	0.82667	0.17273	0.00060	0.14200
BOTTOMS	0.04859	0.81702	0.13438	0.12400
FEED 2	0.38283	0.54394	0.07324	0.26600
REFLUX RATIO	3.06			

RESPONSE

TIME(MINUTES)

BENZENE

TOLUENE

XYLENE

00	0.08874	0.83655	0.07471
0+	0.09269	0.83163	0.07567
1.5	0.07965	0.83838	0.08147
3	0.07426	0.84793	0.07780
5	0.09446	0.82832	0.07722
7	0.07803	0.84136	0.08060
9	0.07152	0.84384	0.07965
11	0.07938	0.83762	0.08300
13	0.07695	0.83998	0.08307
15	0.07391	0.84557	0.08053
17	0.07224	0.84506	0.08270
19	0.07386	0.84143	0.08471
21	0.06456	0.85770	0.07764
23	0.07008	0.84535	0.08457
25	0.06309	0.85523	0.08168
27	0.06738	0.85608	0.07604
29	0.06233	0.85412	0.08356
33	0.06458	0.85133	0.08409
37	0.06574	0.84925	0.08501
41	0.05752	0.85924	0.08325

DATA SET 17
 TOP TRAY VS. TIME
 INITIAL CONDITIONS

MOLE FRACTIONS

RATE

	BENZENE	TOLUENE	XYLENE	LB. MOLES/HR.
FEED 1	0.50083	0.44081	0.05836	0.27600
DISTILLATE	0.35533	0.14420	0.00047	0.14900
BOTTOMS	0.06935	0.80672	0.12393	0.12700
FEED 2	0.31542	0.60174	0.08283	0.27600
REFLUX RATIO	3.06			

RESPONSE TIME (MINUTES)	BENZENE	TOLUENE	XYLENE
00	0.74991	0.19851	0.00159
1	0.78825	0.21012	0.00163
3	0.76814	0.22938	0.00198
5	0.74827	0.24965	0.00208
7	0.71724	0.25058	0.00217
9	0.70075	0.29689	0.00236
11	0.67506	0.32221	0.00272
13	0.65043	0.34639	0.00269
15	0.64289	0.35410	0.00300
17	0.63067	0.36692	0.00240
19	0.61059	0.38638	0.00303
21	0.60379	0.39295	0.00326
23	0.59070	0.40612	0.00318
25	0.57217	0.42455	0.00327
27	0.56619	0.43042	0.00339
29	0.54210	0.45439	0.00350
31	0.53699	0.45952	0.00349
33	0.51901	0.47724	0.00375
35	0.50724	0.48933	0.00343
37	0.51546	0.48103	0.00350
39	0.50691	0.48944	0.00365
41	0.48914	0.50663	0.00423
43	0.48565	0.51063	0.00372
45	0.46783	0.52817	0.00399
475	0.45314	0.54270	0.00417

DATA SET 18

TRAY 4 VS. TIME

INITIAL CONDITIONS

MOLE FRACTIONS

RATE

	BENZENE	TOLUENE	XYLENE	LB. MOLES/HR.
FEED 1	0.55289	0.39281	0.05420	0.27600
DISTILLATE	0.92305	0.07671	0.00024	0.14900
BOTTOMS	0.10230	0.77144	0.12626	0.12700
FEED 2	0.28428	0.63208	0.08364	0.27600
REFLUX RATIO	3.16			

RESPONSE

TIME (MINUTES)

BENZENE

TOLUENE

XYLENE

0	0.67426	0.32051	0.00523
1.5	0.62608	0.36699	0.00693
3	0.60961	0.38286	0.00753
5	0.57987	0.41212	0.00801
7	0.51111	0.47995	0.00895
9	0.49687	0.49414	0.00898
11	0.45011	0.53984	0.01005
13	0.44061	0.54833	0.01106
15	0.39359	0.59508	0.01133
17	0.35662	0.63120	0.01213
19	0.34869	0.63735	0.01195
21	0.34015	0.64778	0.01207
23	0.32685	0.65974	0.01341
25	0.30425	0.68225	0.01350
27	0.27311	0.71293	0.01390
29	0.26596	0.72075	0.01330
31	0.26118	0.72525	0.01358
33	0.24073	0.74517	0.01410
35	0.23306	0.75219	0.01475
37	0.23142	0.75392	0.01466
39	0.22090	0.76398	0.01511
41	0.20765	0.77692	0.01542
43	0.20740	0.77812	0.01448
45	0.20986	0.77440	0.01574

DATA SET 19
DISTILLATE VS. TIME
INITIAL CONDITIONS

MOLE FRACTIONS

RATE

	BENZENE	TOLUENE	XYLENE	LB. MOLES/HR.
FEED 1	0.29994	0.64370	0.05636	0.20200
DISTILLATE	0.55277	0.44510	0.00213	0.11800
BOTTOMS	0.01212	0.87042	0.11746	0.08400
FEED 2	0.51301	0.43323	0.05376	0.20200
REFLUX RATIO	4.36			

RESPONSE

TIME (MINUTES)

BENZENE

TOLUENE

XYLENE

00.	0.55277	0.44510	0.00213
1	0.54097	0.45913	0.00000
3	0.53239	0.41761	0.00000
5	0.59934	0.40066	0.00000
8	0.65467	0.34533	0.00000
10	0.67498	0.32502	0.00000
12	0.69007	0.30993	0.00000
14	0.69855	0.30145	0.00000
17	0.71604	0.28396	0.00000
20	0.74007	0.25993	0.00000
23	0.75168	0.24332	0.00000
26	0.76771	0.23229	0.00000
29	0.78359	0.21641	0.00000
33	0.78409	0.21591	0.00000
36	0.79329	0.20671	0.00000
39	0.79465	0.20535	0.00000
43	0.81158	0.18842	0.00000
47	0.81198	0.18802	0.00000
51	0.81461	0.18539	0.00000
55	0.81007	0.18993	0.00000
59	0.82544	0.17456	0.00000
63	0.83243	0.16757	0.00000
67	0.82567	0.17433	0.00000
71	0.81121	0.18379	0.00000
75	0.83223	0.16777	0.00000
79	0.82969	0.17031	0.00000
83	0.83338	0.16662	0.00000
87	0.84137	0.15863	0.00000
92	0.83901	0.16099	0.00000

DATA SET 20

DISTILLATE VS. TIME

INITIAL CONDITIONS

MOLE FRACTIONS

RATE

	BENZENE	TOLUENE	XYLENE	LB. MOLES/HR.
FEED 1	0.55848	0.39254	0.04898	0.20200
DISTILLATE	0.91518	0.08448	0.00033	0.11300
BOTTOMS	0.07644	0.81464	0.10892	0.08900
FEED 2	0.31796	0.60986	0.07218	0.20200
REFLUX RATIO	3.06			

RESPONSE

TIME (MINUTES)

BENZENE

TOLUENE

XYLENE

00.	0.91518	0.08448	0.00033
1	0.91606	0.08394	0.00000
3	0.90739	0.09261	0.00000
5	0.89882	0.10118	0.00000
7	0.87883	0.12117	0.00000
9	0.87345	0.12655	0.00000
12	0.85310	0.14690	0.00000
15	0.83041	0.16959	0.00000
19	0.82697	0.17303	0.00000
21	0.81712	0.18288	0.00000
24	0.78104	0.21896	0.00000
27	0.75608	0.24302	0.00000
30	0.74880	0.25120	0.00000
33	0.73427	0.26573	0.00000
36	0.77194	0.22806	0.00000
39	0.70200	0.29800	0.00000
42	0.69195	0.30805	0.00000
45	0.69538	0.30462	0.00000
48	0.66786	0.33214	0.00000
51	0.65145	0.34855	0.00000
54	0.63385	0.36615	0.00000
57	0.62838	0.37162	0.00000
60	0.62511	0.37439	0.00000
63	0.62000	0.38000	0.00000
66	0.60705	0.39295	0.00000
69	0.59602	0.40398	0.00000
73	0.59647	0.40353	0.00000
77	0.58043	0.41957	0.00000
81	0.59642	0.40358	0.00000
85	0.58613	0.41387	0.00000
89	0.58802	0.41198	0.00000

DATA SET 22

TRAY 6 VS. TIME

INITIAL CONDITIONS

MOLE FRACTIONS

RATE

	BENZENE	TOLUENE	XYLENE	LB. MOLES/HR.
FEED 1	0.31152	0.61458	0.07391	0.20200
DISTILLATE	0.52191	0.47583	0.00225	0.10900
BOTTOMS	0.01157	0.81975	0.16868	0.09300
FEED 2	0.47678	0.49564	0.02758	0.20200
REFLUX RATIO	4.22			

RESPONSE

TIME(MINUTES)

	BENZENE	TOLUENE	XYLENE
000	0.06459	0.88853	0.04688
04	0.06768	0.88304	0.04928
2	0.08998	0.87103	0.03899
4	0.11163	0.85344	0.03493
6	0.11307	0.85454	0.03240
8	0.12147	0.84569	0.03284
10	0.12962	0.83140	0.03898
12	0.13129	0.83765	0.03107
14	0.13330	0.83500	0.03169
16	0.13450	0.83407	0.03143
18	0.13925	0.83054	0.03020
21	0.14272	0.82722	0.03005
24	0.14622	0.82515	0.02863
27	0.14929	0.82040	0.03030
30	0.14643	0.82454	0.02903
33	0.14800	0.82267	0.02933
36	0.15538	0.81624	0.02838
39	0.15391	0.81846	0.02763
42	0.16124	0.80885	0.02991
45	0.16283	0.80815	0.02902
48	0.16127	0.81157	0.02716
51	0.15997	0.81312	0.02691
54	0.16417	0.80930	0.02653
57	0.16855	0.80543	0.02603
60	0.16250	0.81112	0.02638
63	0.15990	0.81364	0.02646
67	0.16667	0.80713	0.02620
71	0.17216	0.80107	0.02677
75	0.16388	0.81098	0.02514
79	0.16874	0.80703	0.02423
85	0.17703	0.79776	0.02520

DATA SET 12 A
 DETERMINATION OF COMPONENT EFFICIENCIES
 SUPERFICIAL VAPOR VELOCITY 1.04 FT/SEC

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W5	H6 IDENT.
1	1.410	0.085	0.400	0.010	2.030	9.160	1.400	0.270	2.700	0.785	0.850	0.020
2	1.400	0.160	0.670	0.010	2.200	9.480	2.120	0.230	2.670	0.508	0.000	0.000
3	1.270	0.312	1.720	0.020	2.050	9.520	2.250	0.270	2.710	0.310	0.000	0.000
4	1.350	0.640	1.390	0.015	1.920	10.200	2.000	0.310	2.760	0.208	0.000	0.000
5	1.150	0.480	1.900	0.020	1.950	4.850	1.750	0.200	2.510	0.058	0.000	0.000
6	1.280	1.670	1.280	0.055	2.110	9.000	1.600	0.260	2.620	0.062	0.820	0.020
7	1.350	2.480	1.220	0.180	1.950	8.560	2.150	0.230	2.450	0.036	0.000	0.000
8	1.360	3.510	1.420	0.180	1.950	7.370	1.950	0.270	2.750	0.020	0.000	0.000
9	1.500	5.660	1.800	0.230	1.850	6.330	2.050	0.260	0.000	0.000	0.000	0.000

DATA SET 12 B
 DETERMINATION OF COMPONENT EFFICIENCIES
 SUPERFICIAL VAPOR VELOCITY 1.12 FT/SFC

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H6	EFFICIENT.
1	1.450	0.237	0.000	0.000	2.100	8.900	1.500	0.260	2.800	0.740	0.900	0.050	
2	1.400	0.485	1.200	0.020	2.020	9.330	1.860	0.240	2.710	0.475	0.000	0.000	
3	1.330	0.780	1.190	0.060	2.000	8.930	1.900	0.260	2.820	0.280	0.000	0.000	
4	1.270	1.080	1.350	0.065	1.900	7.070	1.420	0.230	2.750	0.130	0.000	0.000	
5	1.320	2.430	1.900	0.090	2.080	8.680	1.750	0.240	2.650	0.113	0.000	0.000	
6	1.500	3.980	1.950	0.120	2.050	8.120	1.650	0.230	2.570	0.052	0.000	0.000	
7	1.560	5.370	1.890	0.220	2.120	6.830	2.450	0.230	2.750	0.026	0.000	0.000	
8	1.550	3.470	1.500	0.150	1.900	2.700	1.670	0.140	2.700	0.007	0.000	0.000	
9	1.710	3.500	1.750	0.170	1.900	2.720	1.750	0.120	2.790	0.007	0.000	0.000	

DATA SET 13
DETERMINATION OF COMPONENT EFFICIENCIES
SUPERFICIAL VAPOR VELOCITY 1.15 FT/SEC

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H6 IDENT.
1	1.220	0.970	1.850	0.030	2.020	9.060	1.250	0.310	2.300	0.720	1.110	0.065
2	1.170	1.550	1.390	0.090	1.930	8.660	1.200	0.340	2.250	0.465	2.000	0.030
3	1.190	2.460	1.500	0.130	1.950	8.230	2.250	0.310	2.070	0.298	1.400	0.032
4	1.250	4.070	1.600	0.220	2.120	7.950	1.750	0.220	2.220	0.206	0.550	0.020
5	1.290	5.820	1.380	0.360	1.900	7.230	1.800	0.360	2.170	0.160	1.380	0.031
6	1.310	6.530	1.810	0.360	1.910	6.890	1.650	0.320	2.250	0.108	1.600	0.005
7	1.620	7.770	1.720	0.260	2.000	5.730	1.750	0.230	2.450	0.050	0.750	0.003
8	1.570	8.690	1.850	0.320	1.900	4.390	1.650	0.230	2.600	0.026	0.800	0.001
9	3.620	5.040	2.560	0.230	1.880	3.250	2.150	0.160	2.700	0.011	0.000	0.000
10	1.140	0.782	1.480	0.045	2.070	8.300	2.200	0.270	2.390	0.725	1.110	0.054
11	1.190	1.460	2.200	0.045	2.000	8.510	2.400	0.250	2.200	0.542	1.800	0.030
12	1.180	2.220	1.500	0.115	1.950	7.960	2.250	0.320	2.430	0.000	1.400	0.411
13	1.270	3.840	1.150	0.280	1.900	8.320	2.100	0.320	2.220	0.398	1.280	0.031
14	1.210	4.310	1.280	0.300	1.880	7.700	1.900	0.380	2.250	0.183	1.380	0.015
15	1.340	5.800	1.500	0.280	2.000	7.280	1.780	0.290	2.300	0.105	0.950	0.024
16	1.600	6.940	1.600	0.240	2.000	6.060	1.750	0.230	2.450	0.056	1.200	0.005
17	1.620	8.500	1.500	0.440	1.890	4.930	1.950	0.220	2.800	0.028	0.000	0.000

DATA SET 14 A
DETERMINATION OF COMPONENT EFFICIENCIES
SUPERFICIAL VAPOR VELOCITY 0.99 FT/SEC

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H6 IDENT.
1	1.220	1.530	1.580	0.050	1.990	8.230	1.900	0.290	2.580	0.610	1.300	0.045
2	1.230	2.160	1.500	0.130	1.940	7.710	1.850	0.320	2.420	0.382	1.000	0.050
3	1.250	3.190	1.890	1.350	1.900	7.050	1.900	0.320	2.500	0.250	1.040	0.020
4	1.500	4.570	1.230	0.240	2.000	6.570	1.600	0.240	2.500	0.190	0.850	0.019
5	1.300	5.680	1.400	0.260	1.860	5.400	1.600	0.220	2.250	0.132	0.000	0.000
6	1.530	6.520	1.500	0.260	1.900	4.730	1.400	0.280	2.900	0.076	0.000	0.000
7	1.420	7.470	1.900	0.280	1.780	4.180	1.900	0.240	2.720	0.042	0.000	0.000
8	1.530	8.400	1.450	0.440	1.730	3.340	1.300	0.220	1.800	0.022	0.000	0.000
9	1.550	9.360	1.500	0.480	1.620	2.460	1.750	0.140	2.300	0.010	0.000	0.000
10	1.180	1.350	2.000	0.056	1.990	8.280	1.800	0.330	2.500	0.732	1.500	0.062
11	1.250	2.030	1.100	0.140	2.000	7.980	2.200	0.260	2.400	0.562	1.300	0.050
12	1.300	2.990	1.600	0.125	1.930	7.540	1.850	0.300	2.440	0.447	1.600	0.027
13	1.410	4.240	1.450	0.200	1.950	7.000	2.360	0.310	2.620	0.410	1.250	0.020
14	1.450	4.700	1.150	0.260	1.900	6.620	2.000	0.260	2.630	0.180	0.800	0.015
15	1.370	5.650	2.100	0.170	1.820	5.580	2.200	0.180	2.550	0.094	0.000	0.000
16	1.350	6.930	1.700	0.320	1.740	4.890	1.500	0.270	2.390	0.051	0.000	0.000
17	1.440	8.500	2.100	0.230	1.740	3.660	1.300	0.220	2.560	0.024	0.000	0.000

DATA SET 14 B
 DETERMINATION OF COMPONENT EFFICIENCIES
 SUPERFICIAL VAPOR VELOCITY 1.25 FT/SEC

	W1	H1	N2	H2	W3	H3	W4	H4	W5	H5	W6	H6 IDENT.
1	1.240	1.250	1.700	0.065	2.120	7.780	1.850	0.270	2.670	0.580	1.750	0.040
2	1.470	1.475	1.450	0.065	2.040	5.640	2.100	0.210	2.530	0.250	1.400	0.030
3	1.210	3.320	1.400	0.160	1.990	7.280	1.700	0.310	2.530	0.256	1.350	0.022
4	1.290	4.260	1.850	0.160	1.940	6.000	1.450	0.230	2.500	0.142	0.750	0.015
5	1.490	6.430	1.490	0.230	1.860	5.920	1.500	0.250	2.490	0.130	1.000	0.011
6	1.530	6.880	1.300	0.440	1.890	4.880	1.400	0.230	2.530	0.066	0.000	0.000
7	1.530	8.480	1.250	0.440	1.900	4.340	1.620	0.120	2.610	0.038	0.000	0.000
8	1.600	9.460	1.550	0.460	1.660	3.360	2.100	0.140	2.390	0.018	0.000	0.000
9	3.320	5.220	1.550	0.520	1.640	2.200	1.700	0.145	2.430	0.007	0.000	0.000
10	1.400	1.157	1.700	0.055	2.300	7.970	1.950	0.210	2.560	0.665	1.650	0.045
11	1.260	1.985	1.850	0.080	1.920	7.820	1.850	0.270	2.390	0.480	1.630	0.015
12	1.360	2.880	1.480	0.110	1.920	7.320	1.850	0.270	2.370	0.370	1.600	0.030
13	1.340	4.550	1.640	0.145	2.070	7.200	1.750	0.230	2.540	0.350	1.820	0.017
14	1.300	5.560	1.600	0.230	1.880	6.880	1.730	0.280	2.430	0.153	1.230	0.010
15	1.400	6.880	1.380	0.480	1.860	5.930	1.920	0.240	2.610	0.088	0.900	0.007
16	1.480	8.130	1.820	0.270	1.870	4.730	2.000	0.150	2.300	0.042	0.000	0.000
17	1.780	8.800	1.400	0.500	2.240	2.940	1.700	0.135	2.880	0.018	0.000	0.000

17	1.600	8.500	1.700	0.280	1.850	4.620	1.750	0.210	2.500	0.030	0.000	0.000	19
18	1.610	8.280	1.900	0.300	1.800	4.360	1.900	0.210	2.600	0.028	0.000	0.000	21
19	1.570	7.860	2.400	0.300	1.890	4.050	1.900	0.180	2.500	0.025	0.000	0.000	23
20	1.600	7.720	2.400	0.230	1.950	3.820	1.900	0.170	2.520	0.022	0.000	0.000	25
21	1.600	8.320	2.050	0.260	1.850	4.090	1.800	0.220	2.580	0.026	0.000	0.000	27
22	1.600	8.550	1.850	0.370	2.050	4.060	1.430	0.210	2.570	0.026	0.000	0.000	29
23	1.600	8.600	1.700	0.310	1.880	4.260	1.850	0.130	2.550	0.027	0.000	0.000	31
24	1.610	8.680	2.300	0.280	2.010	3.970	1.900	0.200	2.530	0.025	0.000	0.000	33
25	1.600	8.650	2.700	0.240	1.900	3.980	2.100	0.190	2.500	0.025	0.000	0.000	35
26	1.620	8.760	1.800	0.340	1.840	4.050	2.000	0.220	2.520	0.025	0.000	0.000	39

DATA SET 15
TOP TRAY VS. TIME

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H6IDENT.
1	1.400	5.120	2.000	0.220	1.970	6.200	2.420	0.220	2.520	0.711	3.250	0.023 F01
2	1.570	8.280	2.100	0.320	1.760	4.195	2.550	0.135	2.540	0.018	0.000	0.000 DIS
3	1.270	0.285	1.400	0.150	1.900	7.880	1.800	0.320	2.920	1.310	2.300	0.050 BOT
4	1.500	6.130	1.600	0.250	1.930	5.470	1.650	0.210	2.430	0.609	1.100	0.250 F02
5	1.500	6.700	2.250	0.230	1.850	5.680	2.600	0.220	2.540	0.040	0.000	0.000 00
6	1.440	7.110	2.200	0.220	1.950	5.890	2.000	0.200	2.400	0.041	0.000	0.000 .25
7	1.500	6.940	2.000	0.300	1.950	5.820	1.900	0.260	2.460	0.042	0.000	0.000 1
8	1.560	7.040	1.700	0.300	1.950	5.460	1.500	0.320	2.460	0.038	0.000	0.000 2
9	1.500	6.730	2.000	0.250	1.840	5.310	2.000	0.220	2.460	0.036	0.000	0.000 3
10	1.540	6.960	1.800	0.290	1.840	5.070	1.700	0.250	2.430	0.034	0.000	0.000 5
11	1.480	7.370	1.900	0.310	1.870	4.800	1.600	0.250	2.450	0.033	0.000	0.000 7
12	1.500	7.880	1.870	0.350	1.830	4.980	1.600	0.270	2.400	0.033	0.000	0.000 9
13	1.680	7.940	1.890	0.290	1.860	4.800	1.800	0.220	2.400	0.032	0.000	0.000 11
14	1.530	7.850	1.700	0.320	1.870	4.580	1.480	0.230	2.320	0.029	0.000	0.000 13
15	1.540	7.920	1.700	0.330	1.890	4.450	1.600	0.240	2.440	0.029	0.000	0.000 15
16	1.550	8.120	2.130	0.320	1.930	4.370	1.800	0.220	2.560	0.029	0.000	0.000 17

DATA SET 16
TRAY 8 VS. TIME

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H5IDENT.
1	1.430	5.220	1.500	0.200	1.830	4.830	1.650	0.200	2.580	0.580	1.850	0.025 F01
2	1.730	5.330	1.600	0.170	1.860	1.217	1.800	0.042	0.148	0.052	0.120	0.014 DIS
3	1.310	0.684	1.850	0.025	2.130	8.560	2.150	0.210	2.650	1.300	2.300	0.042 F0T
4	1.380	5.400	1.750	0.200	2.120	6.010	1.750	0.190	2.540	0.776	2.300	0.025 F02
5	1.400	1.244	2.400	0.025	2.270	8.620	2.100	0.220	2.600	0.767	2.100	0.032 00
6	1.320	1.267	1.400	0.050	2.030	8.830	2.050	0.250	2.430	0.780	1.000	0.038 0+
7	1.250	1.080	1.400	0.042	1.970	8.680	1.900	0.210	2.410	0.783	1.700	0.042 1.5
8	1.280	1.037	1.400	0.045	2.160	8.460	1.950	0.230	2.500	0.764	1.700	0.041 3
9	1.280	1.277	1.800	0.042	2.000	8.570	2.100	0.260	2.430	0.743	2.100	0.045 5
10	1.330	1.050	2.100	0.035	2.100	8.650	2.400	0.220	2.530	0.792	1.500	0.040 7
11	1.200	1.062	1.900	0.045	2.180	8.520	2.100	0.220	2.620	0.765	1.350	0.040 9
12	1.300	0.985	1.900	0.042	1.970	8.370	2.000	0.220	2.530	0.740	1.450	0.042 11
13	1.300	0.967	1.900	0.042	2.000	8.330	2.500	0.220	2.570	0.737	1.600	0.042 13

14	1.220	0.980	1.590	0.045	1.970	8.420	1.900	0.240	2.430	0.750	1.200	0.040	15
15	1.320	0.990	1.200	0.052	2.080	8.850	2.100	0.230	2.590	0.800	1.300	0.045	17
16	1.280	0.925	1.890	0.035	1.950	8.400	2.200	0.170	2.530	0.750	1.100	0.042	19
17	1.270	0.880	0.900	0.050	2.090	8.570	1.500	0.260	2.380	0.770	1.400	0.050	21
18	1.260	0.987	2.200	0.042	2.080	8.850	2.300	0.260	2.630	0.805	1.850	0.040	23
19	1.280	0.967	1.100	0.050	2.180	9.270	1.700	0.270	2.540	0.870	1.300	0.050	25
20	1.320	0.985	1.400	0.040	2.180	9.070	1.900	0.210	2.420	0.830	1.250	0.045	27
21	1.360	0.880	1.200	0.035	2.140	9.120	2.100	0.240	2.580	0.855	1.600	0.032	29
22	1.250	0.872	1.200	0.040	2.000	8.630	1.800	0.240	2.510	0.780	1.400	0.040	33
23	1.330	0.882	1.400	0.041	2.000	9.120	2.200	0.230	2.500	0.837	1.750	0.040	37
24	1.240	0.817	1.500	0.035	2.070	8.820	2.350	0.220	2.530	0.805	1.700	0.035	41

DATA SET 17
TOP TRAY VS. TIME

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H6IDENT.
1	1.510	6.780	1.750	0.250	2.030	5.280	1.650	0.220	0.265	6.160	2.650	0.022 F01
2	1.880	5.220	1.600	0.190	1.700	0.738	1.600	0.420	0.238	0.032	0.000	0.000 DIS
3	1.320	0.805	2.100	0.022	1.960	7.520	2.250	0.210	2.600	1.005	2.000	0.040 B01
4	1.340	4.000	1.400	0.160	2.050	5.930	1.850	0.220	2.580	0.751	2.520	0.022 F02
5	1.630	9.700	2.500	0.270	1.750	2.620	1.600	0.150	2.730	0.016	0.000	0.000 00
6	1.710	9.690	2.300	0.300	1.900	2.740	2.200	0.100	0.278	0.175	0.000	0.000 1
7	1.710	9.460	1.850	0.400	1.910	3.005	2.100	0.110	0.232	0.210	0.000	0.000 3
8	1.670	9.420	2.000	0.380	1.880	3.320	2.250	0.110	0.284	0.219	0.000	0.000 5
9	1.590	8.490	2.100	0.320	1.830	3.435	2.100	0.120	0.263	0.222	0.000	0.000 7
10	1.600	8.620	1.780	0.310	1.850	3.720	1.900	0.150	0.263	0.250	0.000	0.000 9
11	1.570	8.620	1.620	0.250	1.890	4.035	2.000	0.110	0.275	0.273	0.000	0.000 11
12	1.510	8.280	1.850	0.300	1.830	4.320	2.050	0.150	0.258	0.284	0.000	0.000 13
13	1.530	8.210	2.100	0.270	1.800	4.520	2.800	0.140	0.262	0.318	0.000	0.000 15
14	1.530	7.820	2.150	0.310	1.810	4.580	2.900	0.130	0.216	0.303	0.000	0.000 17
15	1.560	7.780	1.700	0.280	1.920	4.690	2.400	0.170	0.264	0.322	0.000	0.000 19
16	1.560	7.470	2.000	0.270	1.870	4.740	2.250	0.220	0.273	0.328	0.000	0.000 21

17	1.500	7.550	1.600	0.320	1.770	5.220	1.630	0.220	0.243	0.356	0.000	0.000	23
18	1.540	7.130	1.700	0.300	1.970	4.920	1.450	0.250	0.259	0.345	0.000	0.000	25
19	1.570	6.740	1.680	0.280	1.870	5.100	1.550	0.240	0.253	0.356	0.000	0.000	27
20	1.470	6.920	2.150	0.270	1.960	5.200	1.990	0.220	0.246	0.384	0.000	0.000	29
21	1.490	6.960	1.650	0.270	1.930	5.420	1.750	0.260	0.244	0.392	0.000	0.000	31
22	1.370	6.620	1.650	0.310	1.790	5.560	1.750	0.250	0.239	0.394	0.000	0.000	33
23	1.400	6.930	2.000	0.270	1.870	5.930	2.450	0.230	0.239	0.394	0.000	0.000	35
24	1.520	6.460	1.830	0.240	1.930	5.540	2.600	0.230	0.243	0.390	0.000	0.000	37
25	1.450	6.520	2.050	0.260	1.880	5.790	2.200	0.230	0.230	0.425	0.000	0.000	39
26	1.400	6.280	2.400	0.260	2.000	5.520	2.100	0.220	0.270	0.410	0.000	0.000	41
27	1.510	6.270	1.750	0.260	2.060	5.740	2.000	0.240	0.233	0.443	0.000	0.000	43
28	1.260	6.200	2.000	0.280	1.810	5.910	1.800	0.250	0.230	0.422	0.000	0.000	45
29	1.330	6.340	2.100	0.240	2.030	6.000	2.600	0.170	0.245	0.456	0.000	0.000	47.5

DATA SET 18
TRAY 4 VS. TIME

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H6IDENT.
1	1.550	7.400	2.130	0.300	1.860	5.170	2.200	0.240	2.500	0.620	1.400	7.045 F01
2	1.880	5.620	2.300	0.220	1.790	0.572	1.750	0.035	0.190	0.021	0.000	0.000 DIS
3	1.380	1.240	2.130	0.042	1.910	7.920	2.770	0.320	2.650	1.090	2.200	0.055 B0T
4	1.420	3.889	2.130	0.140	2.090	7.010	2.040	0.300	2.530	0.920	0.000	0.000 F02
5	1.600	8.450	2.500	0.350	1.880	4.050	1.900	0.240	0.250	0.584	0.140	0.041 0
6	1.530	8.520	2.100	0.400	1.930	4.680	1.750	0.320	0.246	0.815	0.120	0.069 1.5
7	1.620	8.130	2.100	0.320	1.900	5.150	1.800	0.260	0.233	0.943	0.195	0.069 3
8	1.630	7.500	2.250	0.280	1.870	5.470	2.100	0.260	0.233	0.998	0.110	0.081 5
9	1.500	6.420	1.700	0.400	1.950	5.560	1.800	0.320	0.240	0.989	0.110	0.072 7
10	1.570	6.600	1.800	0.350	1.980	6.180	2.050	0.320	2.360	0.110	0.105	0.100 9
11	1.470	6.210	2.050	0.310	2.050	6.440	2.100	0.290	2.520	0.114	0.108	0.084 11
12	1.500	5.770	1.900	0.290	1.920	6.720	2.100	0.290	2.500	0.119	0.230	0.072 13
13	1.390	5.510	1.900	0.270	2.000	6.920	2.360	0.310	2.430	0.125	0.185	0.087 15
14	1.300	5.090	1.500	0.330	2.020	7.090	1.600	0.340	2.400	0.131	0.180	0.087 17
15	1.380	4.920	1.850	0.250	2.040	7.380	1.900	0.330	2.430	0.135	0.175	0.056 19

16	1.460	4.620	1.320	0.270	2.080	7.420	1.780	0.290	2.420	0.137	0.160	0.069	21
17	1.460	4.270	1.800	0.200	2.030	7.520	1.800	0.240	2.530	0.141	0.160	0.069	23
18	1.420	4.160	1.550	0.200	2.030	7.820	1.720	0.330	2.480	0.147	0.175	0.060	25
19	1.420	3.730	1.700	0.170	2.200	7.660	1.500	0.230	2.500	0.150	0.190	0.060	27
20	1.380	3.780	1.470	0.170	2.130	7.970	2.150	0.230	2.430	0.150	0.115	0.060	29
21	1.400	3.610	1.600	0.190	2.100	8.060	2.300	0.270	2.400	0.154	0.110	0.081	31
22	1.390	3.400	1.700	0.180	2.290	8.070	2.200	0.280	2.430	0.160	0.190	0.062	33
23	1.280	3.290	1.700	0.190	2.060	8.070	2.350	0.270	2.400	0.157	0.190	0.069	35
24	1.380	3.220	1.350	0.170	2.100	8.270	2.100	0.280	2.360	0.165	0.160	0.081	37
25	1.340	3.040	1.300	0.210	2.070	8.240	2.100	0.320	2.370	0.165	0.160	0.082	39
26	1.280	2.820	1.400	0.160	2.050	7.970	2.220	0.260	2.390	0.157	0.170	0.069	41
27	1.430	2.370	1.000	0.220	2.230	8.350	1.500	0.320	2.300	0.173	0.140	0.088	43
28	1.370	2.850	1.450	0.220	2.090	8.500	2.050	0.300	2.400	0.175	0.140	0.075	46

DATA SET 19
DISTILLATE VS. TIME

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H6 INENT.
1	1.360	4.100	1.500	0.180	2.000	7.120	2.140	0.260	2.500	0.575	1.850	0.030 FDI
2	1.610	7.280	2.100	0.270	1.920	5.840	1.900	0.240	0.310	0.167	0.420	0.030 DIS
3	1.400	0.146	0.130	0.075	2.120	8.320	2.180	0.230	2.510	1.092	1.600	0.050 BOT
4	1.580	6.950	2.000	0.260	1.950	5.650	1.900	0.230	2.520	0.625	2.250	0.028 FDI
5	1.610	7.280	2.100	0.270	1.920	5.840	1.900	0.240	0.310	0.167	0.420	0.030 00
6	1.520	7.070	1.500	0.280	1.840	5.800	1.950	0.260	0.000	0.000	0.000	0.000 1
7	1.620	7.420	1.880	0.280	1.820	5.580	1.750	0.260	0.000	0.000	0.000	0.000 3
8	1.590	3.930	1.400	0.220	1.950	2.550	2.400	0.082	0.000	0.000	0.000	0.000 5
9	1.650	4.080	1.600	0.210	1.850	2.260	2.400	0.090	0.000	0.000	0.000	0.000 8
10	1.660	4.260	1.500	0.200	1.870	2.160	2.100	0.070	0.000	0.000	0.000	0.000 10
11	1.630	4.440	1.400	0.240	1.860	2.075	1.900	0.080	0.000	0.000	0.000	0.000 12
12	1.720	4.550	1.100	0.230	2.120	1.890	1.500	0.070	0.000	0.000	0.000	0.000 14
13	1.750	4.730	1.450	0.230	2.180	1.792	1.950	0.062	0.000	0.000	0.000	0.000 17
14	1.700	4.720	1.850	0.250	1.960	1.720	1.800	0.080	0.000	0.000	0.000	0.000 20
15	1.720	4.880	1.700	0.200	1.970	1.670	2.050	0.055	0.000	0.000	0.000	0.000 23
16	1.710	4.900	1.900	0.190	1.850	1.605	2.300	0.065	0.000	0.000	0.000	0.000 26

17	1.720	4.960	1.400	0.260	1.790	1.556	1.600	0.070	0.000	0.000	0.000	29
18	1.780	5.000	1.550	0.270	1.880	1.550	1.700	0.066	0.000	0.000	0.000	33
19	1.760	4.930	1.500	0.230	1.850	1.445	1.600	0.062	0.000	0.000	0.000	36
20	1.750	5.020	1.650	0.220	1.850	1.445	1.850	0.062	0.000	0.000	0.000	39
21	1.790	5.170	1.680	0.220	1.760	1.427	1.900	0.065	0.000	0.000	0.000	43
22	1.840	5.160	1.480	0.240	1.980	1.310	1.600	0.060	0.000	0.000	0.000	47
23	1.780	5.260	1.690	0.260	1.850	1.367	1.700	0.060	0.000	0.000	0.000	51
24	1.730	5.210	1.400	0.220	1.900	1.310	1.610	0.055	0.000	0.000	0.000	55
25	1.850	5.150	1.500	0.260	1.980	1.200	1.500	0.065	0.000	0.000	0.000	59
26	1.800	5.380	1.600	0.240	1.870	1.240	1.300	0.055	0.000	0.000	0.000	63
27	1.800	5.320	1.600	0.270	1.990	1.195	1.900	0.060	0.000	0.000	0.000	67
28	1.690	5.360	1.400	0.340	1.800	1.385	1.850	0.067	0.000	0.000	0.000	71
29	1.830	5.270	1.500	0.220	2.040	1.150	1.600	0.055	0.000	0.000	0.000	75
30	1.830	5.180	1.600	0.240	1.980	1.156	1.800	0.055	0.000	0.000	0.000	79
31	1.720	4.880	1.750	0.220	1.800	1.092	1.800	0.058	0.000	0.000	0.000	83
32	1.780	5.200	1.700	0.280	1.780	1.155	1.800	0.060	0.000	0.000	0.000	87
33	1.790	5.220	1.900	0.240	1.820	1.155	2.100	0.055	0.000	0.000	0.000	92

DATA SET 20
DISTILLATE VS. TIME

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H6 IDENT.
1	1.500	6.170	2.050	0.270	1.770	4.380	1.800	0.210	2.620	0.430	1.150	0.037 F01
2	1.760	5.330	1.820	0.260	1.900	0.538	0.225	0.225	0.026	0.188	0.000	0.000 D15
3	1.180	0.959	1.500	0.035	1.950	7.320	1.900	0.320	2.580	0.850	2.000	0.050 R0T
4	1.320	3.870	1.520	0.220	1.900	6.230	1.900	0.250	2.600	0.622	1.550	0.040 F02
5	1.760	5.330	1.820	0.260	1.900	0.538	0.225	0.225	0.026	0.188	0.000	0.000 00
6	1.730	5.360	1.800	0.250	1.750	0.562	2.400	0.028	0.000	0.000	0.000	0.000 1
7	1.770	5.260	1.650	0.250	1.860	0.598	2.000	0.029	0.000	0.000	0.000	0.000 3
8	1.780	5.300	1.750	0.230	1.750	0.701	2.200	0.036	0.000	0.000	0.000	0.000 5
9	1.770	5.370	1.600	0.250	1.940	0.790	1.500	0.052	0.000	0.000	0.000	0.000 7
10	1.730	5.080	1.600	0.260	1.760	0.850	1.600	0.048	0.000	0.000	0.000	0.000 9
11	1.820	5.130	1.750	0.200	2.000	0.950	1.600	0.042	0.000	0.000	0.000	0.000 12
12	1.830	5.090	1.400	0.200	2.080	1.075	1.500	0.050	0.000	0.000	0.000	0.000 15
13	1.730	5.070	1.900	0.200	1.830	1.192	1.600	0.048	0.000	0.000	0.000	0.000 19
14	1.790	9.280	2.400	0.310	1.800	2.420	1.800	0.125	0.000	0.000	0.000	0.000 21
15	1.690	9.070	2.050	0.390	1.810	2.820	1.900	0.120	0.000	0.000	0.000	0.000 24
16	1.580	9.560	2.050	0.330	1.750	3.260	2.000	0.135	0.000	0.000	0.000	0.000 27

17	1.630	9.040	2.200	0.320	1.860	3.155	2.000	0.120	0.000	0.000	0.000	0.000	30
18	1.600	8.700	1.900	0.330	1.790	3.315	2.200	0.125	0.000	0.000	0.000	0.000	33
19	1.660	8.800	2.200	0.300	1.850	3.555	2.400	0.115	0.000	0.000	0.000	0.000	35
20	1.540	9.070	2.050	0.310	1.970	3.555	2.050	0.150	0.000	0.000	0.000	0.000	32
21	1.630	8.780	2.100	0.340	1.900	4.000	1.700	0.170	0.000	0.000	0.000	0.000	42
22	1.680	8.550	2.050	0.320	1.830	4.060	1.500	0.220	0.000	0.000	0.000	0.000	45
23	1.620	8.120	1.900	0.290	1.930	4.000	1.990	0.160	0.000	0.000	0.000	0.000	43
24	1.620	7.920	2.200	0.270	1.990	4.120	1.700	0.160	0.000	0.000	0.000	0.000	51
25	1.550	8.140	1.980	0.260	1.930	4.480	1.500	0.200	0.000	0.000	0.000	0.000	54
26	1.600	8.070	1.900	0.320	1.960	4.660	1.850	0.160	0.000	0.000	0.000	0.000	57
27	1.650	7.760	1.900	0.270	2.050	4.450	1.560	0.190	0.000	0.000	0.000	0.000	60
28	1.610	7.860	2.100	0.270	1.900	4.860	1.700	0.190	0.000	0.000	0.000	0.000	63
29	1.550	7.700	1.950	0.280	1.950	4.720	1.800	0.180	0.000	0.000	0.000	0.000	65
30	1.550	7.650	1.900	0.240	1.920	4.960	1.600	0.200	0.000	0.000	0.000	0.000	69
31	1.520	7.620	1.600	0.260	1.820	5.040	1.820	0.220	0.000	0.000	0.000	0.000	73
32	1.480	7.560	2.100	0.250	1.880	5.140	1.700	0.190	0.000	0.000	0.000	0.000	77
33	1.600	7.630	2.350	0.190	1.920	5.030	2.030	0.170	0.000	0.000	0.000	0.000	81
34	1.560	7.820	2.300	0.250	1.920	5.300	2.100	0.220	0.000	0.000	0.000	0.000	85
35	1.630	8.000	1.900	0.240	1.930	5.550	2.000	0.220	0.000	0.000	0.000	0.000	89

DATA SET 22
TRAY 6 VS. TIME

	W1	H1	W2	H2	W3	H3	W4	H4	W5	H5	W6	H6IDENT.
1	1.340	3.750	1.200	0.170	1.820	6.520	1.500	0.200	2.430	0.682	1.200	0.024 F01
2	1.470	6.500	2.000	0.230	1.900	5.520	1.650	0.170	0.262	0.211	0.290	0.012 D1S
3	1.280	0.132	0.800	0.009	1.900	7.520	1.800	0.240	2.600	1.305	1.950	0.050 B0T
4	1.470	5.740	1.600	0.190	1.830	5.680	1.700	0.190	2.390	0.280	1.100	0.019 F02
5	1.170	0.848	1.100	0.040	1.970	8.300	2.000	0.230	2.230	0.444	2.000	0.016 000
6	1.200	0.890	1.900	0.040	2.000	8.500	1.900	0.220	2.370	0.459	2.700	0.012 0+
7	1.200	1.200	1.500	0.042	2.000	8.370	2.000	0.210	2.370	0.362	2.100	0.013 2
8	1.250	1.385	1.750	0.057	1.950	8.210	2.000	0.250	2.400	0.313	2.300	0.012 4
9	1.250	1.415	1.500	0.060	1.990	8.110	1.650	0.260	2.300	0.305	1.600	0.014 5
10	1.260	1.532	1.900	0.057	1.980	8.210	2.100	0.230	2.370	0.305	2.390	0.011 8
11	1.230	1.410	2.000	0.050	1.900	7.060	2.100	0.220	2.430	0.303	1.500	0.009 10
12	1.280	1.518	1.800	0.050	1.900	7.810	1.700	0.270	2.300	0.277	1.400	0.012 12
13	1.280	1.610	2.150	0.055	1.930	8.090	2.200	0.220	2.270	0.296	2.300	0.014 14
14	1.300	1.600	2.000	0.050	1.950	7.940	2.000	0.230	2.370	0.284	1.750	0.011 16
15	1.260	1.718	2.000	0.067	1.940	8.080	1.900	0.260	2.280	0.288	1.500	0.014 18
16	1.260	1.680	1.850	0.067	1.880	7.860	2.000	0.270	2.240	0.273	1.750	0.017 21

17	1.310	1.820	2.350	0.060	1.980	8.270	1.900	0.300	2.230	0.290	1.800	0.014	24
18	1.280	1.860	1.900	0.055	1.930	8.080	2.050	0.250	2.380	0.280	1.600	0.012	27
19	1.310	1.780	2.100	0.056	2.000	7.880	2.300	0.220	2.400	0.268	1.400	0.012	30
20	1.230	1.880	2.000	0.067	1.950	7.920	2.700	0.220	2.410	0.263	2.800	0.009	33
21	1.300	1.912	2.400	0.060	2.000	7.930	1.600	0.270	2.370	0.265	1.650	0.015	36
22	1.270	1.905	2.000	0.065	1.970	7.870	2.200	0.220	2.300	0.260	1.500	0.016	39
23	1.270	1.912	1.750	0.062	1.880	7.720	1.900	0.260	2.500	0.248	1.400	0.014	42
24	1.300	1.925	1.900	0.057	1.900	7.780	2.000	0.250	2.400	0.256	1.500	0.012	45
25	1.260	2.015	2.100	0.055	1.930	7.930	1.370	0.240	2.310	0.256	1.150	0.014	48
26	1.250	2.075	1.800	0.062	1.960	8.060	2.000	0.210	2.300	0.259	1.900	0.012	51
27	1.300	2.077	2.100	0.060	1.980	8.060	2.050	0.230	2.380	0.256	1.150	0.010	54
28	1.360	2.105	2.000	0.052	2.000	8.140	2.000	0.220	2.350	0.256	1.750	0.012	57
29	1.250	2.140	2.200	0.055	2.000	8.050	2.000	0.180	2.380	0.250	2.000	0.011	60
30	1.220	2.095	2.000	0.055	1.940	8.030	2.000	0.210	2.330	0.250	1.700	0.010	63
31	1.260	2.092	2.050	0.062	1.930	7.950	1.900	0.230	2.320	0.245	2.200	0.010	67
32	1.270	2.130	2.050	0.065	1.890	8.020	1.900	0.220	2.380	0.244	1.600	0.012	71
33	1.270	2.188	2.000	0.065	2.000	8.260	1.900	0.240	2.290	0.255	1.400	0.015	75
34	1.300	2.120	1.700	0.070	2.000	7.900	1.600	0.260	2.310	0.235	1.400	0.013	79
35	1.270	2.132	1.700	0.085	1.890	7.720	2.100	0.270	2.320	0.226	2.500	0.011	85