THE UNIVERSITY OF MICHIGAN

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PROPYLENE-PROPANE ADSORPTION IN A PACKED SILICA GEL ADSORPTION BED

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NOMENCLATURE

Symbol	Dimension	
a		Beattie Bridgeman constant
a		coefficients for temperature dependent fugacity ratio correlation
a_s	cm^2/gm	specific area of adsorbent particle for mass transfer (area of equivalent sphere)
a_x	cm^2	cross-sectional area of column
A_0		Beattie Bridgeman constant
b		coefficients for pressure dependent cross-correlation of fugacity ratio
B_0		Beattie Bridgeman constant
c		coefficient of liquid specific volume correlation
c		Beattie Bridgeman constant
d		coefficient of saturation temperature correlation
D	cm^2/sec	diffusivity of mixed adsorbed gases in gel
D_{AB}	cm^2/sec	gas phase diffusivity of propylene into propane
D_{ass}	cm^2/sec	assumed value of D
e		coefficients of temperature function correlation (defined by Equation (B4))
E		error in a computed value
F	mg-mol/cm/gm	rate function defined by Equation (A45)
f	cm^3/cm^3	voids fraction in packed adsorption bed
g		coefficients of (Gy) power series fit
G	mg-mols/sec	molar flow rate
i		a counter used in the computer flowsheets

Symbol	Dimension	
j		a counter used in the computer flowsheets
j_D		j factor for mass transfer
k_y	mg-mol/ cm^2/sec	mass transfer coefficient in concentration units
k		a counter used in the computer flowsheets
L	gm	amount of silica gel in cell
m_A, m_B	mg-mols/gm	average bulk concentration of propylene and propane respectively on the adsorbent.
m'_A, m'_B	mg-mols/gm	pure phase adsorptive capacities of silica gel for propylene and propane respectively.
m_g		number of constants in power series fit to (Gy) data
n_{an}		number of analyses in one data set
n_c		number of series cells
n_p		number of points fit on each break-through curve during reduction to diffusion coefficients calculations.
n_r		number of concentric shells used in the finite difference solution of the diffusion equation.
p_A, p_B	atm	partial pressure of propylene and propane respectively
p^*_A, p^*_B	atm	interface partial pressure of propylene and propane respectively.
P	atm	total system pressure
q		coefficients of Q_A power series fit
Q_A, Q_B	mg-mols/ gm/sec	rate of increase of average concentration of propylene and propane respectively on the silica gel
R	atm cm^3/ mg-mol/°K	gas constant

Symbol	Dimension	
r	cm	radial distance of a point from the center of the adsorbent particle (considered as a sphere)
r_0	cm	radius of the equivalent spherical particle
Re		Reynolds Number $2r_0fv\rho_M/\mu$
R_1,R_2,R_3		rates defined by Equations (56),(58) and (A82) respectively
s	mg-mols/gm	total adsorbed gas concentration at any point within the equivalent spherical particle
$s*$	mg-mols/gm	total gas concentration at r_0
s_A,s_B	mg-mols/gm	concentration of propylene and propane respectively at any point within the equivalent spherical particle .
Sc		Schmidt number
t	sec	time
T	°K	temperature
T_c		critical temperature
T_R		reduced temperature
u	cm/sec	net velocity of molecular species
u		variable defined in Appendix A, Sec. B only
v		variable defined in Appendix A, Sec. B only
v	cm/sec	fluid free space velocity in adsorbent column
$\underline{V}$	cm^3/mg-mol	specific volume
y		mole fraction of propylene in gas phase
$y*$		mole fraction of propylene at interface
y_0		inlet mol fraction of propylene
x	cm	distance through the beds
X_1,X_2,X_3		variables used in the iterative determination of points on the plug-flow model grid, correspond to y, v and s* respectively.

Symbol	Dimension	
z	cm	distance across the gas film
α		a group defined by Equation (A72)
α_{AB}		adsorptive relative volatility of propylene to propane
β		zeroes of Equation (A20)
γ		group defined by Equation (27)
δ		group defined by Equation (28)
δ...		a small amount
ϵ	Kcal/gm-mol	adsorption potential
Θ	cm^2	term used in simplification of diffusion equation; defined by Equation (A2)
μ	gm/cm sec	viscosity
ρ_M	gm/cm^3	mass density
ρ	$mg\text{-}mol/cm^3$	molar density
ρ_A, ρ_B	$mg\text{-}mol/cm^3$	partial molar densities
ρ_s	gm/cm^3	bulk density of silica gel bed
τ		dummy integration variable occurring in Equations (A32), (A33), and (26).
φ	cm^3/gm	adsorbed volume per unit weight of adsorbent
ϕ		viscosity function defined by Equations (B9) and (B10)
ψ		group defined by Equation (15)

ABSTRACT

The kinetics of a binary gas-solid adsorbent system have been studied under the follwing flow system: A series of three shallow packed beds of silica gel were saturated with pure propane gas. A stream of pure propylene was then passed through the series beds at constant flow rate. Concentration histories were measured at the outlet of each bed as a function of time. Similar experiments were run with propylene initially on the bed and propane as the eluent gas. A range of pressures from one atmosphere to 4.3 atmospheres, temperatures of 0°C., 25°C. and 49°C. and particles of .117 cm., .198 cm., and .28 cm. in diameter were employed both in propane desorption and propylene desorption runs.

The results were analyzed in terms of a series resistance formed by gas phase film diffusion followed by homogeneous spherical particle diffusion. Gas phase film resistance was estimated from existing correlations and an average value of the effective diffusion coefficient of 3.65×10^{-5} sq. cm. per sec. was obtained in the partial diffusion model. This was within the experimental accuracy independent of temperature and pressure.

The derived coefficient was used to reconstruct some of the concentration histories obtained experimentally and showed moderately good correlation.

INTRODUCTION

When a gas mixture is passed through a packed bed of adsorbent which is saturated with a gas of composition different from the equilibrium composition corresponding to that of the passing gas, each component of the mixture is adsorbed at a particular rate depending upon how much of that component is already on the adsorbent. Components not present in the gas but adsorbed on the solid are given off until an average composition of adsorbed gas is reached which is in equilibrium with the gas passing the particles.

This equilibrium composition for hydrocarbon gases has been studied by Lewis et al.(14,15,16) but the kinetics of this type of "adsorptive displacement" seem not to be available. The purpose of this investigation was to examine the kinetics of a binary hydrocarbon (propylene-propane) displacement process on a solid adsorbent (silica gel).

The choice of a binary system seems to be justified by the same argument as is frequently mentioned in connection with vapor-liquid mass transfer studies: i.e., the binary system is the simplest possible choice since only one concentration variable is needed. The equations for mass transfer across the boundary layer film, for example, can be solved explicitly for the rate of each of the two components in certain special cases. This would not be possible for ternary or higher systems. In addition, the analytic techniques are usually considerably easier than for multi-component systems.

The propylene-propane-silica gel system was chosen for investigation on several accounts. First, there was a fairly complete set of equilibrium data available over the range of pressures necessary. Secondly, the heats of adsorption and desorption for each gas were almost identical so that in the displacement reaction, isothermal operation could be assumed. Experimental evidence later backed this up. Thirdly, a very precise, convenient and rapid method of analysis was available in the form of gas chromatography.

The potential value of a selective adsorption process for the separation of propylene and propane was also an incidental factor in the choice of this system.

The Model

Where the adsorbent saturated with a binary gas of one composition is contacted with the same binary gas of a composition other than the equilibirum composition in a constant pressure flow system, it does not seem likely that pressure gradients of any size will develop within the porous structure of the gel. Since the reaction is really one of displacement, the rates of adsorption and desorption would appear to be dependent upon the rates of diffusion of the two components past each other through the gel and across the concentration gradient or gas film on the outside of the particle. The actual adsorption reaction, as has been noted by various authors is probably very rapid compared to the diffusion step.

The model was based upon homogeneous radial diffusion in the particle rather than diffusion along an idealized pore. It was felt that both models would exhibit the same general behavior and the one chosen would be the most useful.

Background Material

A. Adsorption Rates

In his comprehensive review of the kinetics of chemisorption of gases on solids, Low(17) mentions only one investigation of the "Rapid Sorption by Porous Solids", that by Sutherland and Winfield(22). These authors measured rates of gas uptake by various porous solids in a constant volume system by means of pressure decrease. The systems examined were isopropyl alcohol - $Al_2O_3 \cdot H_2O$, ethanol - thorium (IV) oxide, water - thorium (IV) oxide, water - $Al_2O_3 \cdot H_2O$, water - -Al_2O_3 and methylvinylcarbinol - thorium (IV) oxide. Initial pressures of from 1.5 to 4 mm. Hg. were used.

Sutherland and Winfield developed equations for the following three possible cases:

1) Transient Knudsen flow into pores of the adsorbent accompanied by adsorption on and desorption from the walls of the pores.

2) The special case of the above when adsorption and desorption were so rapid that adsorption equilibrium could be assumed.

3) Adsorption which is so slow that the transport processes cannot influence the rate at which gas is taken up by the adsorbent. The rate of adsorption and desorption thus determines the rate of gas uptake.

The data of Winfield indicated that case 2) was the realistic scheme.

Ward(24) considered gas uptake in the hydrogen-copper system to be partly due to solution of the hydrogen in copper and then diffusion into the particles. He derived an expression for the rate q from the spherical diffusion equations.

$$q = A\left[\frac{4}{3}\pi R^3 - \frac{8R^3}{\pi}\sum_{n=1}^{\infty}\frac{1}{n^2}\exp(-kn^2\pi^2 t/R^2)\right]$$

where R is the radius of the copper spheres, and k is a constant.

Glueckauf(8) assumes that particle diffusion is the controlling resistance in chromatographic displacements and with a solution of the diffusion equation examines several empirical rate equations as to their applicability with various types of isotherms.

B. Saturation Behavior of Packed Adsorption Beds

The problem of adsorption (or ion exchange) on a packed bed where the component to be adsorbed is present only in small quantities has been solved by various authors with various simplifying assumptions. The stipulation of "trace adsorption", of course, ensures that the velocity of the gas through the bed is constant.

Among these solutions should be mentioned the work of Hiester and Vermeulen(9) who made dimensionless solutions for a general class of problems where the kinetics of adsorption could be described by a second order kinetic equation and the equilibrium isotherms were linear.

Acrivos(1) outlined in general terms the method of characteristics as applied to the adsorption in a fixed bed problem. It is this method which is pursued in the following mathematical work.

EXPERIMENTAL METHOD AND TREATMENT OF DATA

The experimental apparatus used in this investigation consisted of three shallow (1 inch) beds of silica gel in series. Before the first bed and between each of the successive beds were located small orifice meters for flow-rate determination and sample points for the withdrawal of gas samples. Thermocouples were mounted just below the adsorbent bed support screen and just above the bed. These were used to check the designed isothermal operation of the apparatus. A constant temperature bath surrounded the three cells and connecting tubing.

The general method was to saturate the three adsorbent beds with pure propylene and then introduce a measured constant flow of pure propane to the beds in series. Flow-rates were observed and samples taken for analysis by gas chromatograph at intervals until essentially pure propane was being taken off the last cell. Periodically during a run which lasted for an average of 25 to 30 minutes, temperatures were read in the gas stream by the thermocouples.

After saturation with propane, the inlet gas was changed to propylene and the procedure repeated until essentially pure propylene was issuing from the last cell. In this cyclic way, concentration history data could be obtained for both propane desorption into propylene and propylene desorption into propane.

The data so obtained were curve fit as the product of concentration and flow-rate (corrected for dead space in the columns) and the curve fits differentiated with respect to time to obtain an expression for adsorption or desorption rates. These were then used to iteratively deduce a value of the diffusion coefficient consistent with a homogeneous spherical diffusion model.

For a few cases, the value of the diffusion coefficient obtained above was tested by reconstruction of the concentration histories based upon a plug-flow bulk flow model and a rate governed by homogeneous spherical diffusion into the adsorbent particles.

APPARATUS

The overall layout of the experimental apparatus is shown in Figure 1. Components of the adsorption cell are shown in Figure 2, 3 and 4. Following is a detailed description of the major components of the apparatus.

A. Adsorption Cells

Three identical cells were used in series. The body of the cell shown in Figure 2 is made from standard galvanized two-inch pipe machined out to receive a force-fit liner. The top of the body has twenty-four to the inch threads and is machined to a smooth gasket fit. The bottom of the body has standard two-inch pipe threads to receive the bottom conical cap. A clamping support of 3/4 inch angle iron is welded to the body. The liner is of two parts, one forced in from the bottom, the other from the top. Between them a fine stainless steel screen (200 mesh) silica gel support is held. The overall height of the body exclusive of the top and bottom caps is 3 and 3/4 inches. The screen support is mounted 1 and 1/4 inches above the bottom of the body.

The top cap shown in Figure 3 is machined out of three-inch hexagon bar stock steel. It is one inch in height and is bored out to a depth of three-quarters of an inch. The inside surface is smooth machined for a gasket fit. One central hole is threaded to receive three-eighths inch copper tube fitting and four holes, ninety degrees apart are drilled on a circle whose radius is 3/4 inch and are threaded to receive one-quarter inch copper tube fittings.

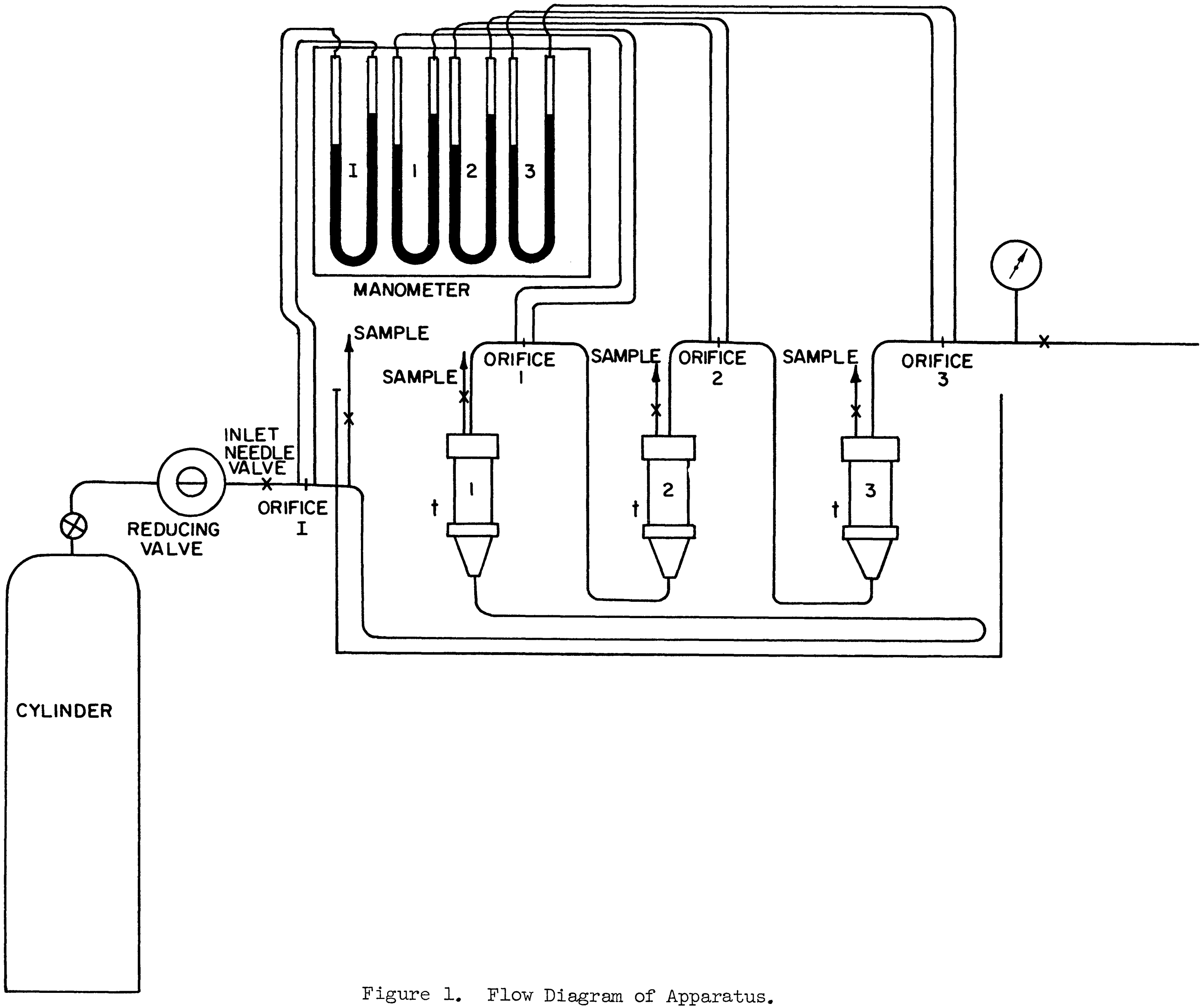

Figure 1. Flow Diagram of Apparatus.

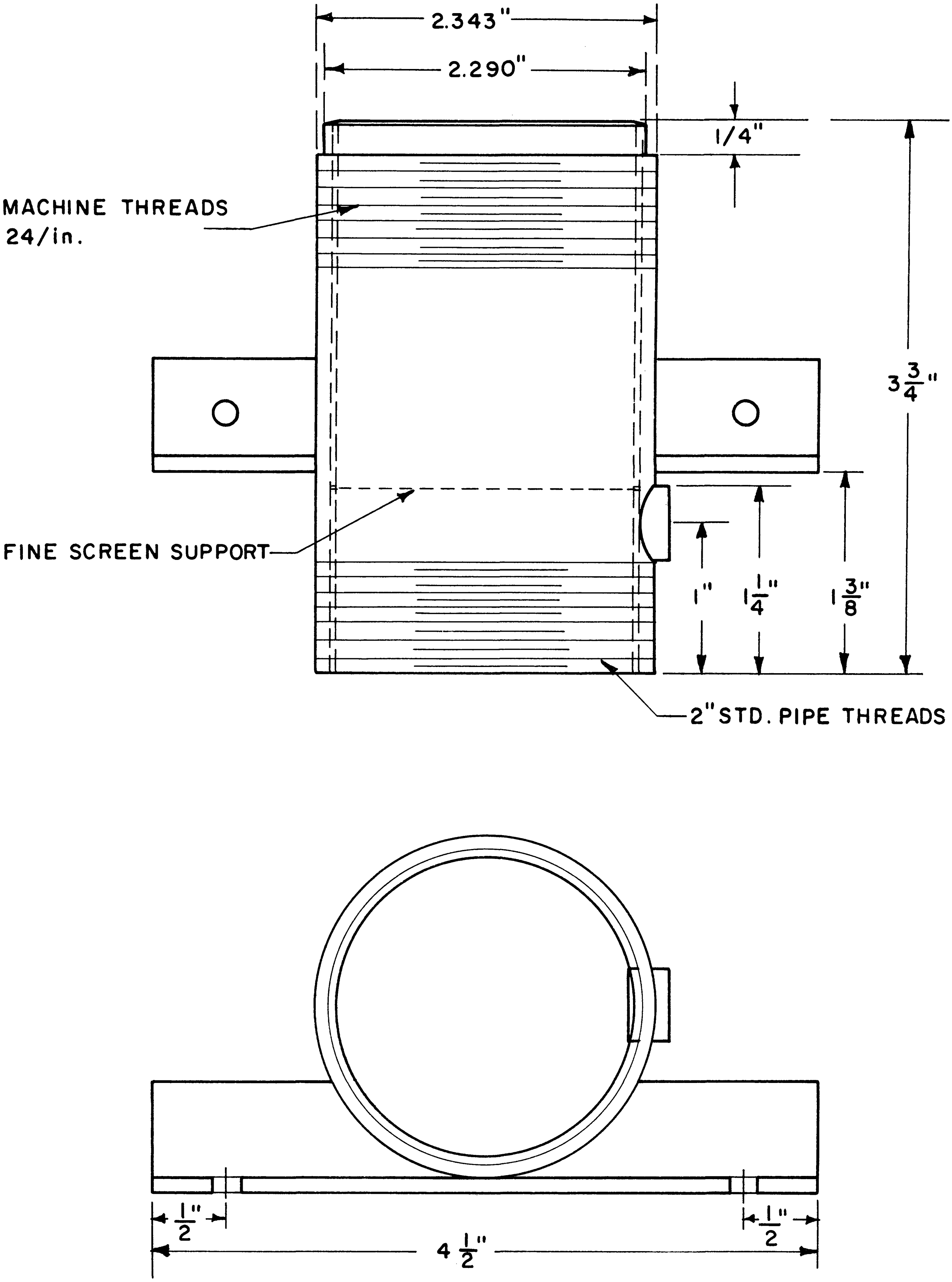

Figure 2. Adsorption Cell Cap.

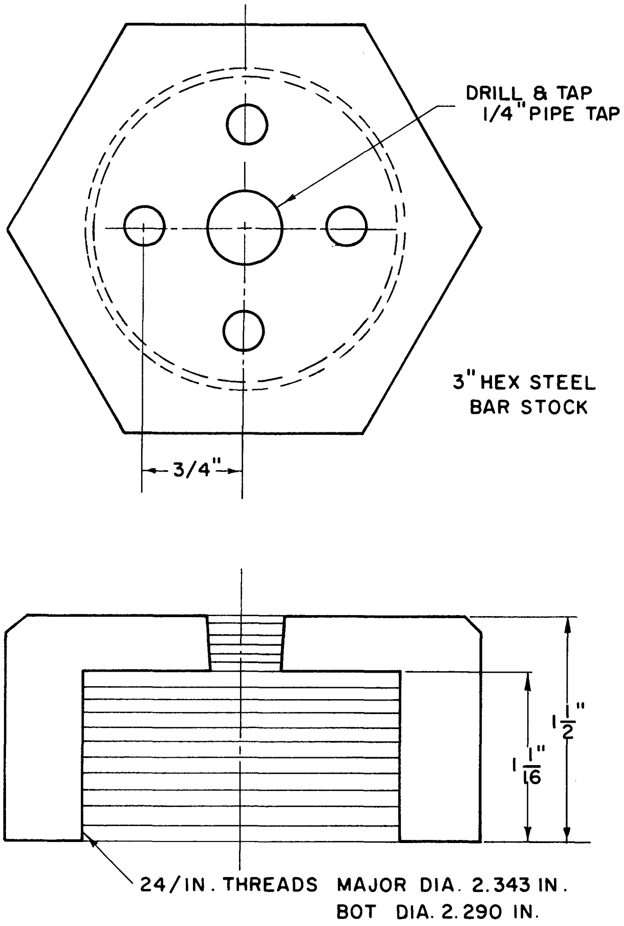

Figure 3. Adsorption Cell Body.

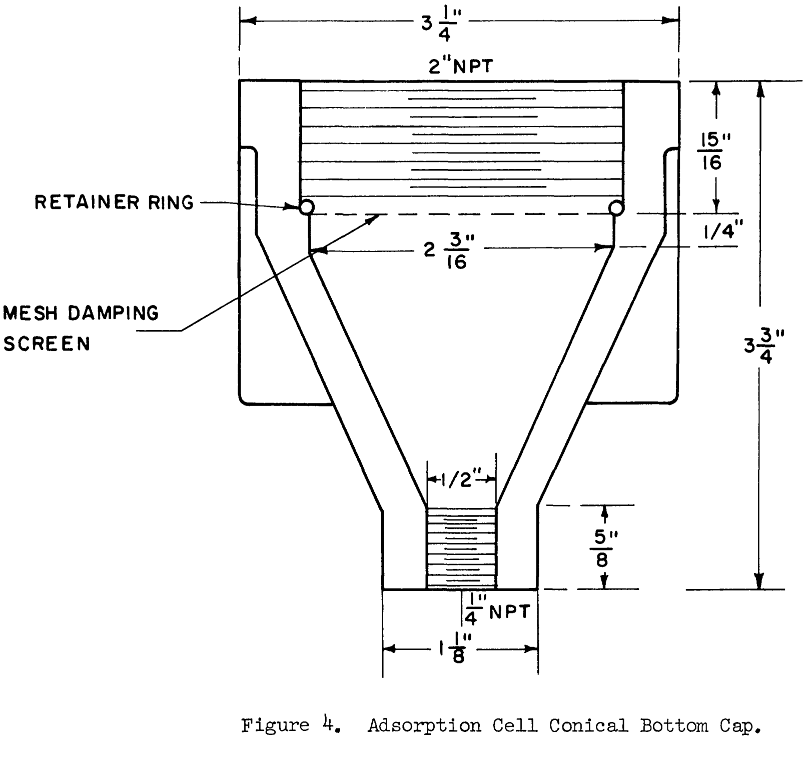

Figure 4. Adsorption Cell Conical Bottom Cap.

The bottom cap shown in Figure 4 is a specially designed gradual enlargement. It is cast in iron and machined to receive a three-eighths inch copper tube fitting at the small end, the inside is cut to a smooth taper. At the top of the cap a fine (200 mesh) screen is clamped. The purpose of the gradual enlargement and damping screen is to ensure as flat a velocity profile in the entrance of the cell as possible. The top is threaded to fit onto the threaded lower part of the cell body. The overall height of the bottom cap is 3 and 3/4 inches.

The gasket for the top cap is cut from one-eighth inch teflon.

B. Constant Temperature Bath

The constant temperature bath is 23 by 6 by 11 inches and is constructed from twenty-two gauge galvanized iron soft-soldered at all joints except the back removable panel. This is fastened by means of 3/16 inch sheet metal screws on a spacing of 2 inches. A gasket is provided for the back panel. This panel is also cut 3 inches from the top and hinged at that point so that the top can be loosened and swung down to provide easy access to the cell caps when they are to be removed.

During runs at 0°C., ice is packed around the cells mounted in the bath. At other temperatures water is in the bath and the temperature is regulated by a bi-metallic on-off type controlling device and a 500 watt immersion heater. The current supplied to the heater can be adjusted by means of a variable resistor supplied with voltmeter and ammeter. In this way optimum heating current can be found for each operating temperature.

In the bottom of the bath a coil of one-quarter inch copper tubing of length 64 inches is placed to serve as a pre-heater or cooler for the gas going to the first cell. Thermocouple measurements showed that temperature never varied from the bath temperature by more than one-half a degree at any time during a run.

C. Flow-meters

Flowrates are measured at four points in the system; namely, at the inlet to cell number 1, at the exit of cells number 1, 2 and 3. Measurement was by means of the pressure drop across a small orifice of diameter .02 inches mounted in the lines.

The orifice fixtures were machined from one-half inch brass round bar stock. A one-inch piece of the stock was bored from both ends to a depth of 17/32 inch, and to a diameter to provide a snug push fit for 3/8 inch copper tubing. The bottom of the hole was bored out square leaving a partition approximately 1/16 inch wide at the center of the piece. This partition was then carefully center-drilled and pierced with an orifice hole of diameter .02 inches.

The orifice fixtures are fastened by sweating and soldering the 3/8 inch tubing into the bottomed holes in either end.

The manometer taps are one-eighth copper tubing soldered into holes bored as close to the orifice fittings as possible.

The manometer U-tubes are made of 1/3 inch OD by 2mm ID capillary tubing and are provided with a construction at the bottom to prevent oscillation. They are fastened at the top into fittings made from standard elbow type 3/8 inch copper tubing fittings with the compression rings replaced with rubber O-rings. This type of fastening was found to be quite satisfactory at all ranges of pressure and vacuum.

Needle valves are provided in each manometer connection so that they could be isolated when the system is under vacuum.

The manometer fluid used is Acetylene Tetrabromide colored for easy reading with Methyl Red. This fluid has a specific gravity of 2.876 and provides the correct range of pressure drops over the required range of velocity measurements.

All four flowmeters were calibrated with propane and propylene measured by downward displacement of water.

D. Thermocouples

Thermocouple fittings were made from copper-constantan double wire passed through the center of a one-eighth OD stainless steel tube and then brazed into the tip. This tube was then mounted by means of a compression fitting bored out to let the tube pass all the way through and extend into the gas stream.

Thermocouples are mounted below each adsorbent bed through the wall of the cell and above the bed through the top cap.

Thermocouple EMF's were measured with a Leeds and Northrup Type K Potentiometer. A multipoint switch was provided to which all thermocouples were connected. This allowed rapid reading of all points.

E. Sampling System

Samples for analysis are taken in glass sample bulbs of approximately 30 cc. capacity. They are fitted with one opening closed by a stopcock and a 10/30 ground glass joint is provided for fastening to the sampling manifold and to the gas chromatography unit.

The sampling manifold as shown in Figure 5 is designed so that the sample bulb and the leads from the sampling valve can be evacuated prior to the taking of a sample. Four sample points are provided for: inlet to cell number 1, and outlets of cells 1, 2 and 3.

Each sampling system is provided with a connection to the main vacuum header, a ground glass joint to fit the sample tube and a mercury manometer to measure the vacuum and to act as a safety valve. Connection from glass-ware to metal sampling valve at the cells is provided by tygon tubing. All other parts of the leads from the cell to the sample tube and including the manometer are made from 2 mm. capillary tubing to cut down on the volume of gas necessary in each sample.

Vacuum is drawn on the main header by a Cenco Hyvac 7 pump. A cold trap is provided in the line to trap condensible gases.

The entire sampling assembly is mounted on a flexaframe and can be disconnected and removed en mass so that the back of the apparatus is accessible.

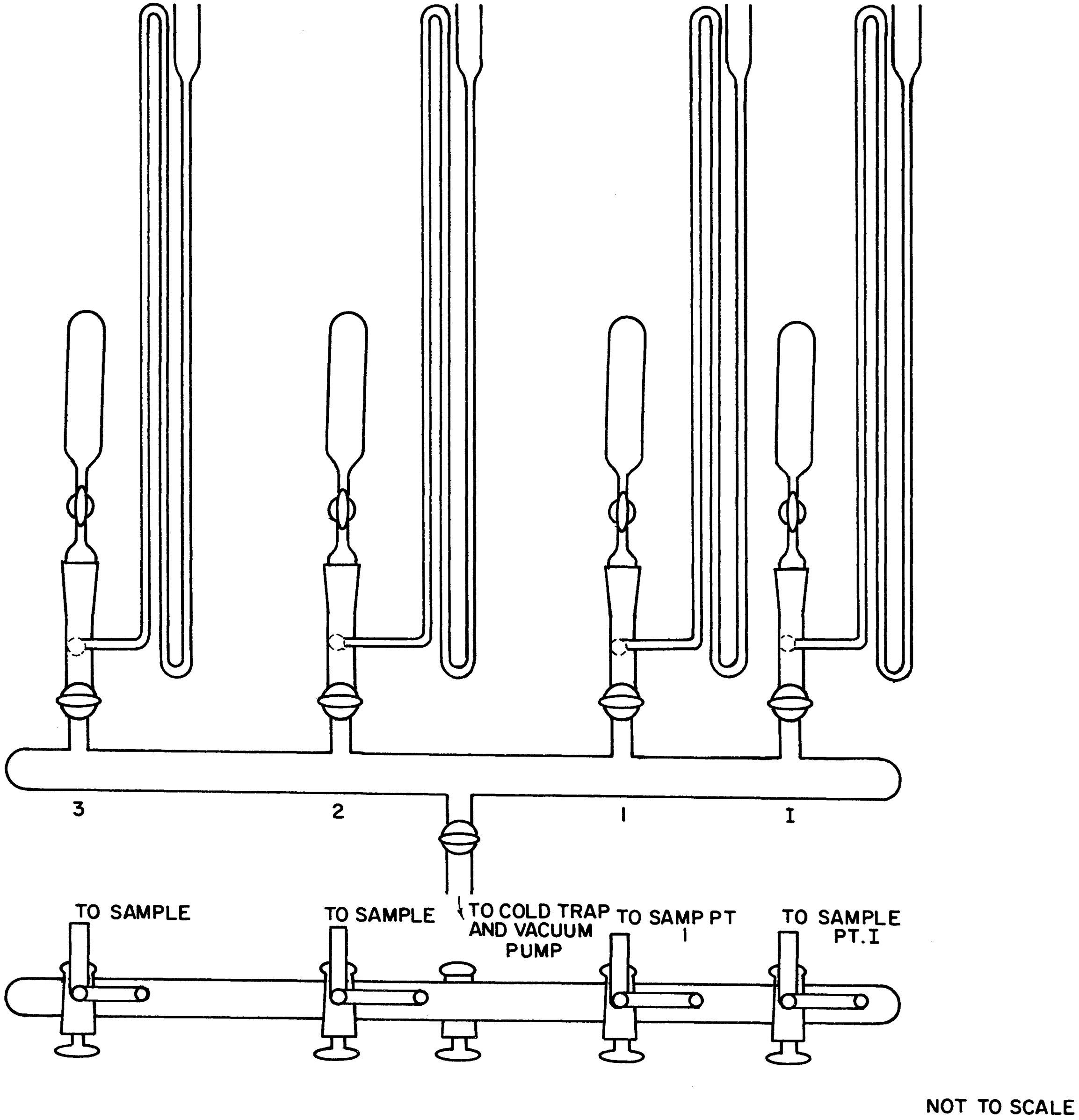

Figure 5. Sampling Manifold.

EXPERIMENTAL MATERIALS

The propane and propylene used in this investigation were supplied by the Phillips Petroleum Company. They were supplied as 99 mol percent purity but subsequent analysis showed that the propane was at least 99.9 mol percent with undetectible impurities on the gas chromatograph. The propylene analyzed 99.6 mol percent pure with the only detectible impurity being propane.

The silica gel was purchased from the Davison Company in several mesh sizes. These were further refined so that material used passed through the indicated mesh size or stuck in the screen but would not enter or pass through the next smaller screen.

TABLE I

Mesh Size	8	10	15
Bulk Density	.706	.700	.700
Voids Fraction as Packed	.42	.42	.42
B.E.T. Surface Area sq.m./gm. (measured with Nitrogen)	872	--	830
Pore Volume cc./gm.	47	--	47

EXPERIMENTAL PROCEDURE

A. Preparation of New Silica Gel Beds

Fifty cubic centimeters of gel as measured in a graduated cylinder were weighed and then put into each cell. Since the cross sectional area a_x of the column is 20.3 square centimeters, the depth of gel in each bed is 2.46 cm. The bed is evenly distributed and then the cap is screwed into place and turned down firmly on the teflon gasket.

After all connections have been made and pressure tested with compressed air, the system is put under vacuum. Care must be taken that the manometer valves are all completely shut so as to prevent the sucking of the fluid back into the pressure tap lines. The pressure gauge is shut off.

The system is kept under vacuum and at a water bath temperature of about 80°C. for 2 to 3 days. The system pressure usually quickly attains a minimum of a tenth of a millimeter of mercury as measured by a McLeod gauge and maintains this during the period of pulling down.

B. Preparation of Beds for a Run

Before a run, the beds are filled with one pure gas and allowed to come to equilibrium at whatever pressure and temperature the run is to be made. Experience showed that this need not be much more than an hour at any temperature or pressure used.

Just before the run, the connection from the pressure regulating valve to the main flow regulating valve is broken and the gas cylinders switched. The remaining gas in the leads up to the opening is then purged with the second pure gas and then the connection re-made.

C. Run Procedure

The timer is started and the main regulating valve opened at time zero. Since the volume of the leads and pre-heater is 300 cc., it requires a determinable amount of time, depending upon the flow-rate used, for the gas to reach the first cell. During this period of time, the flow-rate and the pressure in the cells must be adjusted by use of the two valves upstream of the cells and downstream. It was found that once this was carefully done, the conditions remained adequately constant, usually without any further adjustment during the course of the run.

Samples are taken according to a pre-determined schedule. It is important to keep the total volume of samples low, especially during low flow-rate runs. It was found possible to make replicate runs to fill in the concentration histories as the reproducibility was quite good.

Pressure drop readings from the flow-rate manometers are recorded during some of the replicate runs.

D. Analysis

Gas samples are analyzed by vapor-solid chromatography. The column is of quarter inch copper tubing, three feet long and packed with Burrel 200-mesh chromatography grade silica gel. The column is at room temperature, the carrier gas is helium and the flow-rate is maintained at approximately 250 cc./min. The peaks are recorded on a Brown 0-2 mv. recorder equipped with a mechanical integrator supplied by the Disc Integrator Corporation.

A typical chromatogram is shown in Figure 6. One analysis requires 2 and 1/2 minutes.

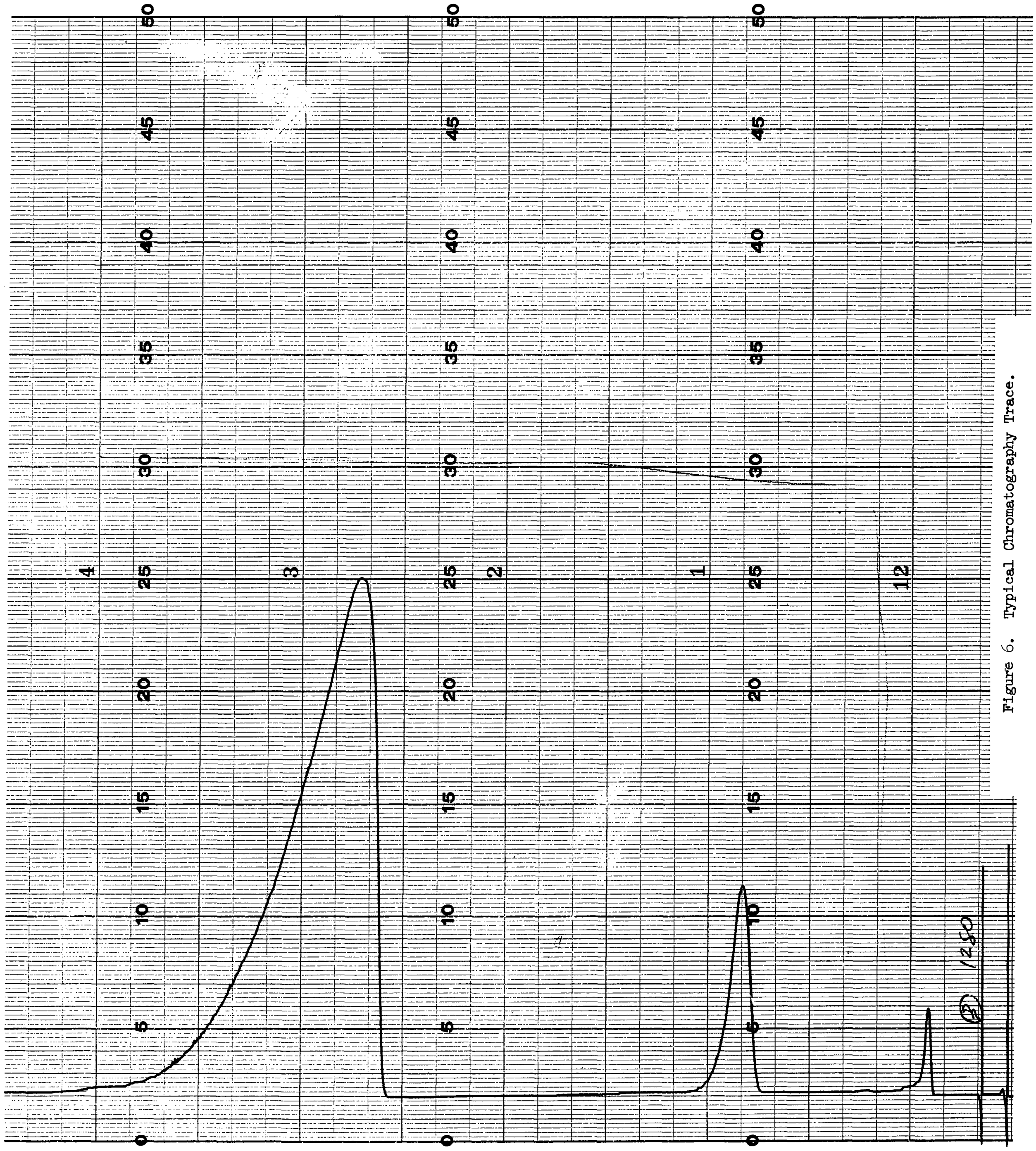

Figure 6. Typical Chromatography Trace.

THEORY

A. Development of the Mass Transfer Model

1. Assumptions

The model to be developed here considers two mass transfer steps in series; namely, diffusion across a gas film and then diffusion into the particle with a constant relative volatility at the interface. The actual adsorption reaction is considered to be infinitely rapid.

The concentration of adsorbed propylen and propane are assumed to follow an expression of the form below which was found by Lewis(14) to hold for average concentration at equilibrium.

$$\frac{s_A}{m'_A} + \frac{s_B}{m'_B} = 1 \tag{1}$$

where m' = average equilibrium capacity of adsorbent for the gas mg-mols/gm.

s = point concentration of adsorbed gas (function of radius) mg-mols/gm.

This equilibrium assumption is in a way related to the assumption of the infinitely rapid adsorption step since it is as consequence of that condition that all available adsorption sites must be filled at all times. Equation (1) says, in effect, that the fraction of available sites for adsorption of propylene actually filled with propylene, plus the fraction of sites available for adsorption of propane, actually filled with propane, must be equal to one. The number of available sites will be different for the two gases, being higher for the unsaturated one. The sites will, however, be on the same adsorption surface and so if one gas is adsorbed, by stearic hindrance, the other gas is not adsorbed on that accupied surface.

The assumption of pointwise equilibrium is consistent with the experimental relations of Lewis as shown below. By definition

$$m_A = \frac{\int_0^{r_o} r^2 s_A dr}{\int_0^{r_o} r^2 dr} = \frac{3}{r_o^3} \int_0^{r_o} r^2 s_A dr \qquad (2)$$

with a similar expression for m_B

Hence

$$\frac{m_A}{m_A'} + \frac{m_B}{m_B'} = \frac{3}{r_o^3} \int_0^{r_o} \left[\frac{s_A}{m_A'} + \frac{s_B}{m_B'}\right] r^2 dr = \frac{3}{r_o^3} \int_0^{r_o} r^2 dr = 1 \qquad (3)$$

It is further assumed that transport through the solid phase can be treated as Fick's Law type diffusion through a homogeneous sphere.

The diffusion coefficient is considered to be independent of concentration.

2. Mathematical Formulation of the Diffusion Model

The transport of propylene (component A) and that of propane (component B) are governed by the diffusion equations in spherical coordinates:

$$\frac{\partial s_A}{\partial t} = D_A \left[\frac{2}{r} \frac{\partial s_A}{\partial r} + \frac{\partial^2 s_A}{\partial r^2}\right] \qquad (4)$$

$$\frac{\partial s_B}{\partial t} = D_B \left[\frac{2}{r} \frac{\partial s_B}{\partial r} + \frac{\partial^2 s_B}{\partial r^2} \right] \qquad (5)$$

From (1)

$$s_B = m_B' - \frac{m_B'}{m_A'} s_A \qquad (6)$$

Differentiate twice with respect to radius.

$$\frac{\partial s_B}{\partial r} = - \frac{m_B'}{m_A'} \frac{\partial s_A}{\partial r} \qquad (7)$$

$$\frac{\partial^2 s_B}{\partial r^2} = - \frac{m_B'}{m_A'} \frac{\partial^2 s_A}{\partial r^2} \qquad (8)$$

Differentiate (6) with respect to time.

$$\frac{\partial s_B}{\partial t} = - \frac{m_B'}{m_A'} \frac{\partial s_A}{\partial t} \qquad (9)$$

Substitute (7), (8), and (9) into (5) and cancel.

$$\frac{\partial s_A}{\partial t} = D_B \left[\frac{2}{r} \frac{\partial s_A}{\partial r} + \frac{\partial^2 s_A}{\partial r^2} \right] \qquad (10)$$

Equation (10) implies that for this model it is necessary to consider the diffusion coefficients equal

$$D_A = D_B \qquad (11)$$

The result of (11) is that there is only one independent diffusion equation in the set (4) and (5). It may be written in terms of the concentration of either propylene or propane or in terms of the sum of the concentrations. We will use the latter.

Define:

$$s = s_A + s_B \tag{12}$$

Solve for s_A and s_B separately in the two equation system (12) and (1).

$$s_A = \frac{s + m_B'}{\psi} \tag{13}$$

and

$$s_B = \frac{s(\psi - 1) + m_B'}{\psi} \tag{14}$$

where

$$\psi = \frac{m_A' - m_B'}{m_A'} \tag{15}$$

By definition, Q_A is the rate of increase of average propylene concentration (bulk basis) on the silica gel; Q_B is the rate of increase of average propane concentration. In other words:

$$Q_A = \frac{\partial m_A}{\partial t} \tag{16}$$

$$Q_B = \frac{\partial m_B}{\partial t} \tag{17}$$

A boundary condition on the diffusion equation showing the flux of material into the particle may be derived in terms of the total concentrations:

$$D \frac{4\pi r_0^2}{(4/3)\ \pi r_0^3} \left(\frac{\partial s}{\partial r}\right)_{r_0} = Q_A + Q_B \tag{18}$$

or

$$\left(\frac{\partial s}{\partial r}\right)_{r_0} = \frac{r_0(Q_A + Q_B)}{3\ D} \tag{19}$$

If we differentiate Equation (3) with respect to time and use definitions (16) and (17) we get the following condition which must hold between the rates:

$$\frac{1}{m'_A} Q_A + \frac{1}{m'_B} Q_B = 0 \tag{20}$$

Substitute Q_B as can be solved for in Equation (20) into (19). We then get a boundary condition in terms of one rate Q_A only.

$$\left(\frac{\partial s}{\partial r}\right)_{r_0} = \frac{r_0 \psi}{3D} Q_A \tag{21}$$

We are now in a position to make a complete statement of the boundary value problem involved in the diffusion model.

$$s_t = D \left[\frac{2}{r} s_r + s_{rr}\right] \tag{22}$$

$$s_r(r_0,t) = \frac{r_0\psi}{3D}\, Q_A(t) \tag{23}$$

$$s(0,t) \qquad \text{bounded for all } t \tag{24}$$

$$s(r,0) = S_0 \tag{25}$$

The method of Laplace Transforms(5) is employed to give an analytic solution in terms of an infinite sine series. Details of the solution are given in Appendix A; the series solution is given here.

$$s(r,t) = m(t) - \frac{2}{3}\,\frac{r_0^3\psi}{D}\,\frac{1}{r}\sum_{n=1}^{\infty} \gamma_n\,\delta_n \sin(\beta_n r/r_0) \tag{26}$$

where

$$\gamma_n = (-1)^n \frac{\sqrt{1+\beta_n^2}}{\beta_n^3} \tag{27}$$

$$\delta_n = \exp(-\beta_n^2 Dt/r_0^2)\cdot\sum_{n=0}^{\infty}\left(-\frac{r_0^2}{\beta_n^2 D}\right)^j Q_A^{(j)}(0)$$

$$- \sum_{n=0}^{\infty}\left(-\frac{r_0^2}{\beta_n^2 D}\right)^j Q_A^{(j)}(t) \tag{28}$$

and β_n are the successive roots of the equation

$$\tan \beta_n = \beta_n \tag{29}$$

The notation "$Q_A^{(j)}(t)$" denotes the j^{th} derivative of $Q_A(t)$ with respect to t.

The average concentration $m(t)$ is given by

$$m(t) = S_0 + \psi \int_0^t Q_A(\tau)\, d\tau \tag{30}$$

3. Development of the Gas Film Mass Transfer Relation

From kinetic considerations as outlined by Treybal$^{(23)}$, the partial pressure gradient across a gas film due to the inter-diffusion of two gases may be written:

$$-dp = \beta\rho_A\rho_B(u_A - u_B)dz \tag{31}$$

By definition,

$$Q_A = u_A\rho_A a_s \tag{32}$$

$$Q_B = u_B\rho_B a_s \tag{33}$$

Therefore,

$$-dp_A = \frac{\beta}{a_s}(Q_A\rho_B - Q_B\rho_A)\, dz \tag{34}$$

Now if we assume that the Perfect Gas Law holds,

$$\rho_A = p_A/RT \tag{35}$$

Now the diffusion coefficient D_{AB} may be defined as follows:

$$D_{AB} = R^2T^2/\beta P \tag{37}$$

If we now substitute this into (34), we get

$$-dp_A = \frac{RT}{D_{AB}Pa_s}(Q_A p_B - Q_B p_A)dz \qquad (38)$$

Now

$$p_A + p_B = P \qquad (39)$$

Therefore

$$-dp_A = \frac{RT}{D_{AB}Pa_s}[PQ_A - (Q_A + Q_B)p_A]dz \qquad (40)$$

Rearrange

$$\frac{-dp_A}{Q_A[P - (\frac{Q_A + Q_B}{Q_A})\,p_A]} = \frac{RT\ dz}{D_{AB}Pa_s} \qquad (40a)$$

If now Q_A and Q_B are constant across the diffusion path z, we may integrate this expression.

$$\frac{1}{Q_A + Q_B}\log_e\left[\frac{P - (\frac{Q_A + Q_B}{Q_A})\,p_A{}^*}{P - (\frac{Q_A + Q_B}{Q_A})\,p_A}\right] = \frac{RT\ z}{D_{AB}Pa_s} \qquad (41)$$

By definition

$$\frac{D_{AB}P}{RT\ z} = k_y \qquad (42)$$

Therefore

$$Q_A + Q_B = k_y a_s \log_e\left[\frac{P - (\frac{Q_A + Q_B}{Q_A})\,p_A{}^*}{P - (\frac{Q_A + Q_B}{Q_A})\,p_A}\right] \qquad (43)$$

Now as a result of the equilibrium restriction imposed by Equation (20), rate Equation (43) can be written in terms of Q_A only.

$$Q_A = \frac{k_y a_s}{\psi} \log_e \left[\frac{P - \psi p_A{}^*}{P - \psi p_A} \right] \tag{44}$$

The mass transfer coefficient k_y may be estimated from the Colburn j_D factor correlation.

$$j_D = \frac{k_y (Sc)^{2/3}}{f\ v\ \rho} = f(RE) \tag{45}$$

The specific area a_s may be estimated from Figure 16 of the Appendix B, the source of which is Hougen and Watson, Chemical Process Principles.(12)

4. Interfacial Relations

We assume adsorption equilibrium at the interface. Thus any resistance to adsorption will be included in the effective difussion coefficient

$$\frac{p_A{}^*}{p_B{}^*} \frac{s_B{}^*}{s_A{}^*} = \alpha_{AB} \tag{46}$$

$$p_A{}^* + p_B{}^* = P$$

Substitute for $s_A{}^*$ and $s_B{}^*$ values from (13) and (15) and for $p_B{}^*$ from the above physical restraint into Equation (46).

$$\frac{p_A^*}{P - p_A{}^*} \quad \frac{s^*(\psi - 1) + m_B'}{s^* - m_B{}'} = \alpha_{AB}$$

Solve for p_A^* and substitute for ψ its definition from Equation (15).

$$p_A^* = \frac{P}{1 + \dfrac{m_B'(m_A' - s^*)}{m_A'(s^* - m_B')} \dfrac{1}{\alpha_{AB}}} \tag{47}$$

B. Development of the Plug-Flow Model

1. Basis

It was desireable to use the derived diffusion coefficient to predict the experimental concentration histories as an additional check on the consistency of the data processing step. As has been mentioned previously, the adsorption cells were designed with a long conical gradual enlargement and a fine damping screen below each bed. These were to ensure a flat velocity profile across the bed and the subsequent development of the flow model assumes no radial bed gradients in velocity or concentration.

Flow rates used in this study were low with a maximum Reynolds number of 10. On this basis, eddy diffusion was not taken into consideration and no term for longitudinal diffusion was put into the flow equations.

No temperature gradients were ever detected in the system during any run as might be expected from the very similar heats of adsorption of propylene and propane. These heats of adsorption were obtained as the slope of a Clausius-Clapeyron type plot of $\log_e P$ vs 1/T at constant amount of gas adsorbed. The Lewis(14,15) equilibrium data provided values of 5260 cal. per gm. mol for propylene and 5480 cal. per gm. mol for propane.

As a result of the above, the equations were set up without heat effects.

The rate of adsorption was governed by the diffusion of mixed gas in the particle. Gas film resistance is taken into consideration. All mass transfer processes were taken the same as those used in the previous section and all assumptions stated there apply equally to this section.

2. Development of the Differential Equations

We take a mass balance around a differential volume of the adsorbent bed as shown in Figure 7 of volume $a_x dx$. Since the mass balance will refer specifically to propylene unless otherwise noted, we drop the subscript and write y for y_A, etc.

The net amount of propylene added to the element in dt seconds through fluid flow is

$$\left\{v\rho y - \left[v\rho y - \frac{\partial}{\partial x}(v\rho y)\, dx\right]\right\} fa_x dx$$
$$= - \frac{\partial}{\partial x}(v\rho y)\, fa_x dx dt \tag{48}$$

The net amount of propylene added to the element in dt seconds due to transfer from the solid phase is

$$-\rho_s Q_A a_x\, dx\, dt \tag{49}$$

The net accumulation of propylene in the vapor phase of the element in dt seconds is

$$\left\{\left[\rho y + \frac{\partial}{\partial t}(\rho y)\, dt\right] - \rho y\right\} fa_x\, dx$$
$$= \frac{\partial}{\partial t}(\rho y)\, fa_x\, dx\, dt \tag{50}$$

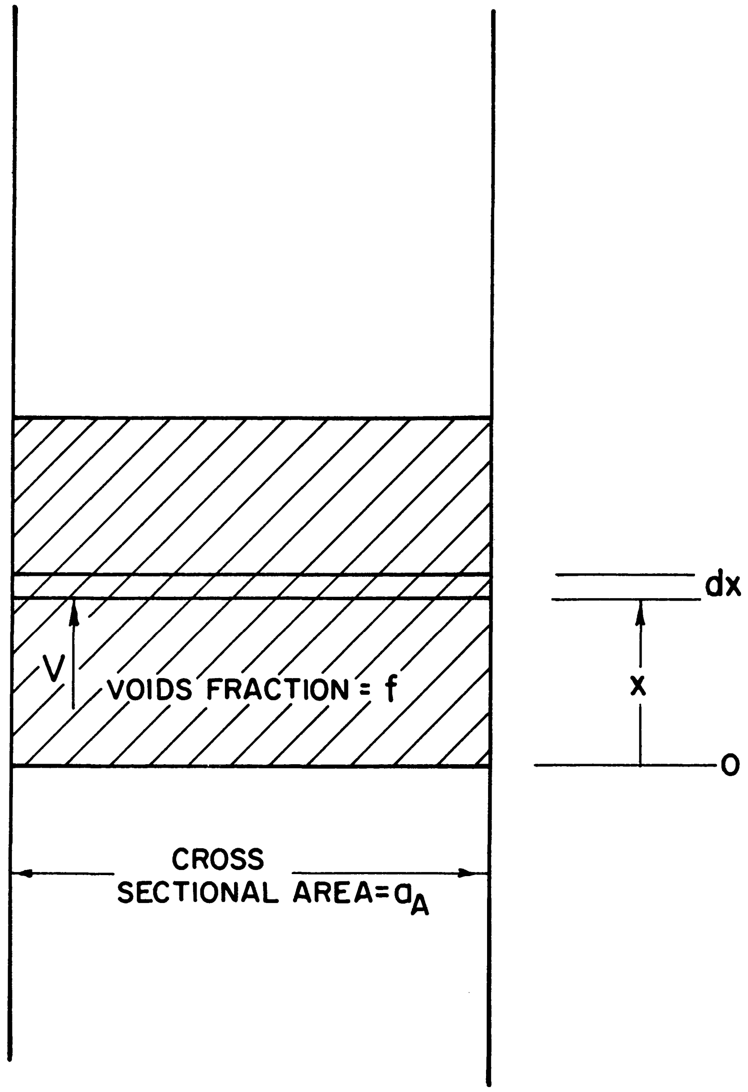

Figure 7. Schematic sketch of one Adsorption Bed Showing Terms Used in Mathematic Derivation of the Plug-Flow Model.

The complete differential mass balance on propylene in the gas phase can then be assembled and common terms cancelled to give the following differential equation:

$$\frac{\partial}{\partial x}(v\rho y) + \frac{\partial}{\partial t}(\rho y) + \frac{\rho_s}{f} Q_A = 0 \qquad (51)$$

Similarly a mass balance can be derived on the whole gas stream:

$$\frac{\partial}{\partial x}(v\rho) + \frac{\partial \rho}{\partial t} + \frac{\rho_s}{f}(Q_A + Q_B) = 0 \qquad (52)$$

Equation (51) can be simplified. Expand the applicable terms to

$$y[\frac{\partial}{\partial x}(v\rho) + \frac{\partial \rho}{\partial t}] + (v\rho)\frac{\partial y}{\partial x} + \rho\frac{\partial y}{\partial t} + \frac{\rho_s}{f} Q_A = 0 \qquad (53)$$

Substitute for the square bracketed term its equivalent from Equation (52) and rearrange.

$$\frac{\partial y}{\partial x} + \frac{1}{v}\frac{\partial y}{\partial t} = -\frac{\rho_s}{fv}[(1 - y)Q_A - yQ_B] \qquad (54)$$

Finally substituting from Equations (15) and (20), we get

$$\frac{\partial y}{\partial x} + \frac{1}{v}\frac{\partial y}{\partial t} = R_1 \qquad (55)$$

where

$$R_1 = -\frac{\rho_s}{fv}(1 - \psi y)Q_A \qquad (56)$$

If we make the assumption that the molar gas density remains constant and substitute from (15) and (20) into Equation (52), the following equation develops.

$$\frac{\partial v}{\partial x} = R_2 \qquad (57)$$

where

$$R_2 = - \frac{\psi \rho_s}{f \rho} Q_A \qquad (58)$$

3. Solution Along the Characteristics(1,6,11)

It is convenient to find a solution of Equations (55) and (57) along their so-called characteristic directions. Application of this method reduces the problem to one of solving the following simultaneous ordinary differential equations of first order along the so-called characteristic directions C^+ and C^- as shown in Figure 8. The theory of this method is covered in some generality in Appendix A.

Gas Phase Concentration

$$\left(\frac{dy}{dx}\right)_{C^+} = R_1 \qquad (59)$$

Velocity

$$\left(\frac{dv}{dx}\right)_{C^-} = R_2 \qquad (60)$$

The projections of the characteristic curves into the x-t plane are given by

$$C^+: \quad \frac{dt}{dx} = \frac{1}{x} \qquad (61)$$

$$C^-: \quad \frac{dt}{dx} = 0 \qquad (62)$$

Solution of these equations involves now the simultaneous integration of Equations (59), (60) and (61) in order to obtain the values of y, v and t along the C^- characteristics as functions of x.

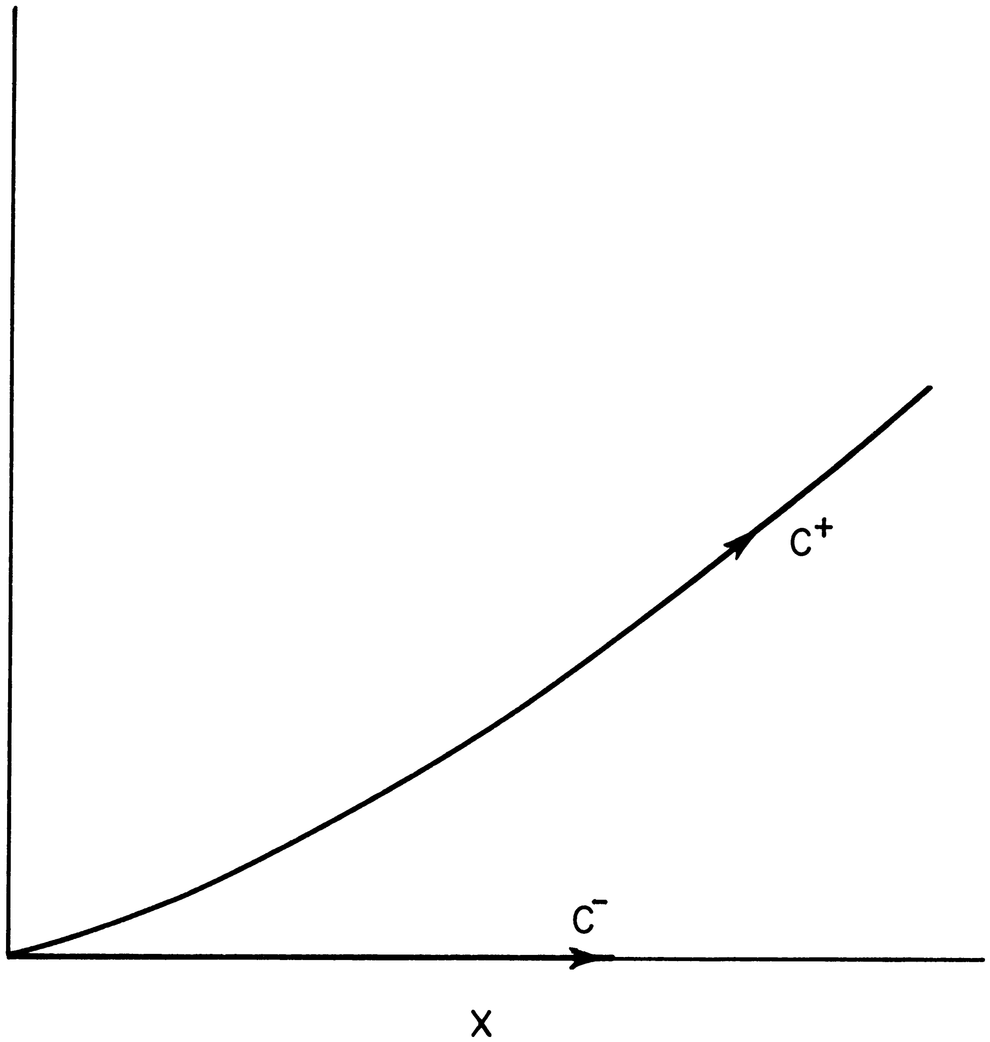

Figure 8. The Characteristic Directions of the Plug-Flow Equations.

The actual integration is carried out by a numerical finite difference scheme, the details of which are outlined in Appendix A.

EXPERIMENTAL DATA

Data observed during runs were analyses at various times, flow rates at the outlet of the three beds at various times during some runs, inlet flow rate and temperature and pressure.

Temperatures within the gas stream were monitored periodically but in no case showed a detectible difference from the bath temperature. Only one temperature is reported for each run.

In the following section, the data are grouped into blocks in which the particle size is constant and sub-blocks in which the temperature was changed. Pressure was changed within these blocks and is indicated for each run.

Analyses are indicated in the following way in the tables to follow: time (secs)/mol fract. propylene. For example, 150/.620 indicates a mol fraction of .620 at time 150 seconds from start up. Flow rates are indicated similarly as time(sec)/flow rate (mg-mol/sec.)

A. Block 1 Data

During this set of runs, the following column data were standard:

Amount of Silica Gel in Bed	1	35.3140	gm.
	2	35.4280	gm.
	3	35.0310	gm.
Height of each bed		2.46	cm.
Particle Mesh size	on	8	
Particle nominal diameter		.28	cm.
Beds void fraction (meas. by Hg displacement)		.42	

TABLE II

EXPERIMENTAL DATA AT PARTICLE DIAMETER OF .28 CMS.

TABLE II

1	2	3	4	5	6	7	8	9
Run No.	Col. Press. atm	Inlet m. f. C_3H_6	Inlet Molar Fl.Rt. mg-mol/sec	Col. No.		ANALYSES*		
Bath Temperature = 0°C								
3		.993	.80	1	60/.178	180/.710	300/.866	420/.973
				2	80/.000	200/.336	320/.636	440/.825
				3	100/.000	220/.037	340/.255	460/.580
4	.97	.000	.78	1	30/.608	150/.209	270/.101	390/.077
				2	50/.897	170/.378	290/.258	410/.183
				3	70/.991	190/.642	310/.408	430/.288
5	3.03	.993	.84	1	40/.000	160/.436	280/.704	400/.829
				2	60/.000	180/.104	300/.406	420/.577
				3	80/.000	200/.000	320/.069	440/.272
6	.97	.000	.78	1	50/.570	150/.286	240/.157	320/.105
				2	70/.825	170/.450	260/.304	340/.244
				3	90/.913	190/.639	280/.459	360/.388
7	.97	.993	.80	1	30/.030	90/.408	190/.708	270/.867
				2	40/.000	100/.050	200/.336	280/.533
				3	50/.000	110/.000	210/.033	290/.162
8	.97	.000	1.07	1	30/.635	90/.303	150/.174	210/.155
				2	40/.881	100/.509	160/.365	220/.268
				3	50/.970	110/.713	170/.521	230/.425
9	.97	.993	.80	1	40/.096	120/.552	210/.754	330/.893
				2	60/.000	140/.124	230/.389	350/.710
				3	80/.000	160/.000	250/.104	370/.367
10	.97	.993	.41	1	100/.000	220/.433	340/.695	540/.896
				2	120/.000	240/.033	360/.160	560/.524
				3	140/.000	260/.000	380/.000	580/.036
11	4.19	.000	1.50	1	60/.556	160/.262	260/.157	420/.099
				2	90/.870	180/.477	280/.266	440/.171
				3	110/.987	200/.698	300/.451	460/.280
12	4.31	.993	1.35	1	60/.065	120/.533	240/.743	360/.866
				2	70/.000	140/.129	260/.472	380/.669
				3	80/.000	160/.018	280/.239	400/.482
13	4.31	.000	.76	1	30/.988	120/.820	210/.481	330/.304
				2	50/.985	140/.980	230/.850	350/.573
				3	70/.984	160/.987	250/.993	370/.795
14	2.31	.993	1.20	1	30/.082	120/.553	210/.773	330/.845
				2	70/.000	140/.238	230/.525	350/.689
				3	90/.000	160/.061	250/.262	370/.533

*seconds/mole fraction C_2H_6

TABLE II (Cont'd.)

	10	11	12	13	14	15	16
3	540/.973	660/.982	780/.991	1080/.993	1380/.993		
	560/.911	680/.945	800/.969	1100/.987	1400/.993		
	580/.763	700/.870	820/.935	1120/.976	1420/.988		
4	510/.060	630/NG	750/.031	1050/NG	1450/.005		
	530/.111	650/.100	770/.064	1070/.054	1470/.018	1890/.005	
	550/.167	670/.158	790/.120	1090/.084	1490/.043	1910/.033	
5	520/.909	640/.943	760/.971	1060/.985	1360/.987	1660/.993	2360/.993
	540/.747	660/.820	780/.907	1080/.954	1380/.973	1680/.980	2380/.992
	560/.459	680/.665	800/.788	1100/.900	1400/.943	1700/.976	2400/.985
6	410/.078	570/.051	690/.061	850/.030	1130/.026		
	430/.193	590/.117	710/.086	870/.065	1150/.048		
	450/.292	610/.260	730/.166	890/.126	1170/.078	1430/.057	1940/.038
7	350/.920	430/.947	510/.965	590/.974	720/.988	900/.989	
	360/.721	440/.822	520/.878	600/.918	730/.950	910/.979	1110/.987
	370/.364	450/.554	530/.706	610/.807	740/.898	920/.945	1120/.970
8	270/.127	400/.072	500/.055	700/.029	1000/.009	1480/.000	
	280/.182	410/.142	510/.111	710/.053	1010/.029	1490/.000	
	290/.351	420/.240	520/.177	720/.117	1020/.060	1500/.036	
9	450/.944	780/.983					
	470/.838	650/.938	800/.965	1000/.982			
	490/.659	670/.857	820/.925	1020/.968			
10	840/.967	1240/.986	1800/.993	2510/.993			
	860/.871	1260/.970	1820/.993	2530/.993			
	880/.552	1280/.909	1840/.984	2550/.993			
11	580/.062	760/.038	880/.037	1100/.010	1400/.000	1800/.000	
	600/.121	780/.076	900/.065	1120/.058	1420/.034	1820/.010	2220/.005
	620/.191	800/.123	920/.091	1140/.084	1440/.052	1840/.022	2240/.005
12	600/.950	900/.973	1200/.986	1500/.993	1800/.993		
	620/.877	920/.958	1220/.972	1520/.985	1820/.993		
	640/.686	940/.874	1240/.959	1540/.983			
13	450/.210	600/.152	800/.113	1100/.049	1500/.039	2000/NG	2500/.000
	470/.389	620/.242	820/.206	1120/.119	1520/.070	2020/.036	2520/.010
	490/.585	640/.451	840/.329	1140/.193	1540/.113	2040/.075	2540/.032
14	450/.942	600/.978	800/.988	1100/.992	1500/.993	2000/.993	
	470/.864	620/.916	820/.206	1120/.984	1520/.993	2020/.993	
	490/.738	640/.848	840/.930	1140/.973	1540/.990	2040/.993	

TABLE II (Cont'd.)

1	2	3	4	5	6	7	8	9
Run No.	Col. Press atm	Inlet m. f. C_3H_6	Inlet Molar Fl.Rt. mg-mol /sec	Col. No.		A N A L Y S E S		
Bath Temperature = 0°C								
15	2.37	.000	1.20	1	30/.797	120/.358	210/.175	330/.114
				2	50/.973	140/.531	230/.344	350/.259
				3	70/.984	160/.739	250/.543	370/.321
16	.97	.993	.41	1	150/.273	270/.579	400/.798	650/.920
				2	180/.017	290/.101	420/.237	670/.743
				3	200/.000	310/.000	440/.023	690/.239
17	.97	.000	.78	1	90/.425	200/.209	350/.105	500/.047
				2	110/.612	220/.350	370/.239	520/.147
				3	130/.771	240/.519	390/.273	540/.246
18	.97	.993	.41	1	90/NG	190/.450	290/.672	450/.873
				2	110/.000	210/.022	320/.144	470/.424
				3	130/.000	230/.000	340/.014	490/.051
19	.97	.000	1.07	1	60/.498	170/.208	240/.134	360/.113
				2	70/.669	150/.369	230/.257	340/.198
				3	90/.765	130/.599	220/.415	320/.279
20	.97	.993	.41	1	70/.060	240/.597	380/.820	600/.933
				2	90/.000	260/.084	400/.281	620/.718
				3	110/.000	280/.005	420/.020	640/.274
21	.97	.000	.50	1	40/.818	160/.434	380/.194	500/.092
				2	60/.927	180/.632	400/.	520/.210
				3	80/.973	200/.800	420/.464	540/.346
22	.97	.993	1.17	1	30/.174	110/.686	170/.815	250/.917
				2	50/.035	120/.386	180/.565	260/.758
				3	70/.005	130/.070	190/.325	270/.515
23	.97	.000	.50	1	100/.595	250/.236	450/.150	550/.089
				2	120/.780	270/.428	470/.263	570/.202
				3	140/.921	290/.677	490/.415	590/.347
24	.97	.993	1.17	1	50/.341	140/.781	230/.869	310/.928
				2	70/.075	150/.490	240/.698	320/.838
				3	90/.005	170/.214	250/.416	240/.697
25	3.70	.000	2.04	1	40/.600	120/.215	200/.118	280/.087
				2	60/.898	140/.399	220/.224	300/.159
				3	80/.970	160/.581	240/.356	320/NG

TABLE II (Cont'd.)

	10	11	12	13	14	15	16
15	450/.074 470/.143 490/.227	600/.053 620/.104 640/.173	800/.031 820/.061 840/.122	1100/.022 1120/.042 1140/.094	1500/.010 1520/.026	2000/.000 2020/.010	
16	1000/.987 1020/.956 1040/.810	1500/.993 1520/.985 1540/.958					
17	650/.039 670/.095 690/.165	800/.034 820/.080 840/.139	970/.018 990/.042 1010/.103	1300/.003 1320/.021 1340/.045	1700/.000 1720/.002 1740/.026		
18	650/.946 670/.800 690/.302	920/.983 940/.936 960/.766	1120/.988 1140/.961 1160/.884	1370/.990 1390/.978 1410/.943			
19	440/.053 460/.134 480/.214	620/.011 600/.070 590/.145	840/.013 820/.047 800/.103	1140/.005 1120/.026 1100/.059	1340/.002 1320/.014 1300/.041	1540/.000 1520/.009 1500/.026	
20	780/.966 800/.881 820/.560	1060/.983 1080/.948 1100/.863	1300/.987 1320/.978 1340/.938	1600/.993 1620/.988 1640/.975	2000/.988		
21	620/.068 640/.142 660/.279	740/.064 760/.117 780/.219	900/.025 920/.055 940/.161	1100/.018 1120/.057 1140/.116	1300/.004 1320/.037 1340/.099	1600/.000 1620/.022 1640/.068	2000/.038
22	350/.944 370/.874 390/.767	450/.964 470/.922 490/.866	600/.979 620/.958 640/.927	800/.988 820/.977 840/.965	1000/.990 1020/.986 1040/.983		
23	700/.067 720/.149 740/.261	820/.045 840/.123 860/.217	1000/.032 1020/.085 1040/.157	1200/.010 1220/.058 1240/.120	1400/.008 1420/.038 1440/.101	1700/.007 1720/.017 1740/.073	2200/.003 2220/.015 2240/.036
24	400/.962 420/.902 440/.799	520/.976 540/.940 560/.898	700/.984 720/.973 740/.953	900/.992 920/.982 940/.972	1100/.993 1120/.988 1140/.984	1300/.993 1320/.990 1340/.988	1620/.991 1640/.990
25	370/.060 380/.118 400/.215	440/.040 460/NG 480/.159	520/.034 540/.071 560/.119	600/.024 620/.051 640/.106	700/.016 720/NG 740/.069	800/.005 820/.019 840/.049	1000/.000 1020/NG 1040/.033

TABLE II (Cont'd.)

1	2	3	4	5	6	7	8	9
Run No.	Col. Press. atm	Inlet m. f. C_3H_6	Inlet Molar Ft.Rt. mg-mol /sec	Col. No.	A N A L Y S E S			
Bath Temperature = 26°C								
26	.96	.993	.81	1	30/.151	150/.795	270/.954	390/.974
				2	50/.005	170/.539	290/.852	410/.935
				3	70/.000	190/.168	310/.635	430/.854
27	.96	.000	.40	1	30/.865	150/.343	270/.187	390/.098
				2	50/.973	170/.591	290/.369	410/.192
				3	70/.985	190/.818	310/.554	430/.409
28	.96	.993	.81	1	50/.279	110/.731	200/.884	330/.959
				2	60/.012	120/.288	220/.710	350/.898
				3	70/.005	130/.033	240/.344	370/.770
29	.96	.000	.40	1	100/.553	200/NG	340/.177	450/.130
				2	120/.817	220/.526	360/.296	470/.223
				3	140/NG	240/.737	380/.489	490/.431
30	.97	.993	.48	1	30/.027	100/.395	200/.768	300/.902
				2	40/.000	110/.016	210/.193	310/.558
				3	50/.000	120/.000	220/.005	320/.067
31	.97	.000	.77	1	20/.758	80/.346	140/.259	200/.137
				2	30/.969	90/.663	150/.366	210/.277
				3	40/.989	100/.772	160/.574	220/.442
32	.97	.993		1	50/.038	150/.522	250/.808	350/.914
				2	60/.000	160/.029	260/.220	360/.557
				3	70/.000	170/.005	270/.069	370/NG
33	.97	.000	.77	1	50/.555	170/.180	360/.068	450/.039
				2	60/.750	180/.310	370/.141	460/.111
				3	70/.910	190/.505	380/.253	470/.205
34	.97	.993	.97	1	50/.133	150/.698	250/.869	350/.947
				2	60/.000	160/.260	260/.617	360/.806
				3	70/.000	170/.025	270/.200	370/.438
Bath Temperature = 49°C								
35	.97	.000	.83	1	30/.700	100/.224	170/.140	240/.056
				2	40/.833	110/.359	180/.225	250/.109
				3	50/.965	120/.548	190/.343	260/.260
36	.97	.993	.67	1	30/.059	100/.698	170/.902	240/.965
				2	40/.000	110/.178	180/.614	250/.845
				3	50/.000	120/.008	190/.152	260/.503
37	.97	.000	.83	1	50/.504	130/.199	200/.078	300/.025
				2	60/NG	140/.295	210/.171	310/.098
				3	70/.807	150/.490	220/.283	320/.167

TABLE II (Cont'd.)

	10	11	12	13	14	15	16
26	510/.984	630/.991	750/.992	870/.992	990/.993		
	530/.968	650/.980	770/.988	890/.989	1010/.990	1120/.992	1520/.993
	550/.932	670/.967	790/.985	910/.985	1030/.987	1140/.988	1540/.990
27	510/.098	630/.037	750/.030	870/.013	1100/.007	1400/.005	
	530/.183	650/.129	770/.079	890/.072	1120/.025	1420/.021	
	550/.316	670/.253	790/.179	910/.162	1140/.093	1440/.070	
28	450/.981	590/.990	700/.990	850/.993	1000/.993		
	470/.957	610/.984	720/.986	870/.993	1020/.993		
	490/.903	630/.972	740/.979	890/.987	1040/.989		
29	560/.057	800/.034	1000/.022	1300/.000			
	580/.114	820/.095	1020/.067	1320/.048	1620/.037	2020/.000	
	600/.281	840/.202	1040/.100	1340/.082	1640/.065	2040/.022	
30	400/.963	500/.973	600/.989	800/.993			
	410/.807	510/.912	610/.955	810/.984	1010/.989	1210/.993	
	420/.325	520/.653	620/.856	820/.948	1020/.981	1220/.989	1610/.993
31	260/.103	320/.069	400/.041	500/.030	700/.005	1000/.000	
	270/.217	330/.158	410/.118	510/.066	710/.038	1010/.007	1300/.005
	280/.343	340/.271	420/.207	520/.142	720/.086	1020/.035	1310/.015
32	700/.978	900/.989	1200/.992	1500/.993			
	710/.958	910/.982	1210/.992	1510/.993			
	720/.877	920/.938	1220/.984	1520/.990			
33	600/.025	800/.005	900/.000	1200/.000			
	610/.079	810/.034	910/.015	1210/.005	1510/.000		
	620/.138	820/.072	920/.047	1220/.025	1520/.005		
34	450/.967	550/.978	650/.990	750/NG	850/.990	950/.993	
	460/.868	560/.944	660/.972	760/.974	860/.985	960/.989	1060/.990
	470/.737	570/.874	670/.919	770/.958	870/.977	970/.981	1070/.987
35	350/.024	500/.005	750/.000				
	360/.098	510/.025	760/.005	1010/.000			
	370/.129	520/.061	770/.016	1020/.005	1540/.000		
36	310/.974	390/.983	460/.987	600/.993	700/.993		
	320/.921	400/.967	470/.973	610/.987	710/.993	860/.993	
	330/.754	410/.879	480/.940	620/.976	720/.988	870/.993	1020/.993
37	410/.014	600/.000					
	420/.053	610/.013	910/.000				
	430/.111	620/.066	920/.013				

TABLE II (Cont'd.)

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Run No.	Col. Press. atm	Inlet m. f. C_3H_6	Inlet Molar Fl.Rt. mg-mol /sec	Col. No.		ANALYSES								
Bath Temperature = 49°C														
38	.96	.993	.67	1	60/.431	130/.798	200/.935		- - -					
				2	70/.030	140/.369	210/.726	280/.882	360/.945	430/.968	540/.985			
				3	80/.005	150/.043	220/.300	290/.635	370/.844	440/.911	550/.989			

TABLE III

VELOCITY DATA AT PARTICLE DIAMETER = .28cms.

Run No.	Col No.	FLOWRATE DATA					
26A	1	35/.631	55/.687	75/.717	95/.729	115/.737	135/.747
	2	40/.638	60/.660	80/.675	100/.689	120/.697	140/.713
	3	25/.614	45/.638	65/.653	85/.653	105/.660	125/.661
	1	155/.749	175/.757				
	2	160/.720	180/.729	200/.736	220/.737	240/.741	260/.744
	3	145/.662	165/.662	185/.663	205/.665	225/.674	245/.680
	1						
	2	280/.746	300/.749	320/.752	340/.753	360/.754	380/.754
	3	265/.682	285/.687	305/.692	325/.698	345/.701	365/.705
	1						
	2	510/.769	540/.770	580/.764	610/.767	660/.767	710/.767
	3	405/.714	425/.714	515/.726	585/.730	615/.732	715/.734
	1						
	2						
	3	765/.737	815/.738	915/.743	965/.745	1015/.749	
29	1	20/.428	35/.525	50/.488	65/.477	80/.462	180/.428
	2	25/.467	40/.514	55/.496	70/.495	85/.485	185/.456
	3	30/.493	45/.493	60/.482	75/.482	90/.472	190/.458
	1	320/.422	430/.421	540/.420	770/.418	980/.416	1280/.414
	2	325/.442	435/.439	545/.437	785/.434	985/.429	1285/.424
	3	330/.445	440/.444	550/.441	790/.439	990/.435	1290/.426
30	1	15/.401	95/.423	165/.451	255/.466	365/.472	465/.478
	2	20/.403	100/.405	170/.408	270/.422	370/.443	470/.450
	3	25/.390	105/.390	175/.390	275/.391	375/.392	475/.404
	1	565/.479	865/.479				
	2	570/.460	670/.465	770/.469	870/.470	1070/.471	
	3	575/.419	675/.436	775/.441	875/.444	975/.447	1075/.449
	1						
	2						
	3	1175/.456	1275/.457				
33	1	35/.854	125/.767	245/.761	305/.759	345/.757	425/.756
	2	20/.849	40/.882	130/.814	150/.811	250/.796	310/.794
	3	25/.849	45/.857	135/.817	155/.815	255/.800	275/.798
	1	575/.755	705/.751	985/.748			
	2	580/.785	710/.783	990/.776	1120/.774		
	3	315/.797	355/.796	435/.791	525/.791	715/.785	995/.770

B. Block 2 Data

Throughout the block of data composed of runs number 45 to 55 inclusive, the following column data were standard:

Amount of Silica Gel in each Bed	1	33.5014	gm.
	2	34.0806	gm.
	3	32.8644	gm.
Height of each bed		2.46	cm.
Particle mesh size	on	14	
Particle nominal diameter		.1168	cm.
Bed voids fraction (measured by Hg displacement)		.42	

TABLE IV

EXPERIMENTAL DATA AT PARTICLE DIAMETER OF .117 CMS.

TABLE IV

1	2	3	4	5	6	7	8	9
Run No.	Col. Press. atm	Inlet m. f. C_3H_6	Inlet Molar Fl.Rt. mg-mol /sec	Col. No.	A N A L Y S E S			
Bath Temperature = 0°C								
45	.98	.993	.87	1	50/.020	120/.405	190/.881	260/.966
				2	60/.000	130/.000	200/.200	270/.574
				3	70/.000	140/.000	210/.000	280/.000
46	.98	.000	.86	1	50/.859	120/.411	190/.185	260/.109
				2	60/.981	130/.867	200/.602	270/.414
				3	70/.988	140/.974	210/.870	280/.649
47	.98	.993	.87	1	30/.000	100/.215	160/.705	230/.958
				2	40/.000	110/.000	170/.000	240/.181
				3	50/.000	120/.000	180/.000	250/.000
48	2.30	.000	.88	1	50/.985	130/.653	210/.233	290/.145
				2	60/.993	140/.982	220/.806	300/.566
				3	70/.993	150/.993	230/.978	310/.888
Bath Temperature = 26°C								
49	.96	.993	.63	1	30/.000	110/.560	190/.976	270/.988
				2	40/.000	120/.000	200/.268	280/.947
				3	50/.000	130/.000	210/.000	290/.027
50	.96	.000	.63	1	50/.800	130/.266	210/.105	290/.043
				2	60/.979	140/.708	220/.396	300/.206
				3	70/.993	150/.921	230/.630	310/.379
51	.97	.993	.63	1	70/.097	150/.870	230/.988	310/.993
				2	80/.000	160/.000	240/.830	320/.979
				3	90/.000	170/.000	250/.000	330/.450
Bath Temperature = 0°C								
52	.97	.000	.49	1	50/.974	150/.605	250/.231	350/.140
				2	60/.993	160/.974	260/.760	360/.517
				3	80/.993	170/.993	270/.970	370/.810
53	.98	.993	.52	1	30/.000	130/.068	230/.560	330/.952
				2	40/.000	140/.000	240/.000	340/.076
				3	50/.000	150/.000	250/.000	350/.000
54	.98	.000		1	20/.988	100/.581	180/.250	260/.107
				2	30/.993	110/.905	190/.583	270/.353
				3	40/.993	120/.985	200/.826	280/.554
55	.98	.993	.52	1	100/.019	200/.467	300/.900	400/.986
				2	110/.000	210/.000	310/.005	410/.454
				3	120/.000	220/.000	320/.000	420/.001

TABLE IV (CONT'D)

	10	11	12	13	14	15	16
45	330/.990	400/.991	470/.993	600/.993			
	340/.929	410/.990	480/.993	610/.993	760/.993		
	350/.030	420/.560	490/NG	620/.991	770/.993	1020/.993	
46	330/.055	400/.045	470/.022	600/.008	700/.005	800/.000	1000/.000
	340/.268	410/.188	490/.112	610/.076	710/.050	810/.022	1010/.011
	350/.477	420/.343	500/.251	620/.161	720/.108	820/.074	1020/.041
47	300/.988	370/.993	440/.993				
	310/.852	380/.976	450/.989	520/.992			
	320/.000	390/.433	460/.824	530/.982	600/.990	700/.993	
48	370/.071	450/.043	600/.023	700/.005	900/.000	1200/.000	
	380/.358	460/.236	610/.117	710/.066	910/NG	1210/NG	
	390/.772	470/.481	620/.235	720/.127	920/.084	1220/.038	
49	350/.992	430/.993	510/.993				
	360/.992	440/.993	520/.993	710/.993			
	370/.826	450/.987	530/.989	720/.993	920/.993		
50	370/.028	450/.000	530/.000				
	380/.119	460/.067	540/.038	620/.010	710/.000		
	390/.210	470/.168	550/.119	630/.066	720/.037		
51	390/.993	470/.993					
	400/.991	480/.993					
	410/.974	490/.988					
52	450/.096	550/.056	750/.027	1050/.002	1300/.000		
	460/.365	560/.259	760/.123	1060/.049	1310/.036	1660/.001	
	470/.614	570/.462	770/.267	1070/.125	1320/.082	1670/.048	
53	430/.987	530/.992	630/.993	800/.993			
	440/.688	540/.973	640/.992	810/.993	1010/.993		
	450/.000	550/.049	650/.598	820/.982	1020/.989		
54	344/.069	420/.041	500/.021	600/.002	800/.000	1000/.000	
	350/.228	430/.151	510/.118	610/.067	810/.054	1010/.013	
	360/.377	440/.261	520/.193	620/.132	820/.082	1020/.036	
55	500/.993						
	510/.944	610/.989	710/.993				
	520/.013	620/.400	720/.928	900/.992			

C. Block 3 Data

Throughout the runs numbered 56 to 59, the following column data were standard:

Amount of Silica Gel in each Bed	1	33.8562	gm.
	2	33.5274	gm.
	3	32.0713	gm.
Height of each bed		2.46	cm.
Particle mesh size	on	10	
Particle nominal diameter		.198	cm.
Bed voids fraction (measured by Hg displacement)		.42	

TABLE V

EXPERIMENTAL DATA AT PARTICLE DIAMETER OF .198 CMS.

TABLE V

1	2	3	4	5	6	7	8	9
Run No.	Col. Press.	Inlet m.f. C_3H_6	Inlet molar flow rate	Col. No.	ANALYSES			
Bath Temperature = 0°C								
56	.98	.000	.79	1	30/.906	120/.356	190/.175	260/.104
				2	40/.993	130/.677	200/.497	270/.353
				3	50/.993	140/.924	210/.756	280/.611
57	.98	.993	.68	1	30/.014	100/.251	170/.584	240/.864
				2	40/.000	110/.000	180/.032	250/.158
				3	50/.000	120/.000	190/.000	260/.000
Bath Temperature = 25°C								
58	.98	.000		1	30/.784	100/.250	170/.150	240/.088
				2	40/.983	110/.667	180/.398	250/.277
				3	50/.987	120/.868	190/.652	260/.477
59	.98	.993		1	30/.055	100/.608	170/.924	240/.978
				2	40/.000	110/.049	180/.447	250/.842
				3	50/.000	120/.000	190/.028	260/.248

	10	11	12	13	14	15	16
56	330/.087	400/.054	470/.050	600/.042	700/.011	900/.007	1100/.000
	340/.284	410/.195	480/.142	610/.104	710/.067	910/.045	1110/.030
	350/.477	420/.337	490/.305	620/.228	720/.173	920/.127	1120/.059
57	310/.940	380/.979	450/.983	600/.992	700/.993	900/.993	
	320/.474	390/.750	460/.902	610/.964	710/.989	910/.993	
	330/.005	400/.082	470/.300	620/.828	720/.955	920/.984	
58	310/.057	380/.026	450/.020	600/.000			
	320/.176	390/.108	460/.103	610/.035	800/.046	1010/.000	
	330/.354	400/.266	470/.201	620/.152	810/.035	1020/.054	
59	310/.990	380/.993					
	320/.962	390/.983	460/.988	610/.993	810/.000	1010/.000	
	330/.709	460/.918	470/.975	620/.988	820/.993		

DATA PROCESSING

All calculations in the reduction of the data were programmed for the IBM 704 computer. A complete flowsheet of calculations is shown in Appendix E. In this section the overall sequence and objectives of these calculations are discussed.

The major objective of the data processing was to deduce the magnitude of the diffusion coefficient D involved in the homogeneous spherical diffusion model. As is shown in the Theory section, the diffusion equation may be solved with a boundary condition of an arbitrary input rate function of time, if this function is such that it has a finite number of derivatives. For this reason, use was made of polynomial curve fitting although this lead to considerable interpolation and smoothing to get enough points to make the polynomials describe the expected curves through the experimental points.

A. Mass Balance Calculations

The assumption of point-wise equilibrium results in the molar flow rate G being fixed at any point in space and time by a relation of the form:

$$G = G_0 \left(\frac{1 + \psi y_0}{1 + \psi y}\right) \qquad (63)$$

Derivation of this relation may be seen in Appendix A.

From smoothed curves of the experimental concentration - time data, points are taken at frequent time intervals and the amounts of the desorbing gas passing each of the three sample points per second (Gy) calculated and tabulated. These values are then correlated as functions of time by a polynomial.

The curves are next integrated by taking the analytic integral of the polynomial expression. From the difference of these integrals and after a correction is made for dead space, the loading of the desorbing gas on each bed initially is calculated.

B. Derivation of the Rate Equation Constants

The constants g of the (Gy) curve fits are differenced and divided by the adsorbent amounts in each cell to give the constants q of the rate functions according to the following relations:

$$q_{1,1} = \frac{(Gy)_0 - g_{1,0}}{L_1} \tag{64}$$

$$q_{1,n} = \frac{- g_{1,n}}{L_1} \qquad 2 \leq n \leq m_g \tag{65}$$

$$q_{i,n} = \frac{g_{i-1,n} - g_{i,n}}{L_i} \qquad \begin{array}{l} 2 \leq i \leq n_c \\ 1 \leq n \leq m_g \end{array} \tag{66}$$

If the desorbing gas is propylene, the coefficients q are taken as the coefficients of the rate function Q_A. if the desorbing gas is propane, the coefficients are those of the function Q_B and they are transformed to those of Q_A via relation (20):

$$q_{i,n} = - \frac{m_A'}{m_B'} q_{i,n} \qquad \begin{array}{l} 1 \leq n \leq m_g \\ 1 \leq i \leq n_c \end{array} \tag{67}$$

C. Iterative Trial and Error Determination of the Diffusion Coefficient

The rate equations derived above are average rates and as such apply most properly at the mid points of the adsorbent beds from which they are derived. As a result, in order to use them in the determination of the diffusion coefficient via the analytic solution, local conditions of molar flow rate and mol fraction must be interpolated at the mid-points. This is done by a standard three point formula.

From these interpolated values, a mass transfer coefficient is computed from the j_D correlation and then from the following rearrangement of Equation (44)

$$y^* = \frac{1}{\psi} - \left(\frac{1}{\psi} - y\right) e^{(\psi Q_A / k_y a_s)} \qquad (68)$$

the interface mol fraction of propylene is computed. Next, from Equation (47) the following relation is derived:

$$s^* = \frac{y^*/\alpha_{AB} + (1 - y^*)}{y^*/\alpha_{AB} m'_A + (1 - y^*)/m'_B} \qquad (69)$$

From this relation, the total gas interface concentration s^* on the adsorbent surface is computed.

Finally a value of the diffusion coefficient D is assumed and the interface total gas concentration is compared as the solution of Equation (26) at radius $r = r_0$. The assumed value of the diffusion coefficient is then corrected as indicated by the discrepancy in the two computed values of s^* and the iterative part of the calculation repeated until this discrepancy is less than an allowable error (usually 1%). The actual method of correction of the assumed value of D based upon this error is taken from a technique due to Gauss and recently described by Wegstein.(25)

This trial and error determination is repeated for four points on each of the break-through curves taken experimentally and finally the derived values of the diffusion coefficient are averaged.

In the section to follow, the data reduction as performed by the computer is reproduced for one run in Table IV and is summarized for the remaining runs in Table VII.

TABLE VI

```
BINARY ADSORPTION KINETICS
MASS BALANCE CLOSURE CALCULATIONS

RUN NUMBER  1
NUMBER OF SERIES CELLS  3
INITIAL SYSTEM PRESSURE                              1.0000 ATMOSPHERES
INITIAL SYSTEM TEMPERATURE (BATH TEMP.)              0.     DEGREES CENT.
MOL FRACTION OF PROPYLENE IN BED INITIALLY           0.
BED VOIDS FRACTION                                   0.4200
BED CROSS-SECTIONAL AREA                            20.3000 SQUARE CM.
ADSORPTIVE RELATIVE VOLATILITY                       0.5000
SILICA GEL LOADED IN EACH CELL            1         35.3140 GRAMS
                                          2         35.4280 GRAMS
                                          3         35.0310 GRAMS
DEPTH OF BEDS                             1          2.4600 CM.
                                          2          2.4600 CM.
                                          3          2.4600 CM.
MAXIMUM (EQUILIBRIUM) LOADING PROPYLENE              3.2737 MG-MOLS/GM.
MAXIMUM (EQUILIBRIUM) LOADING PROPANE                2.5311 MG-MOLS/GM.
ASSUMED INITIAL LOADING OF PROPANE                   2.5311 MG-MOLS/GM.
INLET MASS FLOW RATE                                 0.7961 MG-MOLS/SEC
INLET VOLUMETRIC FLOW RATE                          16.6479 CC/SEC
INLET FREE SPACE VELOCITY                            1.9526 CM/SEC
AREA FOR MASS TRANSFER                              18.5000 SQ. CM.
PARTICLE RADIUS                                      0.1400 CM.
INLET MOL FRACTION PROPANE                           0.0070

UNPROCESSED EXPERIMENTAL DATA WITH FLOWRATES OBTAINED BY EQUILIBRIUM
MASS BALANCE

DATA FOR CELL NO.  1
TIME          G             F            V            X            Q
SECS    MG-MOLS/SEC     CC/SEC       CM./SEC      PROPANE    MG-MOLS/SEC
  17.30      0.6168       12.8949       1.5124       1.0000       0.6168
  20.00      0.6168       12.8949       1.5124       1.0000       0.6168
  50.00      0.6363       13.3027       1.5603       0.8650       0.5504
  80.00      0.6611       13.8207       1.6210       0.7050       0.4660
 110.00      0.6873       14.3697       1.6854       0.5480       0.3766
 140.00      0.7121       14.8895       1.7464       0.4100       0.2920
 170.00      0.7305       15.2738       1.7914       0.3140       0.2294
 200.00      0.7396       15.4651       1.8139       0.2680       0.1982
 230.00      0.7509       15.7002       1.8414       0.2130       0.1599
 260.00      0.7588       15.8668       1.8610       0.1750       0.1328
 290.00      0.7654       16.0054       1.8772       0.1440       0.1102
 320.00      0.7715       16.1326       1.8922       0.1160       0.0895
 350.00      0.7759       16.2248       1.9030       0.0960       0.0745
 380.00      0.7806       16.3227       1.9145       0.0750       0.0585
 410.00      0.7837       16.3886       1.9222       0.0610       0.0478
 440.00      0.7862       16.4408       1.9283       0.0500       0.0393
 470.00      0.7878       16.4741       1.9322       0.0430       0.0339
 500.00      0.7897       16.5124       1.9367       0.0350       0.0276
 530.00      0.7913       16.5461       1.9407       0.0280       0.0222
 560.00      0.7922       16.5654       1.9429       0.0240       0.0190
 590.00      0.7927       16.5751       1.9441       0.0220       0.0174
 620.00      0.7936       16.5944       1.9463       0.0180       0.0143
 650.00      0.7940       16.6041       1.9475       0.0160       0.0127
 680.00      0.7945       16.6138       1.9486       0.0140       0.0111
 710.00      0.7947       16.6187       1.9492       0.0130       0.0103
 740.00      0.7952       16.6284       1.9503       0.0110       0.0087
 770.00      0.7957       16.6382       1.9515       0.0090       0.0072
 800.00      0.7959       16.6430       1.9520       0.0080       0.0064
 830.00      0.7961       16.6479       1.9526       0.0070       0.0056
```

```
 860.00       0.7961      16.6479      1.9526      0.0070      0.0056
 890.00       0.7961      16.6479      1.9526      0.0070      0.0056
 920.00       0.7961      16.6479      1.9526      0.0070      0.0056
 950.00       0.7961      16.6479      1.9526      0.0070      0.0056
 980.00       0.7961      16.6479      1.9526      0.0070      0.0056
1010.00       0.7961      16.6479      1.9526      0.0070      0.0056
1040.00       0.7961      16.6479      1.9526      0.0070      0.0056
1070.00       0.7961      16.6479      1.9526      0.0070      0.0056
1100.00       0.7961      16.6479      1.9526      0.0070      0.0056
1130.00       0.7961      16.6479      1.9526      0.0070      0.0056
1160.00       0.7961      16.6479      1.9526      0.0070      0.0056
1190.00       0.7961      16.6479      1.9526      0.0070      0.0056
1220.00       0.7961      16.6479      1.9526      0.0070      0.0056
1250.00       0.7961      16.6479      1.9526      0.0070      0.0056
1280.00       0.7961      16.6479      1.9526      0.0070      0.0056
1310.00       0.7961      16.6479      1.9526      0.0070      0.0056
1340.00       0.7961      16.6479      1.9526      0.0070      0.0056
1370.00       0.7961      16.6479      1.9526      0.0070      0.0056
1400.00       0.7961      16.6479      1.9526      0.0070      0.0056
1430.00       0.7961      16.6479      1.9526      0.0070      0.0056
1460.00       0.7961      16.6479      1.9526      0.0070      0.0056

PRESSURE IN CELL 1                              1.0510 ATMOSPHERES

DATA FOR CELL NO.  2
TIME          G              F            V            X            Q
SECS   MG-MOLS/SEC      CC/SEC      CM./SEC      PROPANE    MG-MOLS/SEC
  17.30       0.6168      13.0886      1.5351      1.0000      0.6168
  20.00       0.6168      13.0886      1.5351      1.0000      0.6168
  50.00       0.6168      13.0886      1.5351      1.0000      0.6168
  80.00       0.6172      13.0976      1.5362      0.9970      0.6154
 110.00       0.6198      13.1513      1.5425      0.9790      0.6068
 140.00       0.6256      13.2755      1.5571      0.9380      0.5868
 170.00       0.6378      13.5342      1.5874      0.8550      0.5453
 200.00       0.6566      13.9333      1.6342      0.7330      0.4813
 230.00       0.6755      14.3352      1.6814      0.6170      0.4168
 260.00       0.6927      14.7008      1.7242      0.5170      0.3581
 290.00       0.7077      15.0186      1.7615      0.4340      0.3071
 320.00       0.7208      15.2976      1.7942      0.3640      0.2624
 350.00       0.7332      15.5618      1.8252      0.3000      0.2200
 380.00       0.7433      15.7747      1.8502      0.2500      0.1858
 410.00       0.7519      15.9580      1.8717      0.2080      0.1564
 440.00       0.7590      16.1096      1.8895      0.1740      0.1321
 470.00       0.7654      16.2457      1.9054      0.1440      0.1102
 500.00       0.7706      16.3563      1.9184      0.1200      0.0925
 530.00       0.7746      16.4403      1.9283      0.1020      0.0790
 560.00       0.7779      16.5109      1.9365      0.0870      0.0677
 590.00       0.7806      16.5678      1.9432      0.0750      0.0585
 620.00       0.7826      16.6108      1.9482      0.0660      0.0517
 650.00       0.7844      16.6491      1.9527      0.0580      0.0455
 680.00       0.7856      16.6732      1.9556      0.0530      0.0416
 710.00       0.7872      16.7070      1.9595      0.0460      0.0362
 740.00       0.7881      16.7264      1.9618      0.0420      0.0331
 770.00       0.7892      16.7507      1.9647      0.0370      0.0292
 800.00       0.7899      16.7653      1.9664      0.0340      0.0269
 830.00       0.7908      16.7848      1.9687      0.0300      0.0237
 860.00       0.7915      16.7995      1.9704      0.0270      0.0214
 890.00       0.7922      16.8142      1.9721      0.0240      0.0190
 920.00       0.7927      16.8240      1.9733      0.0220      0.0174
 950.00       0.7931      16.8338      1.9744      0.0200      0.0159
 980.00       0.7936      16.8436      1.9756      0.0180      0.0143
1010.00       0.7938      16.8486      1.9761      0.0170      0.0135
1040.00       0.7943      16.8584      1.9773      0.0150      0.0119
1070.00       0.7945      16.8633      1.9779      0.0140      0.0111
1100.00       0.7947      16.8683      1.9785      0.0130      0.0103
1130.00       0.7950      16.8732      1.9790      0.0120      0.0095
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1160.00         0.7952       16.8781       1.9796       0.0110       0.0087
1190.00         0.7954       16.8831       1.9802       0.0100       0.0080
1220.00         0.7957       16.8880       1.9808       0.0090       0.0072
1250.00         0.7957       16.8880       1.9808       0.0090       0.0072
1280.00         0.7959       16.8930       1.9813       0.0080       0.0064
1316.00         0.7959       16.8930       1.9813       0.0080       0.0064
1340.00         0.7959       16.8930       1.9813       0.0080       0.0064
1370.00         0.7961       16.8979       1.9819       0.0070       0.0056
1400.00         0.7961       16.8979       1.9819       0.0070       0.0056
1430.00         0.7961       16.8979       1.9819       0.0070       0.0056
1460.00         0.7961       16.8979       1.9819       0.0070       0.0056

PRESSURE IN CELL 2                                1.0357 ATMOSPHERES

DATA FOR CELL NO.  3
TIME            G            F             V            X            Q
SECS     MG-MOLS/SEC      CC/SEC       CM./SEC       PROPANE     MG-MOLS/SEC
  17.30         0.6168       13.3341       1.5639       1.0000       0.6168
  20.00         0.6168       13.3341       1.5639       1.0000       0.6168
  50.00         0.6168       13.3341       1.5639       1.0000       0.6168
  80.00         0.6168       13.3341       1.5639       1.0000       0.6168
 110.00         0.6168       13.3341       1.5639       1.0000       0.6168
 140.00         0.6171       13.3402       1.5646       0.9980       0.6159
 170.00         0.6185       13.3706       1.5682       0.9880       0.6111
 200.00         0.6205       13.4133       1.5732       0.9740       0.6043
 230.00         0.6240       13.4903       1.5823       0.9490       0.5922
 260.00         0.6292       13.6028       1.5955       0.9130       0.5745
 290.00         0.6362       13.7526       1.6130       0.8660       0.5509
 320.00         0.6464       13.9751       1.6391       0.7980       0.5159
 350.00         0.6619       14.3088       1.6783       0.7000       0.4633
 380.00         0.6770       14.6369       1.7167       0.6080       0.4116
 410.00         0.6908       14.9346       1.7517       0.5280       0.3647
 440.00         0.7035       15.2092       1.7839       0.4570       0.3215
 470.00         0.7144       15.4451       1.8115       0.3980       0.2843
 500.00         0.7243       15.6592       1.8366       0.3460       0.2506
 530.00         0.7328       15.8451       1.8584       0.3020       0.2213
 560.00         0.7406       16.0135       1.8782       0.2630       0.1948
 590.00         0.7471       16.1544       1.8947       0.2310       0.1726
 620.00         0.7542       16.3069       1.9126       0.1970       0.1486
 650.00         0.7603       16.4392       1.9281       0.1680       0.1277
 680.00         0.7657       16.5551       1.9417       0.1430       0.1095
 710.00         0.7702       16.6536       1.9533       0.1220       0.0940
 740.00         0.7746       16.7486       1.9644       0.1020       0.0790
 770.00         0.7784       16.8301       1.9740       0.0850       0.0662
 800.00         0.7810       16.8882       1.9808       0.0730       0.0570
 830.00         0.7833       16.9369       1.9865       0.0630       0.0493
 860.00         0.7849       16.9711       1.9905       0.0560       0.0440
 890.00         0.7860       16.9957       1.9934       0.0510       0.0401
 920.00         0.7874       17.0252       1.9969       0.0450       0.0354
 950.00         0.7881       17.0400       1.9986       0.0420       0.0331
 980.00         0.7894       17.0697       2.0021       0.0360       0.0284
1010.00         0.7901       17.0846       2.0038       0.0330       0.0261
1040.00         0.7910       17.1045       2.0062       0.0290       0.0229
1070.00         0.7915       17.1145       2.0073       0.0270       0.0214
1100.00         0.7922       17.1295       2.0091       0.0240       0.0190
1130.00         0.7927       17.1395       2.0103       0.0220       0.0174
1160.00         0.7931       17.1495       2.0114       0.0200       0.0159
1190.00         0.7936       17.1595       2.0126       0.0180       0.0143
1220.00         0.7938       17.1645       2.0132       0.0170       0.0135
1250.00         0.7943       17.1745       2.0144       0.0150       0.0119
1280.00         0.7945       17.1796       2.0150       0.0140       0.0111
1310.00         0.7947       17.1846       2.0155       0.0130       0.0103
1340.00         0.7950       17.1896       2.0161       0.0120       0.0095
1370.00         0.7952       17.1946       2.0167       0.0110       0.0087
1400.00         0.7954       17.1997       2.0173       0.0100       0.0080
1430.00         0.7954       17.1997       2.0173       0.0100       0.0080
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1460.00       0.7957      17.2047       2.0179       0.0090       0.0072

PRESSURE IN CELL 3                                  1.0170 ATMOSPHERES

CORRELATION OF Q CURVES AS POLYNOMIALS IN TIME

BED NO.1
CORRELATION CONSTANTS
                                           B( 1) =     6.59727079E-01
                                           B( 2) =    -1.80543028E-03
                                           B( 3) =    -1.78389500E-05
                                           B( 4) =     1.38157107E-07
                                           B( 5) =    -4.32362217E-10
                                           B( 6) =     7.54037476E-13
                                           B( 7) =    -7.85644490E-16
                                           B( 8) =     4.85826790E-19
                                           B( 9) =    -1.64533921E-22
                                           B(10) =     2.35100204E-26

COMPARISON OF FIT WITH DATA

   TIME               COMPUTED          EXPERIMENTAL

   17.299            0.62383430        0.61682197
   20.000            0.61752134        0.61682197
   50.000            0.53964930        0.55040489
   80.000            0.45642506        0.46604356
  110.000            0.37670664        0.37663200
  140.000            0.30545699        0.29196978
  170.000            0.24489143        0.22937234
  200.000            0.19538049        0.19821931
  230.000            0.15614463        0.15993238
  260.000            0.12577464        0.13279313
  290.000            0.10260715        0.11022322
  320.000            0.08498239        0.08949627
  350.000            0.07140798        0.07448854
  380.000            0.06064859        0.05854496
  410.000            0.05176080        0.04780870
  440.000            0.04408762        0.03931209
  470.000            0.03722619        0.03387696
  500.000            0.03097926        0.02763832
  530.000            0.02529998        0.02215569
  560.000            0.02023523        0.01901272
  590.000            0.01587387        0.01743849
  620.000            0.01230683        0.01428451
  650.000            0.00959031        0.01270475
  680.000            0.00772860        0.01112316
  710.000            0.00666343        0.01033167
  740.000            0.00628050        0.00874729
  770.000            0.00640941        0.00716106
  800.000            0.00685368        0.00636725
  830.000            0.00740827        0.00557297
  860.000            0.00787964        0.00557297
  890.000            0.00811862        0.00557297
  920.000            0.00801714        0.00557297
  950.000            0.00755432        0.00557297
  980.000            0.00676864        0.00557297
 1010.000            0.00577084        0.00557297
 1040.000            0.00473037        0.00557297
 1070.000            0.00384530        0.00557297
 1100.000            0.00327741        0.00557297
 1130.000            0.00320190        0.00557297
 1160.000            0.00365508        0.00557297
 1190.000            0.00460720        0.00557297
 1220.000            0.00587731        0.00557297
 1250.000            0.00715607        0.00557297
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1280.000             0.00797145      0.00557297
1310.000             0.00801150      0.00557297
1340.000             0.00695560      0.00557297
1370.000             0.00492854      0.00557297
1400.000             0.00275511      0.00557297
1430.000             0.00259032      0.00557297
1460.000             0.00825240      0.00557297

INITIAL LOADING OF PROPANE, CELL NO.1        2.6430 MG-MOLS/GM.
PERCENT ERROR IN MASS BALANCE                4.4204

BED NO.2
CORRELATION CONSTANTS
                                        B( 1) =     5.94994634E-01
                                        B( 2) =     1.08423200E-03
                                        B( 3) =    -6.85988104E-06
                                        B( 4) =    -4.09215873E-08
                                        B( 5) =     2.61373848E-10
                                        B( 6) =    -5.91870731E-13
                                        B( 7) =     7.05440629E-16
                                        B( 8) =    -4.72072154E-19
                                        B( 9) =     1.68073075E-22
                                        B(10) =    -2.48296845E-26

COMPARISON OF FIT WITH DATA

   TIME                COMPUTED        EXPERIMENTAL

  17.299             0.61150853      0.61682197
  20.000             0.61364792      0.61682197
  50.000             0.62840062      0.61682197
  80.000             0.62581984      0.61539025
 110.000             0.60668585      0.60675884
 140.000             0.57346006      0.58683157
 170.000             0.52948545      0.54531781
 200.000             0.47839584      0.48127731
 230.000             0.42369898      0.41678650
 260.000             0.36850186      0.35813204
 290.000             0.31535026      0.30713044
 320.000             0.26615786      0.26237269
 350.000             0.22220293      0.21997279
 380.000             0.18417429      0.18581575
 410.000             0.15224995      0.15639400
 440.000             0.12619532      0.13207116
 470.000             0.10546984      0.11022322
 500.000             0.08933302      0.09247740
 530.000             0.07694256      0.07900881
 560.000             0.06744065      0.06767903
 590.000             0.06002445      0.05854496
 620.000             0.05399642      0.05165301
 650.000             0.04880116      0.04549678
 680.000             0.04404008      0.04163469
 710.000             0.03946964      0.03620899
 740.000             0.03498968      0.03309871
 770.000             0.03061673      0.02920070
 800.000             0.02644985      0.02685645
 830.000             0.02263770      0.02372444
 860.000             0.01933400      0.02137063
 890.000             0.01666917      0.01901272
 920.000             0.01471794      0.01743849
 950.000             0.01347767      0.01586242
 980.000             0.01287074      0.01428451
1010.000             0.01272681      0.01349486
1040.000             0.01283024      0.01191419
1070.000             0.01292671      0.01112316
1100.000             0.01275896      0.01033167
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1130.000              0.01214982      0.00953971
1160.000              0.01097295      0.00874729
1190.000              0.00929376      0.00795441
1220.000              0.00729873      0.00716106
1250.000              0.00536975      0.00716106
1280.000              0.00393795      0.00636725
1316.000              0.00363217      0.00636725
1340.000              0.00449036      0.00636725
1370.000              0.00663794      0.00557297
1400.000              0.00898632      0.00557297
1430.000              0.00922177      0.00557297
1460.000              0.00270089      0.00557297

INITIAL LOADING OF PROPANE, CELL NO.2          2.4119 MG-MOLS/GM.
PERCENT ERROR IN MASS BALANCE                 -4.7099

BED NO.3
CORRELATION CONSTANTS
                                      B( 1) =     6.43359333E-01
                                      B( 2) =    -1.64141883E-03
                                      B( 3) =     2.42935443E-05
                                      B( 4) =    -1.38742559E-07
                                      B( 5) =     3.59710577E-10
                                      B( 6) =    -5.17722636E-13
                                      B( 7) =     4.43524992E-16
                                      B( 8) =    -2.25528368E-19
                                      B( 9) =     6.28952211E-23
                                      B(10) =    -7.40698564E-27

COMPARISON OF FIT WITH DATA

  TIME                COMPUTED         EXPERIMENTAL

  17.299              0.62154762      0.61682197
  20.000              0.61919436      0.61682197
  50.000              0.60677259      0.61682197
  80.000              0.60963723      0.61682197
 110.000              0.61715916      0.61682197
 140.000              0.62245756      0.61586770
 170.000              0.62150721      0.61108338
 200.000              0.61239859      0.60434865
 230.000              0.59473237      0.59221472
 260.000              0.56913114      0.57449524
 290.000              0.53685312      0.55091230
 320.000              0.49949309      0.51585955
 350.000              0.45875800      0.46330140
 380.000              0.41630471      0.41162720
 410.000              0.37363011      0.36472990
 440.000              0.33200329      0.32148278
 470.000              0.29243085      0.28431775
 500.000              0.25564999      0.25059381
 530.000              0.22213869      0.22131992
 560.000              0.19214266      0.19478607
 590.000              0.16570865      0.17259002
 620.000              0.14272391      0.14857505
 650.000              0.12295677      0.12773090
 680.000              0.10609616      0.10948860
 710.000              0.09178854      0.09396543
 740.000              0.07966655      0.07900881
 770.000              0.06937916      0.06616104
 800.000              0.06060555      0.05701650
 830.000              0.05307081      0.04934775
 860.000              0.04655227      0.04395328
 890.000              0.04087643      0.04008674
 920.000              0.03592350      0.03543209
 950.000              0.03161512      0.03309871
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 980.000             0.02789211       0.02841974
1010.000             0.02471540       0.02607413
1040.000             0.02207445       0.02294029
1070.000             0.01991685       0.02137063
1100.000             0.01819780       0.01901272
1130.000             0.01685088       0.01743849
1160.000             0.01577413       0.01586242
1190.000             0.01486965       0.01428451
1220.000             0.01400496       0.01349486
1250.000             0.01310077       0.01191419
1280.000             0.01204027       0.01112316
1310.000             0.01081936       0.01033167
1340.000             0.00947040       0.00953971
1370.000             0.00818022       0.00874729
1400.000             0.00720008       0.00795441
1430.000             0.00699103       0.00795441
1460.000             0.00823867       0.00716106

INITIAL LOADING OF PROPANE, CELL NO.3          2.4657 MG-MOLS/GM.
PERCENT ERROR IN MASS BALANCE                 -2.5836

CONSTANTS FOR RATE EQUATION  1
                                        D( 1) =   2.39581573E-02
                                        D( 2) =  -6.61232311E-05
                                        D( 3) =  -6.53345102E-07
                                        D( 4) =   5.05995411E-09
                                        D( 5) =  -1.58351102E-11
                                        D( 6) =   2.76163504E-14
                                        D( 7) =  -2.87739456E-17
                                        D( 8) =   1.77932309E-20
                                        D( 9) =  -6.02599537E-24
                                        D(10) =   8.61045992E-28

CONSTANTS FOR RATE EQUATION  2
                                        D( 1) =  -2.36317372E-03
                                        D( 2) =   1.05492288E-04
                                        D( 3) =   4.00810540E-07
                                        D( 4) =  -6.53758794E-09
                                        D( 5) =   2.53260756E-11
                                        D( 6) =  -4.91347861E-14
                                        D( 7) =   5.44347274E-17
                                        D( 8) =  -3.49698135E-20
                                        D( 9) =   1.21424130E-23
                                        D(10) =  -1.76472735E-27

CONSTANTS FOR RATE EQUATION  3
                                        D( 1) =   1.78564951E-03
                                        D( 2) =  -1.00632428E-04
                                        D( 3) =   1.15020046E-06
                                        D( 4) =  -3.61160043E-09
                                        D( 5) =   3.63064247E-12
                                        D( 6) =   2.73758560E-15
                                        D( 7) =  -9.67005956E-18
                                        D( 8) =   9.10252297E-21
                                        D( 9) =  -3.88322031E-24
                                        D(10) =   6.43254977E-28
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REDUCTION OF DATA FOR BED NO. 1

DEPTH OF SILICA GEL TO MID-POINT              1.2300 CMS.

POINT NO. 1

TIME POINT OF FIT                           128.7811 SECS.
MASS FLOW RATE                                0.7749 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                0.2000
REYNOLDS NUMBER                               4.6411
SCHMIDT NUMBER                                0.8225
MASS TRANSFER COEFFICIENT                     0.0369 SEC-1
INTERFACE MOL FRACTION                        0.2143
SURFACE CONCENTRATION (TOTAL)                 3.1570 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID        3.0588 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE              11.9158 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL           D             ERROR           DERIV            CORR

  1         10.0000E-06    -2.7585E-01
  2          9.5238E-06    -2.9133E-01     3.2507E 04     -8.9622E-06
  3          1.8486E-05    -1.1666E-01     1.9489E 04     -5.9860E-06
  4          2.4472E-05    -6.4093E-02     8.7822E 03     -7.2981E-06
  5          3.1770E-05    -2.5298E-02     5.3158E 03     -4.7590E-06
  6          3.6529E-05    -8.1942E-03     3.5940E 03     -2.2800E-06
  7          3.8809E-05    -1.4986E-03

COMPUTED DIFFUSION COEFFICIENT            3.8809E-05 SQ CM/SEC


POINT NO. 2

TIME POINT OF FIT                            80.2120 SECS.
MASS FLOW RATE                                0.7551 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                0.4000
REYNOLDS NUMBER                               4.2504
SCHMIDT NUMBER                                0.8751
MASS TRANSFER COEFFICIENT                     0.0361 SEC-1
INTERFACE MOL FRACTION                        0.4214
SURFACE CONCENTRATION (TOTAL)                 3.0334 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID        2.9030 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE              16.4909 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL           D             ERROR           DERIV            CORR

  1          3.8809E-05    -1.2060E-03

COMPUTED DIFFUSION COEFFICIENT            3.8809E-05 SQ CM/SEC


POINT NO. 3

TIME POINT OF FIT                            68.8669 SECS.
MASS FLOW RATE                                0.7460 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                0.5000
REYNOLDS NUMBER                               4.1951
SCHMIDT NUMBER                                0.8760
MASS TRANSFER COEFFICIENT                     0.0359 SEC-1
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INTERFACE MOL FRACTION                          0.5236
SURFACE CONCENTRATION (TOTAL)                   2.9660 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID          2.8591 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE                17.6422 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL             D              ERROR            DERIV            CORR

   1          3.8809E-05     -3.0943E-02
   2          3.6961E-05     -3.7407E-02      3.4980E 03      -1.0694E-05
   3          4.7655E-05     -6.2408E-03      2.9144E 03      -2.1414E-06
   4          4.9796E-05     -1.4625E-03

COMPUTED DIFFUSION COEFFICIENT           4.9796E-05 SQ CM/SEC


POINT NO. 4

TIME POINT OF FIT                              49.1272 SECS.
MASS FLOW RATE                                  0.7290 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                  0.7000
REYNOLDS NUMBER                                 4.3210
SCHMIDT NUMBER                                  0.8311
MASS TRANSFER COEFFICIENT                       0.0358 SEC-1
INTERFACE MOL FRACTION                          0.7278
SURFACE CONCENTRATION (TOTAL)                   2.8113 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID          2.7756 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE                19.6481 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL             D              ERROR            DERIV            CORR

   1          4.9796E-05     -8.0230E-02
   2          4.7425E-05     -8.5495E-02      2.2202E 03      -3.8507E-05
   3          8.5932E-05     -3.2982E-02      1.3637E 03      -2.4185E-05
   4          1.1012E-04     -1.7838E-02      6.2615E 02      -2.8488E-05
   5          1.3861E-04     -6.6939E-03      3.9118E 02      -1.7112E-05
   6          1.5572E-04     -1.9639E-03

COMPUTED DIFFUSION COEFFICIENT           1.5572E-04 SQ CM/SEC
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REDUCTION OF DATA FOR BED NO. 2

DEPTH OF SILICA GEL TO MID-POINT            3.6900 CMS.

POINT NO. 1

TIME POINT OF FIT                         326.4326 SECS.
MASS FLOW RATE                              0.7535 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED              0.2000
REYNOLDS NUMBER                             4.5134
SCHMIDT NUMBER                              0.8227
MASS TRANSFER COEFFICIENT                   0.0364 SEC-1
INTERFACE MOL FRACTION                      0.2078
SURFACE CONCENTRATION (TOTAL)               3.1607 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID      3.0679 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE             6.3698 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL          D            ERROR          DERIV          CORR

   1       1.5572E-04    8.0484E-02
   2       1.6350E-04    8.1080E-02     7.6516E 01     1.0596E-03
   3       1.0900E-04    7.5069E-02     1.1029E 02     6.8066E-04
   4       7.2668E-05    6.5832E-02     2.5422E 02     2.5896E-04
   5       4.8445E-05    5.1501E-02     5.9166E 02     8.7045E-05
   6       3.2297E-05    2.9065E-02     1.3893E 03     2.0920E-05
   7       1.1377E-05   -9.9634E-02     6.1520E 03    -1.6195E-05
   8       2.7573E-05    1.7190E-02     7.2134E 03     2.3831E-06
   9       2.5189E-05    9.4217E-03     3.2597E 03     2.8903E-06
  10       2.2299E-05   -2.3184E-03

COMPUTED DIFFUSION COEFFICIENT          2.2299E-05 SQ CM/SEC

POINT NO. 2

TIME POINT OF FIT                         209.2422 SECS.
MASS FLOW RATE                              0.7137 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED              0.4000
REYNOLDS NUMBER                             4.0176
SCHMIDT NUMBER                              0.8754
MASS TRANSFER COEFFICIENT                   0.0351 SEC-1
INTERFACE MOL FRACTION                      0.4136
SURFACE CONCENTRATION (TOTAL)               3.0383 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID      2.8423 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE            10.2044 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL          D            ERROR          DERIV          CORR

   1       2.2299E-05    6.4867E-02
   2       2.3414E-05    7.0647E-02     5.1842E 03     1.3627E-05
   3       9.7867E-06   -6.8546E-02     1.0214E 04    -6.7109E-06
   4       1.6498E-05    2.4194E-02     1.3819E 04     1.7507E-06
   5       1.4747E-05    6.7538E-03     9.9616E 03     6.7798E-07
   6       1.4069E-05   -9.5206E-04

COMPUTED DIFFUSION COEFFICIENT          1.4069E-05 SQ CM/SEC
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POINT NO. 3

TIME POINT OF FIT                              189.0098 SECS.
MASS FLOW RATE                                   0.6953 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                   0.5000
REYNOLDS NUMBER                                  3.9100
SCHMIDT NUMBER                                   0.8763
MASS TRANSFER COEFFICIENT                        0.0347 SEC-1
INTERFACE MOL FRACTION                           0.5144
SURFACE CONCENTRATION (TOTAL)                    2.9723 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID           2.7949 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE                 10.4206 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL           D            ERROR           DERIV           CORR

   1        1.4069E-05    -1.4241E-02
   2        1.3399E-05    -2.1960E-02      1.1522E 04     -1.9060E-06
   3        1.5305E-05    -1.4487E-03

COMPUTED DIFFUSION COEFFICIENT           1.5305E-05 SQ CM/SEC

POINT NO. 4

TIME POINT OF FIT                              142.7455 SECS.
MASS FLOW RATE                                   0.6609 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                   0.7000
REYNOLDS NUMBER                                  3.9176
SCHMIDT NUMBER                                   0.8313
MASS TRANSFER COEFFICIENT                        0.0341 SEC-1
INTERFACE MOL FRACTION                           0.7146
SURFACE CONCENTRATION (TOTAL)                    2.8224 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID           2.6870 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE                  9.8705 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL           D            ERROR           DERIV           CORR

   1        1.5305E-05    -1.4043E-02
   2        1.4576E-05    -1.9631E-02      7.6681E 03     -2.5601E-06
   3        1.7136E-05    -1.6755E-03

COMPUTED DIFFUSION COEFFICIENT           1.7136E-05 SQ CM/SEC
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REDUCTION OF DATA FOR BED NO. 3

DEPTH OF SILICA GEL TO MID-POINT              6.1500 CMS.

POINT NO. 1

TIME POINT OF FIT                           515.6765 SECS.
MASS FLOW RATE                                0.7535 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                0.2000
REYNOLDS NUMBER                               4.5133
SCHMIDT NUMBER                                0.8230
MASS TRANSFER COEFFICIENT                     0.0364 SEC-1
INTERFACE MOL FRACTION                        0.2070
SURFACE CONCENTRATION (TOTAL)                 3.1611 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID        3.1194 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE               5.7324 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL           D             ERROR            DERIV            CORR

   1        1.7136E-05     -6.8556E-02
   2        1.6320E-05     -7.4435E-02      7.2045E 03      -1.0332E-05
   3        2.6652E-05     -2.7027E-02      4.5886E 03      -5.8901E-06
   4        3.2542E-05     -1.3847E-02      2.2376E 03      -6.1883E-06
   5        3.8730E-05     -4.4874E-03      1.5125E 03      -2.9668E-06
   6        4.1697E-05     -1.0265E-03

COMPUTED DIFFUSION COEFFICIENT            4.1697E-05 SQ CM/SEC


POINT NO. 2

TIME POINT OF FIT                           386.0540 SECS.
MASS FLOW RATE                                0.7139 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                0.4000
REYNOLDS NUMBER                               4.0186
SCHMIDT NUMBER                                0.8757
MASS TRANSFER COEFFICIENT                     0.0351 SEC-1
INTERFACE MOL FRACTION                        0.4113
SURFACE CONCENTRATION (TOTAL)                 3.0398 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID        2.9054 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE               8.5074 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL           D             ERROR            DERIV            CORR

   1        4.1697E-05      7.4038E-02
   2        4.3782E-05      7.6907E-02      1.3762E 03       5.5886E-05
   3        2.9188E-05      4.8429E-02      1.9514E 03       2.4818E-05
   4        4.3704E-06     -3.0771E-01      1.4350E 04      -2.1443E-05
   5        2.5813E-05      3.7432E-02      1.6096E 04       2.3256E-06
   6        2.3488E-05      2.8116E-02      4.0059E 03       7.0187E-06
   7        1.6469E-05     -1.4456E-02      6.0656E 03      -2.3833E-06
   8        1.8852E-05      3.2347E-03      7.4228E 03       4.3577E-07
   9        1.8417E-05      3.0896E-04

COMPUTED DIFFUSION COEFFICIENT            1.8417E-05 SQ CM/SEC


POINT NO. 3
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TIME POINT OF FIT                             341.7726 SECS.
MASS FLOW RATE                                  0.6955 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                  0.5000
REYNOLDS NUMBER                                 3.9111
SCHMIDT NUMBER                                  0.8766
MASS TRANSFER COEFFICIENT                       0.0347 SEC-1
INTERFACE MOL FRACTION                          0.5121
SURFACE CONCENTRATION (TOTAL)                   2.9739 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID          2.8183 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE                 8.7310 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL           D             ERROR            DERIV             CORR

  1        1.8417E-05     2.4712E-02
  2        1.9337E-05     3.0336E-02      6.1080E 03        4.9666E-06
  3        1.4371E-05    -7.1452E-03      7.5467E 03       -9.4680E-07
  4        1.5318E-05     1.5837E-03

COMPUTED DIFFUSION COEFFICIENT            1.5318E-05 SQ CM/SEC


POINT NO. 4

TIME POINT OF FIT                             277.5500 SECS.
MASS FLOW RATE                                  0.6615 MG-MOLS/SEC.
MOL FRACTION OF GAS CONSIDERED                  0.7000
REYNOLDS NUMBER                                 3.9211
SCHMIDT NUMBER                                  0.8316
MASS TRANSFER COEFFICIENT                       0.0341 SEC-1
INTERFACE MOL FRACTION                          0.7117
SURFACE CONCENTRATION (TOTAL)                   2.8248 MG-MOL/GM.
AVERAGE CONCENTRATION (TOTAL) ON SOLID          2.6954 MG-MOL/GM.
RATE OF ADSORPTION OF PROPYLENE                 7.8987 MMG-MOL/GM/SEC

RESULTS OF ITERATIVE DETERMINATION OF DIFFUSION COEFFICIENT

TRIAL           D             ERROR            DERIV             CORR

  1        1.5318E-05     3.7936E-03
  2        1.6083E-05     8.6103E-03      6.2891E 03        1.3691E-06
  3        1.4714E-05    -2.8080E-04

COMPUTED DIFFUSION COEFFICIENT            1.4714E-05 SQ CM/SEC


AVERAGE VALUE OF COMPUTED DIFF. COEFF.    3.6841E-05 SQ CM/SEC

END OF DATA PROCESSING RUN NO.  1
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TABLE VII

SUMMARY OF DATA PROCESSING RUNS

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate G	Bulk m.f. C_3H_6 y	Re	Sc	Mass Trans. Coeff. k_y	I.f. m.f. C_3H_6 y*	Surf. Conc. on Sol. s*	Avg. Conc. on Sol. m	Ads. Rate C_3H_6 $X10^6$ Q_A	Diff. Coeff. $X10^5$ D
1	3,7,9	1	128.9	.775	.800	4.64	.823	.0369	.786	3.157	3.059	11.9	3.88
			80.2	.755	.600	4.25	.875	.0361	.579	3.033	2.903	16.5	3.88
			68.9	.746	.500	4.195	.876	.0359	.476	2.966	2.859	17.6	4.93
			49.1	.729	.300	4.32	.831	.0358	.272	2.811	2.776	19.6	15.6
		2	326.4	.754	.800	4.51	.823	.0364	.792	3.161	3.068	6.37	2.23
			209.2	.714	.600	4.02	.875	.0351	.584	3.038	2.842	10.2	1.41
			189.0	.695	.500	3.91	.876	.0347	.486	2.972	2.795	10.4	1.53
			142.7	.661	.300	3.92	.831	.0341	.285	2.822	2.687	9.87	1.71
		3	515.7	.754	.800	4.51	.823	.0364	.793	3.161	3.119	5.73	4.16
			386.1	.714	.600	4.02	.876	.0351	.589	3.040	2.905	8.51	1.84
			341.8	.696	.500	3.91	.877	.0347	.483	2.974	2.818	8.73	1.53
			277.6	.662	.300	3.92	.832	.0341	.288	2.825	2.695	7.90	1.47
											avg. value of D		3.68
2	6,17	1	25.7	.866	.800	5.18	.832	.0389	.828	3.181	3.091	-24.7	..
			32.8	.840	.600	4.73	.875	.0380	.627	3.064	3.054	-22.1	..
			42.5	.828	.500	4.65	.876	.0377	.521	2.998	3.009	-18.9	48.4
			78.9	.806	.300	4.78	.831	.0376	.315	2.847	2.888	-11.2	8.92
		2	32.9	.948	.800	5.68	.823	.0406	.805	3.168	3.271	-4.65	.17
			78.6	.900	.600	5.07	.875	.0303	.611	3.054	3.192	-9.98	1.25
			103.3	.877	.500	4.93	.876	.0388	.511	2.939	3.142	-8.80	1.312
			195.8	.835	.300	4.94	.831	.0382	.306	2.839	3.004	-4.32	.93
		3	96.8	.950	.800	5.69	.823	.0407	.807	3.169	3.208	-6.55	4.14
			154.9	.900	.600	5.06	.876	.0393	.609	3.052	3.115	-7.14	3.27
			199.9	.877	.500	4.93	.877	.0388	.508	2.987	3.045	-6.50	3.26
			347.1	.835	.300	4.94	.832	.0382	.305	2.838	2.880	-3.59	2.71
											avg. value of D		2.88

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate	Bulk m.f. C_3H_6	Re	Sc	Mass. Trans. Coeff.	I.f. m.f. C_3H_6	Surf. Conc. on Sol.	Avg. Conc. on Sol.	Ads. Rate C_3H_6 X10^6	Diff. Coeff. X10^5
				G	y			k_y	y*	s*	m	Q_A	D
3	8,19	1	17.9	1.19	.800	7.11	.822	.0453	.832	3.183	3.113	-32.8	..
			24.3	1.15	.600	6.48	.875	.0442	.631	3.066	3.068	-29.2	..
			31.7	1.13	.500	6.39	.875	.0440	.528	3.001	3.022	-25.5	33.9
			59.3	1.11	.300	6.56	.831	.0437	.318	2.849	2.895	-15.7	11.4
		2	26.6	1.30	.800	7.79	.822	.0473	.807	3.169	3.46	-7.01	1.13
			53.5	1.23	.600	6.95	.875	.0457	.610	3.053	3.193	-9.80	1.22
			69.0	1.20	.500	6.76	.876	.0452	.511	2.989	3.158	-10.2	1.23
			148.4	1.15	.300	6.79	.831	.0444	.307	2.840	3.001	-6.53	1.29
		3	67.4	1.30	.800	7.81	.823	.0473	.809	3.169	3.210	-9.15	5.55
			105.1	1.23	.600	6.95	.875	.0457	.610	3.053	3.127	-9.90	3.79
			142.7	1.20	.500	6.77	.876	.0452	.509	2.988	2.047	-8.76	4.48
			259.9	1.15	.300	6.79	.831	.0444	.305	2.839	2.878	-4.44	3.52
											avg. value of D		3.73
4	10, 16, 18, 20	1	220.0	.396	.800	2.375	.823	.0267	.211	3.138	3.002	6.85	1.64
			158.2	.386	.600	2.174	.876	.0261	.584	3.016	2.888	8.65	2.09
			136.7	.382	.500	2.125	.877	.0260	.483	2.945	2.844	9.25	2.69
			96.7	.373	.300	2.10	.832	.0259	.280	2.796	2.755	10.3	7.38
		2	565.6	.385	.800	2.308	.823	.0263	.792	3.139	3.053	4.74	1.81
			434.7	.365	.600	2.054	.876	.0254	.588	3.018	2.885	6.28	1.39
			391.8	.356	.500	1.999	.877	.0251	.512	2.952	2.823	6.458	1.39
			306.7	.338	.300	2.002	.832	.0247	.288	2.802	2.700	6.04	1.52
		3	878.6	.385	.800	2.308	.823	.0263	.793	3.140	3.064	4.28	1.74
			737.9	.365	.600	2.054	.876	.0254	.590	3.019	2.902	5.62	1.44
			692.1	.356	.500	1.999	.877	.0251	.489	2.953	2.842	5.75	1.48
			597.0	.333	.300	2.002	.832	.0247	.289	2.803	2.720	5.38	1.71
											avg. value of D		2.19

1 Data Proc. Run No.	2 Info. from Runs	3 Col. No.	4 Time Point of Fit	5 Mol. Flow Rate G	6 Bulk m.f. C_3H_6 y	7 Re No.	8 Sc No.	9 Mass Trans. Coeff. k_y	10 I.f. m.f. C_3H_6 y*	11 Surf. Conc. on Sol. s*	12 Avg. Conc. on Sol. m	13 Ads. Rate C_3H_6 $X10^6$ q_A	14 Diff. Coeff. $X10^5$ D
5	11	1	34.9	1.57	.800	9.40	.775	.0539	.836	4.985	4.860	-38.9	..
			45.9	1.55	.600	8.72	.824	.0531	.632	4.908	4.818	-34.0	..
			68.8	1.53	.400	8.77	.811	.0529	.425	4.813	4.745	-25.9	..
			121.8	1.51	.200	9.52	.738	.0534	.215	4.688	4.635	-14.6	..
		2	60.9	1.64	.800	9.81	.775	.0550	.814	4.978	4.999	-15.7	3.60
			93.2	1.60	.600	9.01	.824	.0539	.617	4.901	4.939	-18.6	3.78
			148.5	1.57	.400	8.957	.811	.0535	.416	4.808	4.834	-16.2	6.09
			300.0	1.53	.200	9.62	.739	.0536	.204	4.681	4.682	-4.08	6.09
		3	138.4	1.64	.800	9.81	.775	.0550	.811	4.976	4.981	-11.8	6.10
			191.6	1.60	.600	9.01	.825	.9539	.625	4.899	4.909	-13.1	6.09
			265.1	1.57	.500	8.95	.811	.0534	.511	4.806	4.811	-11.6	6.09
			485.4	1.53	.200	9.62	.739	.0536	.204	4.681	4.640	-3.68	..
											avg. value of D		5.40
6	13	1	102.4	.797	.800	4.77	.773	.0390	.826	5.014	4.808	-20.2	..
			131.9	.788	.600	4.43	.823	.9384	.624	4.937	4.750	-17.9	..
			170.3	.779	.400	4.46	.810	.0383	.420	4.844	4.683	-15.1	..
			273.8	.771	.200	4.84	.737	.0386	.213	4.722	4.553	-9.21	..
		2	187.8	.832	.800	4.98	.773	.0398	.810	5.009	5.026	-7.74	3.10
			251.4	.813	.600	4.58	.823	.0390	.611	4.932	4.972	-8.25	3.10
			356.2	.796	.400	4.55	.810	.0387	.410	4.839	4.886	-7.14	3.10
			625.5	.779	.200	4.89	.737	.0388	.204	4.716	4.749	-2.86	3.10
		3	309.6	.832	.800	4.98	.774	.0398	.807	5.008	5.008	-5.43	..
			416.4	.814	.600	4.58	.823	.0390	.608	4.931	4.940	-6.32	3.10
			562.9	.795	.400	4.551	.810	.0387	.407	4.838	4.847	-5.49	3.10
			953.3	.779	.200	4.89	.737	.0388	.203	4.715	4.709	-1.85	..
											avg. value of D		3.10

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate	Bulk m.f. C_3H_6	Re No.	Sc No.	Mass Trans. Coeff.	I.f. m.f. C_3H_6	Surf. Conc. on Sol.	Avg. Conc. on Sol.	Ads. Rate C_3H_6 X10^6	Diff. Coeff. X10^5
				G	y			k_y	y*	s*	m	Q_A	D
7	21,23	1	38.6	.554	.800	3.32	.823	.0314	.822	3.168	3.099	-15.7	..
			59.1	.538	.600	3.03	.876	.0307	.620	3.050	3.032	-13.3	..
			74.7	.530	.500	2.98	.877	.0305	.519	2.985	2.987	-11.8	78.8
			129.1	.517	.300	3.06	.832	.0303	.313	2.835	2.867	-7.83	7.83
		2	60.4	.607	.800	3.64	.823	.0328	.804	3.158	3.242	-3.25	.375
			138.3	.577	.600	3.24	.876	.0317	.607	3.042	3.164	-4.957	.844
			167.5	.562	.500	3.16	.877	.0313	.508	2.977	3.131	-4.96	.715
			303.9	.535	.300	3.17	.832	.0308	.305	2.829	2.999	-3.29	.598
		3	164.4	.609	.800	3.64	.823	.0328	.806	3.159	3.191	-4.14	3.42
			252.9	.577	.600	3.25	.876	.0317	.607	3.041	3.102	-4.54	2.22
			313.2	.562	.500	3.16	.877	.0313	.507	2.977	3.040	-4.32	2.01
			515.4	.535	.300	3.17	.932	.0308	.305	2.828	2.875	-2.84	2.01
											avg. value of D		2.00
8	22,24	1	85.3	1.14	.800	6.83	.822	.0444	.785	3.156	3.017	15.4	3.69
			49.5	1.11	.600	6.25	.875	.0435	.576	3.032	2.865	22.5	4.10
			40.0	1.10	.500	6.18	.875	.0433	.472	2.963	2.814	24.9	4.99
			27.3	1.07	.300	6.37	.832	.0431	.266	2.807	2.737	28.6	12.3
		2	221.9	1.11	.800	6.65	.822	.0438	.792	3.161	2.975	7.49	1.35
			133.2	1.05	.600	5.92	.875	.0223	.587	3.039	2.781	11.6	1.11
			107.1	1.02	.500	5.76	.876	.0418	.486	2.973	2.710	12.2	.95
			69.4	.974	.300	5.77	.831	.0411	.287	2.823	2.609	10.9	.71
		3	353.4	1.11	.800	6.65	.823	.0438	.794	3.162	3.100	5.88	3.02
			243.3	1.05	.600	5.92	.876	.0423	.589	3.040	2.900	9.86	2.12
			205.9	1.02	.500	5.76	.876	.0418	.488	2.974	2.814	10.5	1.79
			148.5	.975	.300	5.78	.832	.0411	.288	2.825	2.681	9.60	1.53
											avg. value of D		3.14

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate	Bulk m.f. C_3H_6	Re No.	Sc No.	Mass Trans. Coeff.	I.f. m.f. C_3H_6	Surf. Conc. on Sol.	Avg. Conc. on Sol.	Ads. Rate C_3H_6 X10^6	Diff. Coeff. X10^5
				G	y			k_y	y*	s*	m	Q_A	D
9	25	1	28.3	2.15	.800	12.8	.781	.0622	.844	4.843	4.636	-55.4	..
			34.4	2.12	.600	11.9	.831	.0613	.639	4.762	4.601	-47.1	..
			45.5	2.09	.400	11.9	.818	.0611	.429	4.774	4.550	-34.8	..
			77.5	2.07	.200	12.9	.745	.0616	.213	4.532	4.465	-14.9	..
		2	33.0	2.25	.800	13.4	.782	.0636	.805	4.829	4.905	-6.78	.16
			63.4	2.19	.600	12.3	.831	.0623	.612	4.751	4.866	-14.3	1.00
			69.7	2.14	.400	12.2	.818	.0617	.413	4.655	4.856	-14.9	.42
			177.6	2.09	.200	13.1	.745	.0619	.208	4.529	4.690	-9.62	.83
		3	90.3	2.25	.800	13.4	.782	.0636	.813	4.832	4.828	-17.4	..
			122.9	2.19	.600	12.3	.832	.0623	.614	4.752	4.762	-17.6	8.28
			101.0	2.14	.400	12.2	.819	.617	.415	4.656	4.806	-17.8	1.24
			317.5	2.09	.200	13.1	.750	.0619	.206	4.527	4.506	-6.76	..
										avg. value of D			2.00
10	26,28	1	84.3	.781	.800	4.29	.862	.0375	.787	2.216	2.095	11.9	4.51
			53.5	.751	.600	3.88	.917	.0365	.581	2.083	1.958	16.1	5.44
			36.4	.726	.400	3.81	.903	.0360	.375	1.938	1.862	19.0	10.6
			25.6	.705	.200	4.06	.822	.0369	.170	1.768	1.792	21.1	..
		2	204.5	.747	.800	4.11	.862	.0367	.793	2.220	2.027	6.26	1.47
			136.3	.688	.600	3.55	.920	.0350	.589	2.089	1.859	8.95	1.47
			96.9	.637	.400	3.35	.903	.0338	.387	1.947	1.742	9.39	1.35
			68.2	.593	.200	3.42	.822	.0331	.187	1.784	1.660	8.23	1.62
		3	223.9	.747	.800	4.11	.863	.0367	.793	2.220	2.180	6.25	5.99
			238.9	.688	.600	3.55	.918	.0350	.582	2.088	1.964	9.31	3.23
			192.8	.637	.400	3.34	.904	.0338	.387	1.947	1.823	9.33	2.77
			152.3	.593	.200	3.42	.823	.0331	.188	1.785	1.712	7.67	3.49
										avg. value of D			3.81

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate	Bulk m.f. C_3H_6	Re No.	Sc No.	Mass Trans Coeff.	I.f. m.f. C_3H_6	Surf. Conc. on Sol.	Avg. Conc. on Sol.	Ads. Rate C_3H_6 X10^6	Diff. Coeff. X10^5
				G	y			k_y	y*	s*	m	Q_A	D
11	27,29	1	39.9	.466	.800	2.56	.863	.0293	.819	2.226	2.106	-14.2	..
			57.7	.446	.600	2.30	.919	.0283	.618	2.098	2.032	-11.7	..
			82.1	.427	.400	2.24	.904	.0278	.415	1.957	1.951	-8.94	..
			138.1	.411	.200	2.37	.823	.0277	.209	1.792	1.831	-4.91	5.44
		2	84.1	.536	.800	2.95	.863	.0313	.806	2.218	2.279	-4.89	2.99
			124.8	.492	.600	2.54	.919	.0297	.608	2.091	2.209	-5.61	1.79
			184.7	.456	.400	2.39	.904	.0287	.408	1.952	2.105	-5.04	1.35
			341.4	.425	.200	2.45	.823	.0282	.204	1.787	1.939	-1.81	.72
		3	157.7	.534	.800	2.94	.863	.0312	.806	2.217	2.244	-4.37	4.99
			224.8	.492	.600	2.54	.919	.0297	.607	2.090	2.146	-4.62	2.88
			334.7	.456	.400	2.39	.904	.0287	.406	1.951	1.993	-3.86	3.65
			597.0	.425	.200	2.45	.823	.0282	.203	1.788	1.761	-1.88	..
											avg. value of D		2.98
12	31,33	1	22.0	.907	.800	4.92	.867	.0494	.827	2.143	2.001	-27.5	..
			32.0	.864	.600	4.42	.923	.0391	.625	2.015	1.917	-23.0	..
			51.5	.826	.400	4.29	.908	.0382	.420	1.873	1.791	-16.4	..
			92.3	.794	.200	4.53	.827	.0381	.211	1.709	1.630	-8.45	..
		2	40.3	1.04	.800	5.68	.868	.0432	.806	2.130	2.195	-6.77	2.91
			57.9	.956	.600	4.89	.923	.0410	.608	2.003	2.152	-7.77	1.36
			133.8	.884	.400	4.60	.909	.0396	.408	1.865	2.011	-6.77	1.82
			222.4	.821	.200	4.69	.827	.0388	.203	1.702	1.855	-2.39	1.00
		3	74.1	1.04	4.800	5.68	.868	.0432	.807	2.131	2.179	-7.55	5.40
			118.4	.958	.600	4.90	.923	.0410	.609	2.004	2.960	-8.14	5.40
			188.4	.884	.400	4.60	.909	.0396	.407	1.864	1.893	-6.02	7.71
			355.5	.821	.200	4.69	.828	.0388	.204	1.702	1.675	-2.76	..
											avg. value of D		3.66

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate	Bulk m.f. C_3H_6	Re No.	Sc No.	Mass Trans. Coeff.	I.f. m.f. C_3H_6	Surf. Conc. on Sol.	Avg. Conc. on Sol.	Ads. Rate C_3H_6 X10^6	Diff. Coeff. X10^5
				G	y			k_y	y*	s*	m	Q_A	D
13	12	1	164.5	1.34	.800	8.01	.773	.0500	.786	4.999	5.075	14.3	..
			94.8	1.32	.600	7.44	.823	.0493	.575	4.917	4.942	23.8	..
			67.2	1.31	.400	7.49	.809	.0491	.367	4.816	4.863	30.9	..
			58.3	1.30	.200	8.14	.737	.0496	.164	4.687	4.833	33.9	..
		2	392.5	1.32	.800	7.92	.773	.0497	.792	5.002	4.907	7.99	1.22
			236.1	1.29	.600	7.28	.823	.0487	.586	4.921	4.738	13.4	.88
			161.1	1.27	.400	7.23	.810	.0483	.382	4.824	4.618	16.8	.67
			103.9	1.24	.200	7.77	.737	.0483	.184	4.702	4.519	15.0	.13
		3	627.4	1.32	.800	7.92	.773	.0497	.793	5.003	4.983	6.56	2.49
			415.2	1.29	.600	7.28	.823	.9487	.591	4.923	4.812	9.06	1.35
			297.3	1.27	.400	7.23	.810	.0483	.389	4.828	4.691	10.0	1.00
			207.1	1.24	.200	7.78	.737	.0485	.191	4.707	4.604	7.89	.72
											avg. avlue of		1.06
14	36,38	1	71.8	.627	.800	3.18	.900	.0342	.788	1.525	1.464	11.5	10.0
			50.0	.595	.600	2.84	.958	.0330	.582	1.394	1.351	14.5	16.6
			38.1	.569	.400	2.76	.943	.0324	.377	1.259	1.268	16.4	..
			29.3	.548	.200	2.91	.859	.0323	.173	1.111	1.206	17.6	..
		2	176.6	.587	.800	2.977	.901	.0331	.792	1.527	1.412	7.62	3.97
			219.9	.521.	.600	2.48	.958	.0310	.588	1.398	1.243	9.34	3.14
			98.4	.468	.400	2.27	.943	.0295	.386	1.265	1.121	3.90	2.62
			75.0	.424	.200	2.26	.859	.0285	.187	1.122	1.041	7.32	3.46
		3	292.1	.587	.800	3.00	.901	.0331	.793	1.528	1.522	6.76	31.1
			227.4	.521	.600	2.48	.959	.0310	.589	1.398	1.313	8.35	5.42
			191.7	.469	.400	2.27	.944	.0295	.388	1.266	1.190	7.90	5.42
			158.7	.425	.200	2.26	.859	.0285	.189	1.123	1.090	6.42	9.03
											avg. value of D		6.63

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate	Bulk $\bar{m}$.f. C_3H_6	Re No.	Sc No.	Mass Trans. Coeff.	I.f. m.f. C_3H_6	Surf. Conc. on Sol.	Avg. Conc. on Sol.	Ads. Rate C_3H_6 X10^6	Diff. Coeff. X10^5
				G	y			k_y	y*	s*	m	Q_A	D
15	35,37	1	19.8	1.04	.800	5.29	.900	.0437	.828	1.540	1.288	-33.6	..
			27.5	.970	.600	4.63	.958	.0418	.626	1.422	1.101	-27.2	..
			38.2	.914	.400	4.43	.943	.0407	.422	1.289	1.086	-20.2	..
			65.7	.868	.200	4.62	.859	.0403	.212	1.141	.922	-9.82	..
		2	31.7	1.24	.800	6.31	.900	.0475	.807	1.537	1.617	-8.67	3.13
			52.4	1.10	.600	5.27	.958	.0445	.610	1.412	1.532	-10.4	3.76
			75.7	.995	.400	4.82	.943	.0424	.410	1.281	1.435	-9.25	3.02
			156.6	.905	.200	4.82	.860	.0411	.203	1.134	1.249	-2.62	1.98
		3	55.9	1.24	.800	6.30	.901	.0475	.808	1.538	1.583	-10.7	10.8
			85.9	1.11	.600	5.28	.958	.0445	.610	1.412	1.445	-10.6	15.1
			113.4	.996	.400	4.83	.943	.0424	.407	1.279	1.270	-6.93	..
			244.8	.905	.200	4.81	.859	.0411	.204	1.135	1.071	-3.048	..
											avg. value	of D	6.30
16	45,47	1	94.5	.843	.800	5.05	.823	.0384	.775	3.132	3.054	21.7	8.52
			79.2	.821	.600	4.62	.876	.0376	.510	3.009	2.974	23.8	20.5
			73.2	.812	.500	4.56	.876	.0374	.468	2.941	2.941	24.5	..
			62.8	.793	.300	4.70	.831	.0372	.266	2.786	2.082	25.2	..
		2	232.9	.820	.800	4.91	.823	.0379	.777	3.133	3.013	19.4	5.05
			207.6	.776	.600	4.37	.876	.0366	.572	3.010	2.892	21.7	5.33
			197.4	.756	.500	4.25	.877	.0361	.471	2.943	2.842	21.8	6.05
			180.2	.719	.300	4.26	.832	.0355	.270	.2790	2.757	20.9	18.1
		3	374.1	.820	.800	4.91	.823	.0379	.774	3.131	3.097	22.5	19.6
			247.5	.776	.600	4.37	.876	.0366	.569	3.008	2.954	23.8	13.7
			337.1	.756	.500	4.25	.877	.0361	.469	2.941	2.898	23.5	15.6
			326.5	.718	.300	4.26	.832	.0355	.268	2.787	2.842	22.8	..
											avg. value	of D	12.4

1 Data Proc. Run No.	2 Info. from Runs	3 Col. No.	4 Time Point of Fit	5 Mol. Flow Rate G	6 Bulk m.f. C_3H_6 y	7 Re	8 Sc	9 Mass Trans. Coeff. k_y	10 I.f. m.f. C_3H_6 y*	11 Surf. Conc. on Sol. s*	12 Avg. Conc. on Sol. m	13 Ads. Rate C_3H_6 Q_A	14 Diff. Coeff. X10^5 D
17	46	1	36.8	.942	.800	5.64	.823	.0405	.830	3.163	2.975	-27.8	..
			49.7	.914	.600	5.14	.876	.0396	.629	3.045	2.898	-24.6	..
			56.3	.902	.500	5.07	.876	.0396	.528	2.981	2.862	-23.0	..
			77.0	.878	.300	5.20	.831	.0390	.324	2.834	2.764	-18.6	..
		2	103.7	1.02	.800	6.19	.823	.0424	.816	3.155	3.081	-15.4	..
			128.0	.980	.600	5.51	.876	.0409	.618	3.039	2.993	-16.1	..
			157.9	.956	.500	5.37	.877	.0404	.510	2.975	2.884	-15.7	..
			230.8	.909	.300	5.39	.832	.0398	.315	2.827	2.650	-11.9	..
		3	193.5	1.04	.800	6.21	.823	.0424	.800	2.151	3.100	-9.35	..
			247.8	.981	.600	5.52	.876	.0410	.611	3.035	2.978	-10.0	..
			283.9	.956	.500	5.37	.877	.0404	.511	2.970	2.897	-9.40	..
			389.1	.909	.300	5.39	.832	.0398	.308	2.820	2.711	-5.89	..
											avg. value of D		..
18	48	1	72.8	.938	.800	5.62	.803	.0411	.822	4.174	3.498	-50.4	..
			86.7	.922	.600	5.19	.855	.0404	.620	4.080	3.402	-44.2	..
			108.6	.907	.400	5.19	.8411	.0402	.418	3.968	3.316	-37.9	..
			135.5	.892	.200	5.60	.766	.0404	.212	3.825	3.156	-24.2	..
		2	166.2	.996	.800	5.97	.803	.0423	.806	4.167	4.667	-14.4	..
			212.8	.965	.600	5.43	.855	.0412	.611	4.075	4.532	-23.8	.13
			260.2	.934	.400	5.24	.841	.0414	.414	3.966	4.343	-29.5	.99
			360.4	.906	.200	5.69	.766	.0407	.216	3.828	3.864	-33.4	13.8
		3	292.5	.997	.800	5.97	.804	.0423	.805	4.167	4.114	-10.8	..
			366.8	.965	.600	5.43	.855	.0413	.606	4.042	3.983	-12.4	..
			437.5	.934	.400	5.34	.841	.0407	.405	3.961	3.858	-11.0	..
			568.1	.906	.200	5.69	.766	.0407	.202	3.817	3.699	-5.14	
											avg. value of D		5.00

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate G	Bulk m.f. C_3H_6 y	Re	Sc	Mass. Trans. Coeff. k_y	I.f. m.f. C_3H_6 y^*	Surf. Conc. on Sol. s*	Avg. Conc. on Sol. m	Ads. Rate C_3H_6 Q_A	Diff. Coeff. $X10^5$ D
19	14	1	107.9	1.19	.800	7.11	.802	.0460	.784	4.182	4.077	15.2	2.86
			68.1	1.17	.600	6.57	.854	.0453	.575	4.082	3.968	22.5	3.77
			51.8	1.15	.400	6.58	.840	.0451	.370	3.964	3.910	26.5	7.69
			37.9	1.13	.200	7.13	.765	.0454	.165	3.812	3.852	30.5	..
		2	277.2	1.16	.800	6.99	.803	.9457	.794	4.186	3.881	5.63	.29
			116.2	1.13	.600	6.36	.854	.0445	.592	4.090	3.712	7.58	.090
			85.7	1.09	.400	6.26	.840	.0440	.492	3.978	3.680	6.55	.090
			63.5	1.06	.200	6.67	.765	.0440	.194	3.835	3.660	5.17	.099
		3	464.4	1.17	.800	6.99	.803	.0457	.796	4.187	3.963	3.21	.305
			237.3	1.13	.600	6.37	.854	.0445	.593	4.090	3.802	6.62	.305
			144.9	1.09	.400	6.26	.841	.0440	.392	3.978	3.708	6.70	.173
			89.1	1.06	.200	6.67	.765	.0439	.194	3.836	3.659	4.85	.081
											avg. value of D		1.15
20	15	1	38.2	1.28	.800	7.67	.802	.0477	.834	4.222	4.048	-34.6	..
			52.1	1.26	.600	7.09	.853	.0469	.631	4.028	3.983	-29.6	..
			68.6	1.24	.400	7.08	.840	.0467	.427	4.017	3.918	-24.4	..
			108.5	1.22	.200	7.65	.764	.0470	.217	3.874	3.804	-15.4	..
		2	64.1	1.36	.800	8.15	.802	.0491	.807	4.209	4.260	-6.69	1.00
			85.3	1.32	.600	7.40	.853	.0479	.608	4.117	4.237	-7.94	.51
			121.5	1.27	.400	7.29	.840	.0473	.410	4.007	4.192	-8.85	.51
			277.9	1.23	.200	7.77	.764	.0473	.206	3.865	4.018	-5.54	.70
		3	89.3	1.36	.800	8.14	.802	.0491	.806	4.209	4.275	-6.39	.70
			146.7	1.31	.600	7.41	.854	.0479	.609	4.117	4.210	-8.50	1.14
			237.2	1.28	.400	7.30	.840	.0473	.408	4.006	4.100	-7.55	1.44
			463.8	1.23	.200	7.76	.765	.0473	.203	3.863	3.938	-2.93	1.06
											avg. value of D		.76

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate	Bulk m.f. C_3H_6	Re	Sc	Mass. Trans. Coeff.	I.f. m.f. C_3H_6	Surf. Conc. on Sol.	Avg. Conc. on Sol.	Ads. Rate C_3H_6	Diff. Coeff. X10^5
				G	y			k_y	y*	s*	m	Q_A	D
21	30	1	120.5	.458	.800	2.49	.868	.0290	.789	2.119	1.963	8.09	2.35
			87.4	.440	.600	2.25	.923	.0282	.584	1.988	1.863	10.1	3.51
			63.4	.425	.400	2.21	.909	.0278	.380	1.844	1.777	11.5	7.29
			43.6	.412	.200	2.35	.828	.0278	.177	1.679	1.798	12.6	..
		2	308.9	.437	.800	2.38	.868	.0284	.792	2.121	2.009	5.77	2.61
			238.5	.401	.600	2.05	.923	.027	.588	1.990	1.854	7.34	2.21
			181.1	.370	.400	1.92	.909	.0260	.387	1.849	1.712	7.29	1.95
			134.4	.344	.200	1.96	.828	.0255	.188	1.689	1.608	5.88	2.41
		3	502.1	.437	.800	2.38	.868	.0284	.793	2.122	2.044	4.97	2.83
			413.7	.401	.600	2.04	.924	.0270	.589	1.991	1.875	6.44	2.21
			347.0	.370	.400	1.92	.909	.0260	.489	1.850	1.730	6.30	2.21
			289.6	.343	.200	1.96	.828	.0255	.190	1.690	1.621	5.02	2.58
											avg. value of D		2.92
22	34	1	114.1	.947	.800	5.15	.851	.0417	.785	3.023	3.010	13.9	15.6
			76.6	.923	.600	4.72	.905	.0409	.578	2.907	2.873	19.2	15.6
			57.9	.902	.400	4.69	.891	.0405	.372	2.775	2.787	22.3	..
			44.4	.883	.200	5.04	.811	.0406	.169	2.611	2.717	24.6	..
		2	279.1	.921	.800	5.02	.851	.0412	.792	3.027	2.929	7.69	2.72
			186.4	.874	.600	4.47	.906	.0398	.546	2.913	2.729	11.5	1.79
			137.3	.831	.400	4.31	.891	.0389	.385	2.783	2.600	11.8	1.38
			97.6	.792	.200	4.52	.812	.0386	.186	2.627	2.501	10.1	1.38
		3	440.1	.921	.800	5.02	.851	.0412	.793	3.027	3.090	6.64	..
			324.3	.874	.600	4.47	.906	.0398	.586	2.912	2.862	10.8	5.44
			265.2	.831	.400	4.32	.891	.0389	.386	2.784	2.715	11.2	5.44
			207.5	.792	.200	4.52	.812	.0386	.186	2.628	2.579	9.47	5.44
											avg. value of D		6.08

1 Data Proc. Run No.	2 Info. from Runs	3 Col. No.	4 Time Point of Fit	5 Mol. Flow Rate G	6 Bulk m.f. C_3H_6 y	7 Re	8 Sc	9 Mass Trans. Coeff. k_y	10 I.f. m.f. C_3H_6 y*	11 Surf. Conc. on Sol. s*	12 Avg. Conc. on Sol. m	13 Ads. Rate C_3H_6 Q_A	14 Diff. Coeff. X10^5 D
23	49,51	1	78.3	.607	.800	3.32	.866	.0333	.792	2.161	2.045	17.5	6.21
			66.8	.584	.600	2.99	.921	.0323	.591	2.032	1.976	18.9	13.4
			60.9	.564	.400	2.94	.907	.0319	.390	1.891	1.939	19.3	..
			55.5	.547	.200	3.13	.826	.0318	.189	1.728	1.905	19.4	..
		2	186.5	.580	.800	3.17	.866	.0325	.807	2.162	1.887	15.3	2.31
			165.3	.533	.600	2.73	.922	.0309	.609	2.031	1.774	16.9	2.31
			150.6	.492	.400	2.56	.907	.0298	.390	1.892	1.693	16.4	2.66
			144.3	.457	.200	2.62	.826	.0292	.190	1.729	1.660	15.7	7.88
		3	301.8	.580	.800	3.17	.877	.0325	.792	2.161	2.043	17.2	5.72
			281.0	.533	.600	2.74	.922	.0309	.591	2.032	1.922	18.1	6.56
			265.7	.492	.400	2.57	.907	.0299	.390	1.891	1.833	17.3	11.0
			254.1	.450	.200	2.62	.827	.0292	.190	1.729	1.770	15.9	..
											avg. value of D		6.45
24	50	1	35.9	.746	.800	4.07	.866	.0367	.810	2.164	1.937	-24.3	..
			49.5	.711	.600	3.65	.921	.0356	.609	2.036	1.836	-20.8	..
			65.8	.681	.400	3.55	.907	.0349	.409	1.896	1.760	-17.2	..
			89.4	.655	.200	3.75	.826	.0347	.207	1.736	1.022	-12.3	..
		2	83.7	.856	.800	4.67	.866	.0392	.804	2.160	2.168	-11.1	23.2
			122.1	.787	.600	4.04	.922	.0373	.605	2.033	2.018	-12.1	..
			161.7	.728	.400	3.79	.907	.0360	.405	1.894	1.868	-10.6	..
			230.6	.677	.200	3.88	.826	.0353	.203	1.733	1.677	-6.30	..
		3	149.4	.858	.800	4.68	.866	.0393	.802	2.160	2.112	-8.38	..
			203.4	.788	.600	4.05	.922	.0374	.604	2.032	1.959	-8.40	..
			258.7	.728	.400	3.80	.907	.0361	.403	1.892	1.821	-6.36	..
			366.9	.677	.200	3.88	.825	.0353	.202	1.731	1.662	-3.17	..
											avg. value of D		..

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate	Bulk m.f. C_3H_6	Re	Sc	Mass. Trans. Coeff.	I.f. m.f. C_3H_6	Surf. Conc. on Sol.	Ave. Conc. on Sol.	Ads. Rate C_3H_6	Diff. Coeff. X10^5
				G	y			k_y	y*	s*	m	Q_A	D
25	52	1	64.2	.551	.800	1.38	.823	.0491	.806	3.140	2.961	-17.1	..
			87.1	.534	.600	1.25	.876	.0479	.606	3.021	2.876	-15.3	..
			110.6	.520	.400	1.24	.862	.0474	.405	2.886	2.799	-13.3	..
			149.8	.307	.200	1.33	.785	.0475	.204	2.721	2.693	-10.1	..
		2	174.6	.605	.800	1.51	.824	.0514	.803	3.140	3.092	-8.86	..
			233.4	.573	.600	1.35	.876	.0497	.603	3.020	2.965	-9.71	..
			311.4	.545	.400	1.20	.862	.0485	.403	2.884	2.797	-8.77	..
			436.1	.519	.200	1.36	.785	.0480	.202	2.719	2.594	-5.30	..
		3	309.8	.696	.800	1.514	.824	.0514	.802	3.138	3.104	-5.66	..
			403.7	.574	.600	1.135	.876	.0496	.602	3.019	2.975	-6.04	..
			527.2	.545	.400	1.300	.863	.0485	.402	2.883	2.818	-4.83	..
			436.6	.519	.200	1.359	.785	.0480	.201	2.718	2.645	-2.48	..
											avg. value of D		..
26	53	1	152.2	.505	.800	1.26	.823	.0471	.795	3.143	3.040	13.5	.776
			131.9	.492	.699	1.16	.876	.0460	.595	3.024	2.975	14.5	1.35
			113.8	.481	.400	1.15	.862	.0456	.606	2.887	2.914	15.1	..
			94.6	.470	.200	1.23	.785	.0458	.194	2.721	2.847	15.2	..
		2	367.3	.491	.800	1.23	.823	.0464	.796	3.144	2.953	11.5	.34
			332.6	.465	.600	1.09	.876	.0447	.595	3.024	2.856	12.9	.34
			299.9	.442	.400	1.05	.862	.0437	.395	2.888	2.758	12.9	.44
			264.8	.420	.200	1.09	.785	.9433	.195	2.723	2.658	11.5	.76
		3	570.2	.491	.800	1.23	.824	.0464	.795	3.143	3.057	14.1	.76
			537.9	.465	.600	1.09	.876	.9447	.594	3.024	2.949	14.9	.95
			508.9	.442	.400	1.05	.862	.0437	.394	2.887	2.851	14.5	1.44
			476.9	.420	.200	1.10	.785	.9433	.194	2.722	2.749	13.0	..
											avg. value of D		.80

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Data Proc. Run No.	Info. from Runs	Col. No.	Time Point of Fit	Mol. Flow Rate G	Bulk m.f. C_3H_6 y	Re	Sc	Mass Trans. Coeff. k_y	I.f. m.f. C_3H_6 y*	Surf. Conc. on Sol. s*	Avg. Conc. on Sol. m	Ads. Rate C_3H_6 Q_A	Diff. Coeff. X105 D
27	56	1	30.8	.877	.800	2.19	.823	.0616	.813	3.153	3.031	-25.9	..
			44.7	.851	.600	1.99	.875	.0601	.611	3.035	2.954	-22.0	..
			61.6	.828	.400	1.98	.862	.0595	.410	2.899	2.877	-17.9	..
			98.2	.807	.200	2.11	.785	.0596	.207	2.733	2.755	-11.6	2.04
		2	72.4	.965	.800	2.41	.823	.0645	.805	3.149	3.186	-10.6	2.04
			115.2	.913	.600	2.14	.876	.0622	.606	3.031	3.072	-12.1	2.04
			174.6	.868	.400	2.07	.862	.0608	.406	2.896	2.917	-10.3	2.04
			286.7	.826	.200	2.16	.785	.0603	.203	2.730	2.716	-5.71	..
		3	144.9	.965	.800	2.41	.823	.0645	.804	3.148	3.123	-8.63	..
			219.4	.914	.600	2.15	.876	.0622	.605	3.031	2.962	-9.59	..
			323.2	.868	.400	2.07	.862	.0608	.404	2.895	2.758	-7.41	..
			535.5	.826	.200	2.16	.785	.0603	.202	2.729	2.502	-3.98	..
										avg. value of D			2.04
28	57	1	114.9	.657	.800	1.643	.823	.0535	.792	3.142	2.993	14.6	.56
			96.1	.641	.600	1.504	.876	.0524	.590	3.021	2.926	16.4	.87
			77.5	.625	.400	1.492	.862	.0519	.389	2.884	2.853	17.8	2.45
			54.9	.612	.200	1.602	.785	.0521	.187	2.715	2.758	19.1	..
		2	306.3	.639	.800	1.597	.823	.0528	.793	3.142	3.059	11.9	.90
			258.0	.605	.600	1.420	.876	.0509	.591	3.022	2.914	13.9	.70
			221.6	.575	.400	1.371	.862	.0498	.391	2.885	2.797	13.8	.70
			178.4	.547	.200	1.434	.785	.0493	.192	2.720	2.671	11.3	.97
		3	502.6	.639	.800	1.597	.823	.0528	.793	3.142	3.145	11.8	..
			449.3	.605	.600	1.421	.876	.0509	.591	3.022	2.986	13.9	1.45
			401.3	.575	.400	1.371	.862	.0498	.391	2.885	2.832	13.6	1.45
			354.6	.547	.200	1.434	.785	.0493	.192	2.720	2.698	11.1	2.07
										avg. value of D			1.17

D. Summary of Data Processing Runs

The 25 useable data processing runs yielded an average value of the diffusion coefficient D of 3.65×10^{-5} sq. cm. per sec. The standard deviation was 2.59×10^{-5} and the 95% confidence limits on the expected value of D as computed by the Student "t" method(3) for 25 observations were determined as $(3.65 \pm 1.06) \times 10^{-5}$ sq. cm. per sec.

No effect of temperature or pressure was observed over the range of those variables obtainable in this apparatus. The averaged value of D reported is for all three particle sizes used and for all temperatures and pressures used.

DISCUSSION OF THE DATA PROCESSING RESULTS

A. Adsorptive Relative Volatility

Lewis *et al.*(14), from a series of equilibrium studies reported values of adsorptive relative volatility defined by Equation (46) for the system propylene-propane-silica gel of from .31 to .5. This was for a pressure range of 1 to 7.85 atm.

At atmospheric pressure and above, the reported relative volatility of .31 could not be used in the data reduction step because it consistently gave particle boundary propylene concentrations which indicated extremely high diffusion coefficients (i.e. - very flat, even inversely sloped gradients in the particle) for propylene desorption runs and very small coefficients for propylene adsorption runs.

On the assumption that the value of D should be independent of the direction of propylene flow, the adsorptive relative volatility was adjusted to a value of .5. This was used throughout the data processing runs as reported above. The average of D for 13 propylene adsorption runs was 3.96×10^{-5} sq. cm. per sec. and for 12 propylene desorption runs 3.32×10^{-5} sq. cm. per sec.

B. Nature of the Diffusion Coefficient

Gaseous diffusion coefficients fall normally in the range .1 to 1. sq. cm. per sec. Liquid diffusion coefficients are usually in the range 0.3 to $5. \times 10^{-5}$ sq. cm. per sec.(20) Coefficients for diffusion of gaseous species through solids are normally much smaller of the order of 10^{-10} sq. cm. per sec. The value determined in this investigation falls as might be expected in the liquid range.

The lack of effect of the four-fold change in pressure obtained in this study also indicates that the diffusion is taking place in a highly compressed adsorbed state which amounts to essentially liquid diffusion.

RECONSTRUCTION OF CONCENTRATION HISTORIES

Plug-Flow Model Calculations

In the following section the results of recalculating the concentration histories according to the plug-flow model with adsorption rate controlled by homogeneous particle diffusion with an average D of 3.69×10^{-5} sq. cm./sec are shown for several runs, some composite.

Figure 9 shows the results of calculations on a composite of runs 3, 7, and 9. These runs were made on adsorbent of average diameter .28 cm., with a flow rate of .80 mg-mols/sec at the inlet and at a temperature of 0°C. The pressure was approximately atmospheric. Propane was being desorbed.

Figure 10 contains the graphical results of calculations on 6 and 17. These were at a temperature of 0°C, adsorbent diameter of .28 cm a flow-rate of .78 mg-mols/sec and a pressure of .97 atm. Propylene was being desorbed.

The above two runs were made at the same temperature and pressure with almost identical flow-rates. It is interesting to note the difference in the shape of the curves caused by the relative volatility being different from a value of one.

Figure 11 indicates the results obtained from runs 45 and 47. Conditions here were; temperature - 0°C, pressure - .98 atm., particle diameter - .117 cm. and flow rate - .78 mg-mols/sec. Notice the considerable steepening of the curves due to decreased particle size and thus increased adsorption rates.

Figure 12 contains results from run 56 at 0°C, .98 atm., particle diameter of .98 cm. and flow rate of .79 mg-moles/sec.

Figure 13 presents the results of calculations on run number 52. This run was at .98 atm. pressure, 0°C temperature for a particle diameter of .111 cm. The flow rate at the inlet was .495 mg-mols/sec.

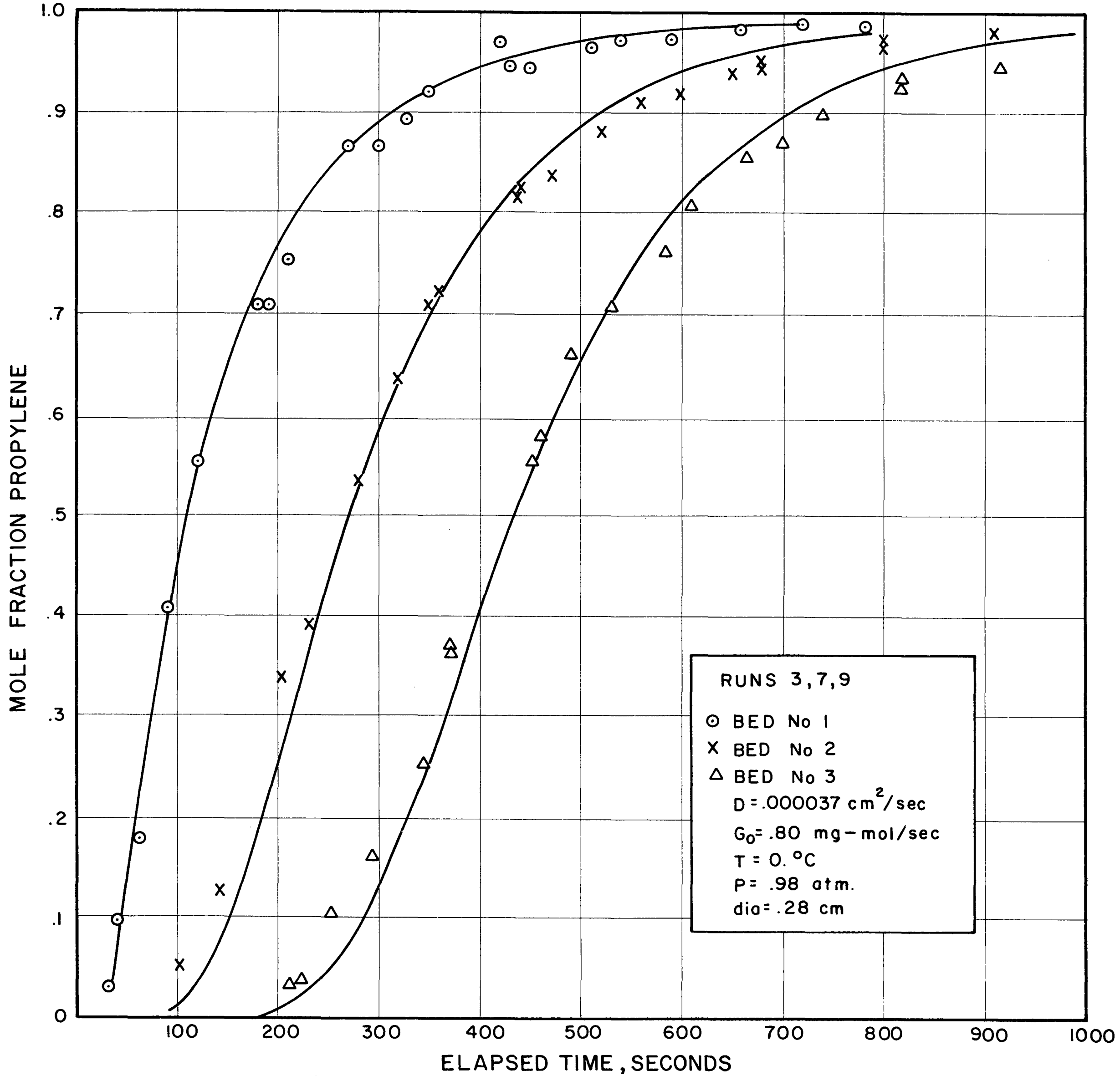


Figure 9. Concentration Histories Reconstructed for Runs 3, 7 and 9.

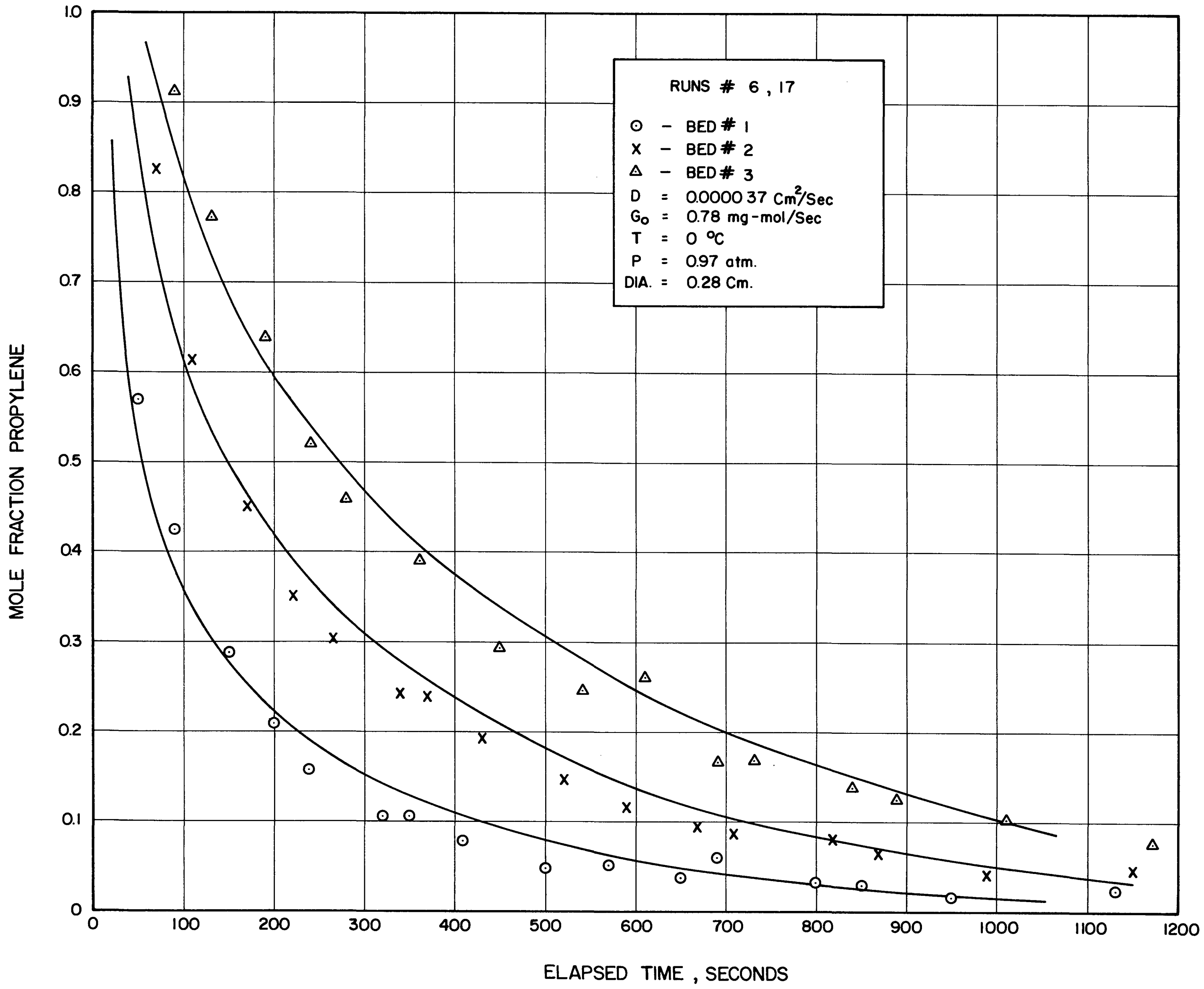


Figure 10. Concentration Histories Reconstructed for Runs 6 and 17.

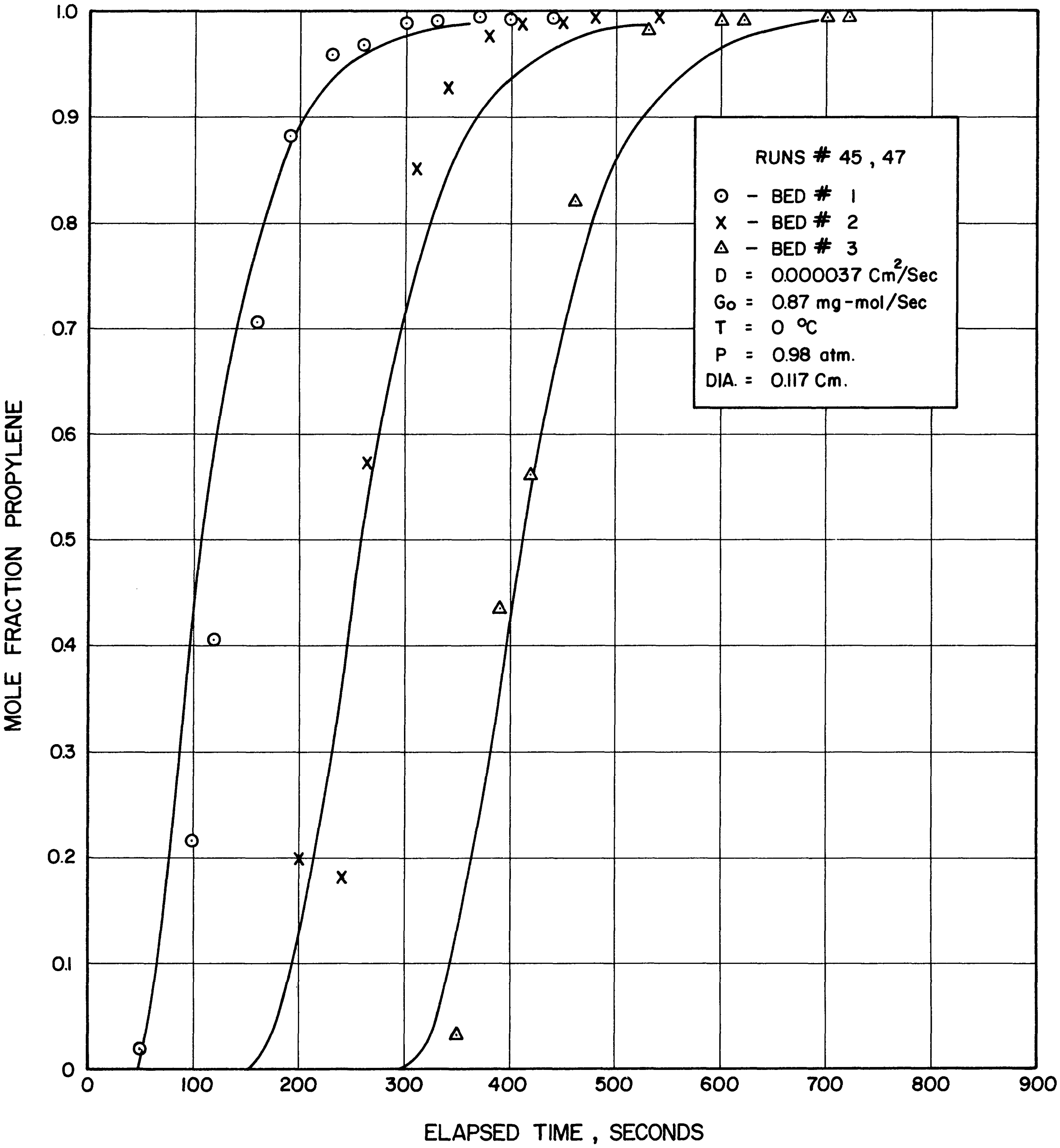


Figure 11. Concentration Histories Reconstructed for Runs 45 and 47.

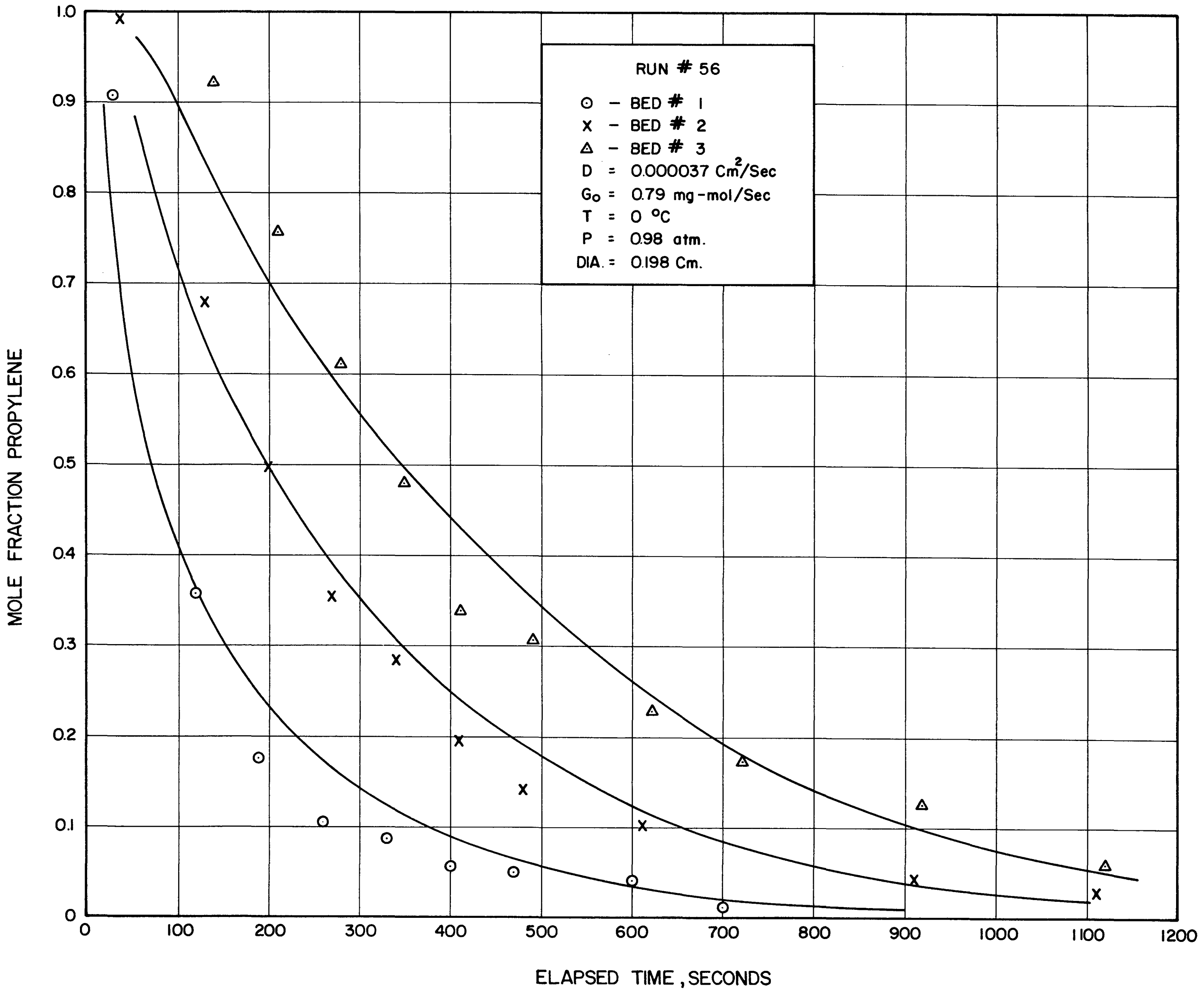


Figure 12. Concentration Histories Reconstructed for Run 56.

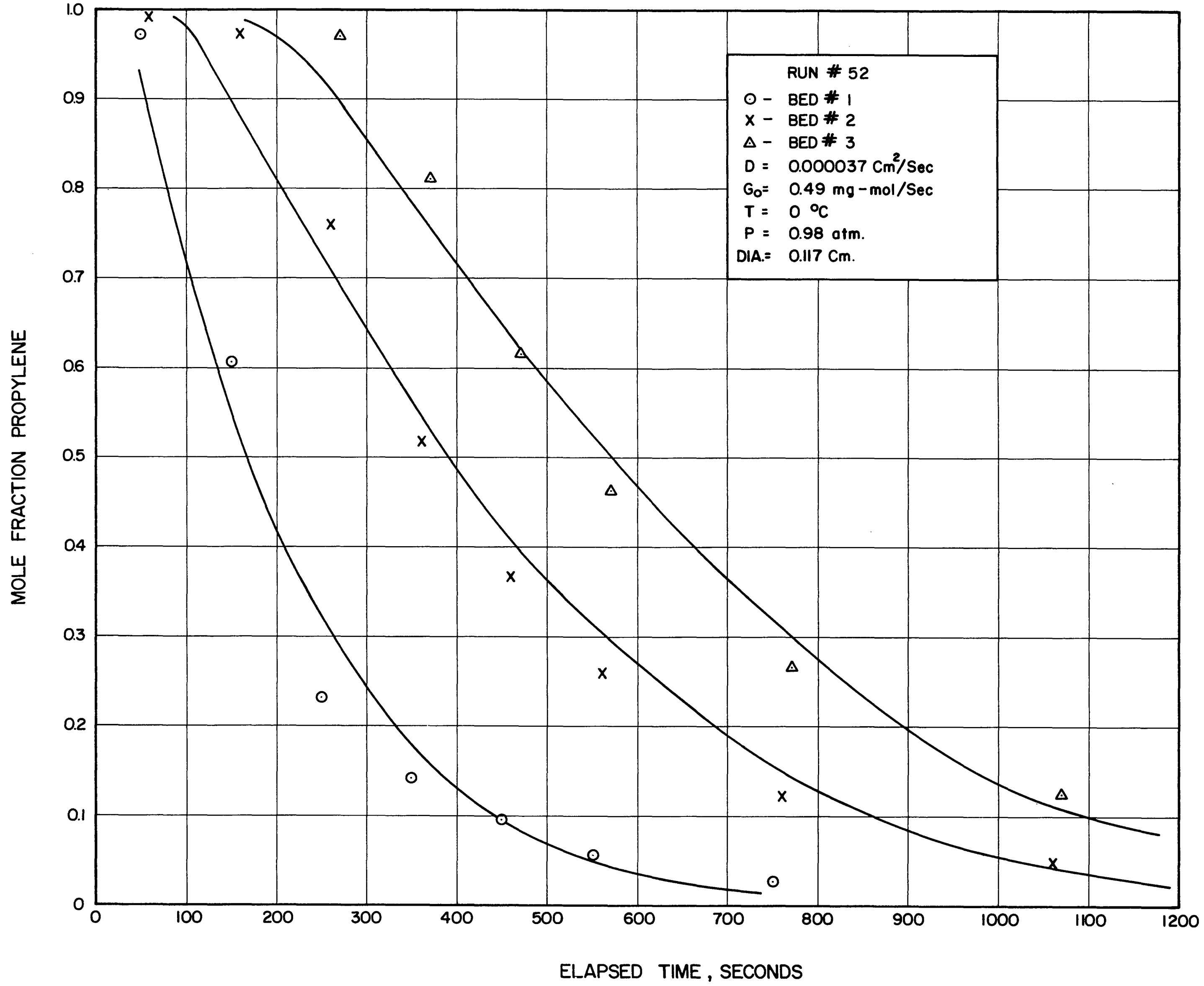


Figure 13. Concentration Histories Reconstructed for Run 52.

CONCLUSIONS AND RECOMMENDATIONS

The purpose of this study was to examine the kinetic behavior of a binary gas-solid adsorbent system; propane-probylene-silica gel being taken as an example. Two separate processes were considered in the adsorption process; namely, passage of the gas through the so-called gas film and diffusion of the adsorbed gases in the particle. The former process was studied from existing correlations. The later process was reduced to a mathematical analysis yielding a coefficient of diffusion of 3.65×10^{-5} sq. cm. per sec. with a standard deviation of 2.06×10^{-5} sq. cm. per sec. During this process, the interface relations were assumed to be governed by a constant adsorptive relative volatility (defined by Equation (46)) of .5.

The use of this diffusion coefficient in the plug-flow model equations led to reconstructed concentration histories in fair agreement over most of the range except the initial few minutes where the adsorption or desorption rate was highest. It was in this region that the most difficulty was encountered in the data reduction step as well. The difficulty in clearly defining the adsorptive relative volatility mentioned earlier may be involved here. Under high transfer rate conditions, it is most unlikely that equilibrium at the interface is really attained at all. As indicated by the results of this study, the effective relative volatility may be a function of mass transfer rate and certainly different from its equilibrium value.

The diffusion model is not the only one which will fit the data. A first order kinetic equation of the following type:

$$Q_A = k_2(y_A^* - m_A/K_{ads}) \tag{70}$$

where k_1 and k_2 are velocity constants in the reaction

$$C_3H_6 \text{ gas } \underset{k_2}{\overset{k_1}{\rightleftarrows}} C_3H_6 \text{ adsorbed}$$

and

$$K_{ads} = k_1/k_2 = (y_A/m_A) \text{ @ equilibrium}$$

will correlate the data to almost the same degree.

This result may be expected if the radial particle concentrations gradients are close to linear, since for D = constant, the diffusion equation may be reduced to an equation of the type (70).

The flowrate data obtained in the study were unfortunately unreliable. They showed, in general, a qualitative adherence to the predicted behavior but not a quantitative one. The comparison of flowrates obtained experimentally and those computed via relation (63) for run number 26 are shown in Figure 14. It is felt that the capillary tube manometers used with the orifice meters were too sluggish in response to allow accurate readings at these low flow rates.

Future Work

An important part of any further kinetic studies of this kind must be an elucidation of the interface relations under conditions of high flux. The use of a constant relative volatility in this work seems to be one of the most important factors in the scatter of the determinations.

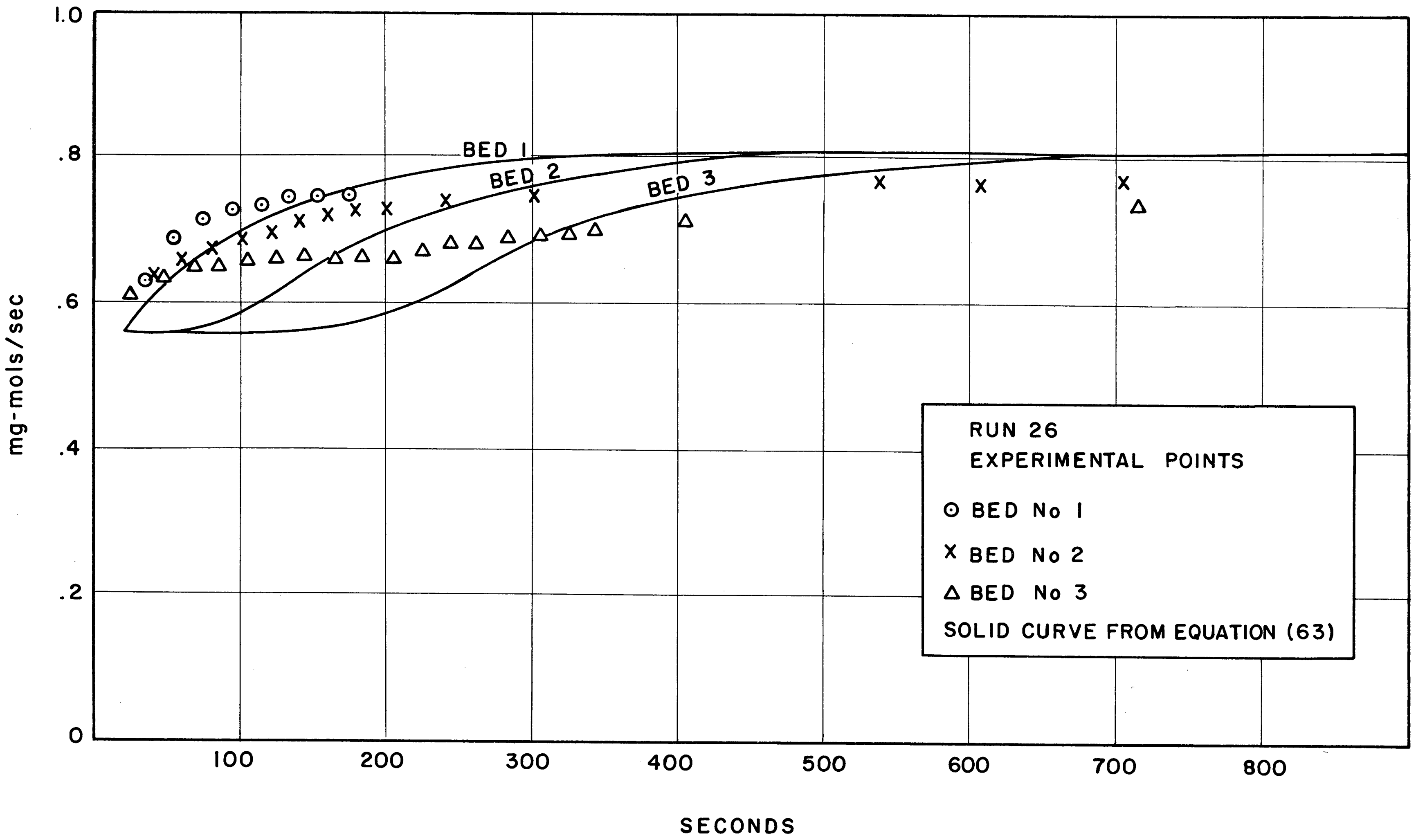


Figure 14. Comparison of Observed and Calculated Velocity Histories for Run 26.

The methods used here could theoretically be extended to multicomponent systems. However, ternary or higher systems present great experimental difficulties both in controlling the experiment and in interpreting the results. For example, a tentative attempt at a nitrogen-propane-propylene-silica gel experiment was made. It was found that with the bed initially saturated with nitrogen, and propane-propylene mixtures passed into it, the whole experiment was over before any readings could be taken. In general, all the components would have to be about equally adsorbed by silica gel in order to get adequate experimental durations.

The method used here to calculate concentration histories could be extended to multicomponent systems. It is probable that some form of first order kinetic equation could be substituted for the complex diffusion equation. The accuracy obtainable would probably be sufficient for design purposes and the attendent saving in computing time would be quite great. Here again, some better relation for unsteady state interface conditions is needed.

APPENDIX A

A. Solution of the Boundary Value Problem Posed in the Diffusion Model(5)

In the Equations (22) to (25), make the substitutions,

$$U = r(S_0 - s) \qquad \text{(A1)}$$

$$\theta = Dt \qquad \text{(A2)}$$

The problem then becomes

$$U_\theta = U_{rr} \qquad \text{(A3)}$$

$$U(0,\theta) = 0 \qquad \text{(A4)}$$

$$\frac{1}{r_0^2} U(r_0,\theta) - \frac{1}{r_0} U_r(r_0,\theta) = -F(\theta) \qquad \text{(A5)}$$

$$U(r,0) = 0 \qquad \text{(A6)}$$

The method of attack will be to first solve the case where boundary condition (A5) is replaced by a constant input function. Let the solution of this case be $V(r,\theta)$. Then,

$$V_\theta = V_{rr} \qquad \text{(A7)}$$

$$V(0,\theta) = 0 \qquad \text{(A8)}$$

$$\frac{1}{r_0^2} V(r_0,\theta) - \frac{1}{r_0} V_r(r_0,\theta) = -1 \qquad \text{(A9)}$$

$$V(r,0) = 0 \qquad \text{(A10)}$$

This solution will then be used via Duhamel's(5) formula to get the solution of the original problem.

Taking the Laplace Transforms of the above set, we get

$$sv = v_{rr} \tag{A11}$$

$$v(0,s) = 0 \tag{A12}$$

$$\frac{1}{r_0^2}\, v(r_0,s) - \frac{1}{r_0}\, v_r(r_0,s) = -\frac{1}{s} \tag{A13}$$

The solution of (A11) subject to the boundary conditions (A12) may be written

$$v(r,s) = B \sinh(\sqrt{s}\ \ r_0) \tag{A14}$$

Substitution of this into the other boundary condition (A13) and rearrangement gives

$$v(r,s) = -\frac{r_0^2\ \sinh(\sqrt{s}\ r_0)}{s(\sinh(\sqrt{s}\ \ r_0) - \sqrt{s}\ \ r_0\cosh(\sqrt{s}\ \ r_0))} \tag{A15}$$

If now the hyperbolic functions are expressed in terms of the first few terms of their series expansion forms, we get

$$v(r,s) = \frac{1}{2s^2}\ \frac{r + \frac{r^3 s}{3!} + \frac{r^5 s^2}{5!} + \frac{r^7 s^3}{7!} + \cdots\cdots}{\frac{r_0}{3!} + \frac{2r_0^3 s}{5!} + \frac{3r_0^5 s^2}{7!} + \cdots\cdots} \tag{A16}$$

From (A16) it can be seen that the function has a pole of order 2 at $s = 0$. Carrying out the division indicated, we can now obtain an expansion in the neighborhood of $s = 0$

$$v(r,s) = \frac{3!\ \ r}{2r_0 s^2} + \frac{r}{2s}\left(\frac{r^2}{r_0} - \frac{2(3!)^2 r_0}{5!}\right) + \sum_{n=0}^{\infty} a_n(r)\ s^n \tag{A17}$$

The first two terms of the solution arise from the first two terms in (A17) as the residue of $e^{zt}v(r,z)$ at $z = 0$. The terms are

$$\frac{3!r\theta}{2r_0} + \frac{r}{2}\left(\frac{r^2}{r_0} - \frac{2(3!)^2 r_0}{5!}\right) \qquad (A18)$$

Equation (A15) contains an infinite number of simple poles at the roots of the equation

$$\sinh(\sqrt{s}\, r_0) - \sqrt{s}\, r_0 \cosh(\sqrt{s}\, r_0) = 0 \qquad (A19)$$

If we assume pure imaginary roots of the form $i\beta/r_0$, Equation (A19) simplifies to

$$\tan \beta_n = \beta_n \qquad (A20)$$

Tables of the first seventeen of these roots are available(13) and they have been extended up to fifty. Table VIII contains the first fifty roots.

The remaining infinite number of terms in the solution come from the residues of $e^{zt}v(r,z)$ at $z = i\beta_n/r_0$.

$$\rho_n(\theta) = \left[\frac{r_0^2 \sinh(\sqrt{z}\, r_0)\, e^{zt}}{\frac{d}{dz}\{z(\sinh(\sqrt{z}\, r_0) - z\, r_0 \cosh(\sqrt{z}\, r_0))\}}\right]_{z = -\frac{\beta_n^2}{r_0^2}} \qquad (A21)$$

$$= \frac{-2r_0^2 \sinh(i\beta_n r/r_0)\, e^{-\beta_n^2\theta/r_0^2}}{\beta_n^2 \sinh(i\beta_n)} \qquad (A22)$$

Now since $\sinh(ix) = i\sin(x)$ we may replace the ratio of hyperbolic sines by the ratio of circular sines. Also in view of the fact that $\tan \beta_n = \beta_n$, we have the two following relations, one of which we use directly and the other will be useful in a subsequent section:

$$\sin(\beta_n) = \frac{(-1)^n \beta_n}{\sqrt{1 + \beta_n^2}} \qquad \text{(A23)}$$

and

$$\cos(\beta_n) = \frac{(-1)^n}{\sqrt{1 + \beta_n^2}} \qquad \text{(A24)}$$

The residue is then

$$\rho_n(\theta) = -2(-1)^n r_0 \frac{\sqrt{1 + \beta_n^2}}{\beta_n^3} \sin(\beta_n r/r_0) e^{-\beta_n^2 \theta / r_0^2} \qquad \text{(A25)}$$

The solution for $V(r,\theta)$ may now be written:

$$V(r,\theta) = \frac{3r\theta}{2r_0} + r\left(\frac{r^2}{2r_0} + \frac{3r_0}{10}\right) - 2r_0^2 \sum_{n=1}^{\infty} \gamma_n \sin(\beta_n r/r_0) e^{-\beta_n^2 \theta / r_0^2} \qquad \text{(A26)}$$

where γ_n is defined by Equation (27).

Substitution of this formal solution into the Equation (A7) and its boundary and initial conditions (A8), (A9), and (A10) shows that they are satisfied.

We now return to the complete problem. Applying the Laplace Transforms to Equation (A3) and its boundary and initial conditions (A4), (A5), and (A6), the following equations arise:

$$su(r,s) = u_{rr}(r,s) \qquad \text{(A27)}$$

$$u(0,s) = 0 \qquad \text{(A28)}$$

$$\frac{1}{r_0^2} u(r_0,s) - \frac{1}{r_0} u_r(r_0,s) = -f(s) \qquad \text{(A29)}$$

A solution of these equations is

$$u(r,s) = -f(s) \frac{r_0^2 \sinh(\sqrt{s}\, r_0)}{\sinh(\sqrt{s}\, r_0) - \sqrt{s}\, r_0 \cosh(\sqrt{s}\, r_0)} \qquad \text{(A30)}$$

or, in terms of the other solution,

$$u(r,s) = sf(s)v(r,s) \qquad \text{(A31)}$$

Duhamel's$^{(5)}$ Formula applies here in the form

$$U(r,\theta) = F(0).V(r,\theta) - \int_0^\theta F'(\theta - \tau).V(r,\theta)d\tau \qquad \text{(A32)}$$

Now if F(t) can be adequately represented by a power series whose derivatives converge to the corresponding derivatives of F(t), the integration in (A32) can be carried out by integration by parts. The resulting solution for $U(r,\theta)$ is as follows:

$$U(r,\theta) = \frac{3r}{r_0} \int_0^\theta F(\tau)d\tau + r\left(\frac{r^2}{2r_0} + \frac{3r_0}{10}\right) F(\theta) - 2r_0^2 \sum_{n=1}^{\infty} \gamma_n \delta_n' \sin(\beta_n r/r_0) \qquad \text{(A33)}$$

where γ_n is defined by Equation (27), page 26, and δ_n' by

$$\delta_n' = e^{-\beta_n^2 \theta/r_0^2} \sum_{j=0}^{\infty} \left(-\frac{r_0^2}{\beta_n^2}\right)^j F^{(j)}(0) - \sum_{j=1}^{\infty} \left(-\frac{r_0^2}{\beta_n^2}\right)^j F^{(j)}(\theta) \qquad \text{(A34)}$$

It can be readily verified that this formal solution satisfies the differential Equation (A3) and the boundary conditions (A4) and (A5). However, in order to show that the solution fulfills the initial condition (A6), it is necessary to prove that for $\theta = 0$, the second and third terms in (A33) cancel. Note that verification of (A33) can be made by an alternate route. Since $V(r,\theta)$ can be verified as a solution of (A7), (A8), (A9) and (A10) and since in general it can be proved that if $U(r,\theta)$ is obtained from this solution via Duhamel's Formula, then $U(r,\theta)$ is guaranteed to be a solution of the whole problem (A3), (A4), (A5) and (A6). We choose the longer route since it leads to a useful simplification of the expression (A33).

It must first be proved that the second term may be expanded in a Sturm-Liouville type series of the sine terms appearing in the third term. We first show that the set

$$\sin(\beta_n r/r_0) \qquad n = 1,2,3,4,\dots\dots \qquad \text{(A34)}$$

is orthogonal over the interval 0 to r_0.

Proof of the Orthogonality of Set (A34)

When $m \neq n$, we evaluate the expression:

$$\int_0^{r_0} \sin(\beta_m r/r_0).\sin(\beta_n r/r_0) = \frac{1}{2}\int_0^{r_0} \cos[(\beta_m-\beta_n)r/r_0]dr$$

$$- \frac{1}{2}\int_0^{r_0} \cos[(\beta_m+\beta_n)r/r_0]dr$$

$$= \frac{r_0\sin[(\beta_m-\beta_n)r/r_0]}{2(\beta_m-\beta_n)} - \frac{r_0\sin[(\beta_m+\beta_n)r/r_0]}{2(\beta_m+\beta_n)}\Bigg]_0^{r_0}$$

$$= \frac{r_0(\sin\beta_m\cos\beta_n - \cos\beta_m\sin\beta_n)}{2(\beta_m - \beta_n)}$$

$$- \frac{r_0(\sin\beta_m\cos\beta_n + \cos\beta_m\sin\beta_n)}{2(\beta_m + \beta_n)} \qquad \text{(A35)}$$

Substitution of relations (A23) and (A24) into the right hand side of (A35) gives:

$$\frac{1}{2}\left[\frac{r_0}{\beta_m - \beta_n}\left(\frac{(-1)^m\beta_m}{\sqrt{1+\beta_m^2}}\,\frac{(-1)^n}{\sqrt{1+\beta_n^2}} - \frac{(-1)^m}{\sqrt{1+\beta_m^2}}\,\frac{(-1)^n\beta_n}{\sqrt{1+\beta_n^2}}\right)\right.$$

$$\left. - \frac{r_0}{\beta_m - \beta_n}\left(\frac{(-1)^m\beta_m}{\sqrt{1+\beta_m^2}}\,\frac{(-1)^n}{\sqrt{1+\beta_n^2}} + \frac{(-1)^m}{\sqrt{1+\beta_m^2}}\,\frac{(-1)^n\beta_n}{\sqrt{1+\beta_n^2}}\right)\right]$$

$$= 0 \qquad \text{(A36)}$$

When m = n, we evaluate the expression:

$$\int_0^{r_0} \sin^2(\beta_n r/r_0) = \frac{1}{2}\int_0^{r_0}[1 - \cos(2\beta_n r/r_0)]\,dr$$

$$= \frac{1}{2}r - \frac{1}{4}r_0/\beta_n \sin(2\beta_n r/r_0)\Big]_0^{r_0}$$

$$= \frac{1}{2}r_0 - \frac{1}{4}r_0/\beta_n \sin(2\beta_n)$$

$$= \frac{1}{2}r_0 - \frac{1}{4}r_0/\beta_n \sin(\beta_n)\cos(\beta_n) \qquad \text{(A37)}$$

Substitute from Equations (A23) and (A24):

$$\int_0^{r_0} \sin^2(\beta_n r/r_0) = \frac{1}{2}r_0 - \frac{1}{2}\frac{r_0}{\beta_n}\,\frac{(-1)^n n}{\sqrt{1+\beta_n^2}}\,\frac{(-1)^n}{\sqrt{1+\beta_n^2}}$$

$$= \frac{r_0}{2}\left(\frac{\beta_n^2}{1+\beta_n^2}\right) \qquad \text{(A38)}$$

The set (A34) is thus seen to be orthogonal over the interval $0 \leq r \leq r_0$. The norm of the functions $\sin(\beta_n r/r_0)$ is shown to be the last expression in (A38) and is non-zero.

Expansion of the Second Term in Equation (A33) in Terms of Orthogonal Set (A34)

In order to complete the proof that solution (A33) satisfies the initial condition (A6), we expand the second term therein in terms of the orthogonal sine functions occurring in the third term.

We wish a series representation of the form

$$r\left(\frac{r^2}{r_0} + \frac{3r_0}{10}\right) = A_1\sin(\beta_1 r/r_0) + A_2\sin(\beta_2 r/r_0) + \ldots. \qquad \text{(A39)}$$

Since the functions are orthogonal, we know that the coefficients A_n are given by:

$$A_n = \frac{\int_0^{r_0} r(\frac{r^2}{r} + \frac{3r_0}{10}) \sin(\beta_n r/r_0)dr}{\int_0^{r_0} \sin^2(\beta_n r/r_0)dr} \qquad \text{(A40)}$$

Integration by parts gives the following:

$$A_n = (-1)^n . 2r_0^{\,2} \frac{\sqrt{1 + \beta_n^2}}{\beta_n^3} \qquad \text{(A41)}$$

Thus

$$r\left(\frac{r^2}{r_0} + \frac{3r_0}{10}\right) = 2r_0^{\,2} \sum_{n=1}^{\infty} \gamma_n \sin(\beta_n r/r_0) \qquad \text{(A42)}$$

If this series representation of the second term in series solution (A33) is placed into the equation, we get the following simplified expression:

$$U(r,\theta) = \frac{3r}{r_0} \int_0^{r_0} F(\tau)\, d\tau - 2r_0^{\,2} \sum_{n=1}^{\infty} \gamma_n \delta_n'' \sin(\beta_n r/r_0) \qquad \text{(A43)}$$

where

$$\delta_n'' = e^{-\beta_n^2\theta/r_0^2} \sum_{j=0}^{\infty} \left(-\frac{r_0^2}{\beta_n^2}\right)^j F^{(j)}(0) - \sum_{n=0}^{\infty} \left(-\frac{r_0^2}{\beta_n^2}\right)^j F^{(j)}(\theta) \tag{A44}$$

The series solution in form (A43) is easily seen to fulfill initial condition (A6).

Re-introduction of Original Variables

From Equation (21)

$$F(\theta) = F(Dt) = \frac{r_0\psi}{3D} Q_A(t) \tag{A45}$$

The derivatives of $F(\theta)$ with respect to θ can be evaluated in terms of derivatives of $Q_A(t)$ with respect to t by successive application of the chain rule. Thus:

$$F^{(1)}(\theta) = \frac{dF(\theta)}{d\theta} = \frac{r_0\psi}{3D}\frac{dQ_A}{dt}\frac{dt}{d\theta} = \frac{r_0\psi}{3D}\frac{dQ_A}{dt}\frac{1}{D} = \frac{r_0\psi}{3D}\frac{1}{D} Q_A^{(1)}(t)$$

$$F^{(2)}(\theta) = \frac{r_0\psi}{3D}\frac{1}{D^2} Q_A^{(2)}(t)$$

$$\cdots\cdots\cdots\cdots\cdots$$

$$F^{(n)}(\theta) = \frac{r_0\psi}{3D}\frac{1}{D^n} Q_A^{(n)}(t) \tag{A46}$$

Substituting these relations and re-substituting for U from Equation (A1) into (A43), we get the final form of the solution (26).

$$s(r,t) = S_0 + \psi \int_0^t Q_A(\tau)\, d\tau - \frac{2r_0^3\psi}{3rD} \sum_{n=1}^{\infty} \gamma_n \delta_n \sin(\beta_n r/r_0) \tag{26}$$

TABLE VIII(13)

FIFTY ROOTS OF THE EQUATION $\text{TAN}\beta_n = \beta_n$

n	β_n	n	β_n	n	β_n
1	4.4934	18	58.1022	35	111.5176
2	7.7253	19	61.2447	36	116.6595
3	10.9041	20	64.3871	37	117.8013
4	14.0662	21	67.5295	38	120.9431
5	17.2208	22	70.6717	39	124.0949
6	20.3713	23	73.8139	40	127.2266
7	23.5195	24	76.9570	41	130.3685
8	26.6661	25	80.0981	42	133.5103
9	29.8116	26	83.2503	43	136.6520
10	32.9564	27	86.3824	44	139.7937
11	36.1006	28	89.5243	45	142.9354
12	39.2444	29	92.6662	46	146.0772
13	42.3979	30	95.8081	47	149.2189
14	45.5311	31	98.9501	48	152.3607
15	48.6741	32	102.0920	49	155.5024
16	51.8170	33	105.2339	50	158.6441
17	54.9597	34	108.3757		

B. Method of Characteristics for a General Set of Two Simultaneous Quasi-Linear First-Order Differential Equations(6,11)

Consider the set

$$A_1u_x + B_1u_y + C_1v_x + D_1v_y = R_1 \qquad (A47)$$

$$A_2u_x + B_2u_y + C_2v_x + D_2v_y = R_2 \qquad (A48)$$

We assume that these equations have integral surfaces on which u and v are at least sectionally continuous. We are interested in the intersection of these two to form one which is the solution surface of the simultaneous equations.

In particular, we are going to look for a space curve or family of space curves on this integral surface along which the derivatives in the above equations may be discontinuous.

Provided that u and v are continuous along space curve C on the integral surface, infinitesimal changes in u and v along C may be obtained from infinitesimal changes in x and y along the projection of C into the x-y plane via the relations

$$du_C = u_xdx + u_ydy \qquad (A49)$$

$$dv_C = v_xdx + v_ydy \qquad (A50)$$

Now Equations (A47), (A48), (A49) and (A50) constitute four equations in four unknowns - the derivatives u_x, u_y, v_x and v_y.

By Cramer's Rule, these equations provide a unique solution for u_x, u_y, v_x and v_y unless the determinant of the coefficients is zero. Now since we are looking for an indeterminancy which may allow

u_x to be discontinuous, let us set this determinant equal to zero.

$$\begin{vmatrix} A_1 & B_1 & C_1 & D_1 \\ A_2 & B_2 & C_2 & D_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{vmatrix} = 0 \qquad \text{(A51)}$$

After expansion, rearrangement and division through by $-dx^2$, this determinant yields the following quadratic equation in dy/dx which must hold along the curve C on which the equation set is indeterminate

$$a\left(\frac{dy}{dx}\right)^2 + b\left(\frac{dy}{dx}\right) + c = 0 \qquad \text{(A52)}$$

where

$$a = A_1C_2 - A_2C_1 \qquad \text{(A53)}$$

$$b = -\,(A_1D_2 - A_2D_1 + B_1C_2 - B_2C_1) \qquad \text{(A54)}$$

$$c = B_1D_2 - B_2D_1 \qquad \text{(A55)}$$

Hence, the slopes of the projections of characteristics C^+ and C^- are given by the respective roots of (A52).

$$\frac{dy}{dx} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \qquad \text{(A56)}$$

Along the lines in the x-y plane defined by Equation (A56) the set (A47) - (A50) does not possess a unique solution and in particular, the set cannot be solved for u_x; hence no solution exists unless the numerator determinant in Cramer's Rule is also zero. In that case there are an infinite number of solutions; hence the required indeterminacy on u_x.

An important classification of equations follows from (A56). If $b^2 - 4ac < 0$, the equation set is termed elliptic and there are no characteristic directions in the real plane. If $b^2 - 4ac = 0$, the set is parabolic and there is only one characteristic direction through a point in the x-y plane. In the most important case where $b^2 - 4ac > 0$, the set is termed hyperbolic and there are two characteristic directions through each point in the x-y plane.

By equating the numerator determinant of Cramer's Rule for u_x to zero, we can now derive an equation which provides a restriction on the total derivatives of u and v with respect to x along C^+ and C^-.

$$\begin{vmatrix} R_1 & B_1 & C_1 & D_1 \\ R_2 & B_2 & C_2 & D_2 \\ du & dy & 0 & 0 \\ dv & 0 & dx & dy \end{vmatrix} = 0 \qquad \text{(A57)}$$

After expansion, rearrangement and division through by dx^2, (A57) yields the following expression:

$$e\left(\frac{du}{dx}\right)_C + f\left(\frac{dv}{dx}\right)_C + g = 0 \qquad \text{(A58)}$$

where

$$e = \left[(B_1C_2 - B_2C_1)\left(\frac{dy}{dx}\right)_C - (B_1D_2 - B_2D_1)\right] \qquad \text{(A59)}$$

$$f = -(C_1D_2 - C_2D_1)\left(\frac{dy}{dx}\right)_C \qquad \text{(A60)}$$

$$g = (C_1R_2 - C_2R_1)\left(\frac{dy}{dx}\right)_C^2 - (D_1R_2 - D_2R_1)\left(\frac{dy}{dx}\right)_C \qquad \text{(A61)}$$

Application of the Method of Characteristics to Equations (55) and (57)

The coefficients take on the following values:

$$A_1 = 1 \qquad A_2 = 0$$

$$B_1 = 1/v \qquad B_2 = 0$$

$$C_1 = 0 \qquad C_2 = 1$$

$$D_1 = 0 \qquad D_2 = 0$$

Hence

$$a = 1$$

$$b = -1/v$$

$$c = 0$$

The discriminant $b^2 - 4ac$ is positive and non-zero, hence the set is hyperbolic and has two characteristic directions given by

$$\frac{dt}{dx} = \frac{\frac{1}{v} \pm \sqrt{(\frac{1}{v})^2}}{2}$$

$$\frac{dt}{dx} = \frac{1}{v} \quad \text{along } C^+ \tag{61}$$

$$\frac{dt}{dx} = 0 \quad \text{along } C^- \tag{62}$$

Equations involving the total derivatives of y and v along the characteristics are now obtained from (A58). Refer to Figure 8.

$$C^+: \qquad e = \frac{1}{v}\frac{1}{v} = \frac{1}{v^2}$$

$$f = 0$$

$$g = -(\frac{1}{v})^2$$

Hence

$$\left(\frac{dy}{dx}\right)_{C^+} = R_1 \qquad (55)$$

C^-: $e = 0$

$f = 0$

$g = 0$

Since Equation (57) involves only the derivative of v along the characteristic C^- already, it introduces a degeneracy into the equations at this point. That is, along C^-

$$0 . \left(\frac{dy}{dx}\right)_{C^-} - 0 . \left(\frac{dv}{dx}\right)_{C^-} - 0 = 0$$

We thus take Equation (57) as the correct expression of the total derivative of v with respect to x along the direction C^-.

C. Finite Difference Approximation to Plug-Flow Model Equations(10)

For solution along the characteristic lines, we choose a finite difference grid constructed as in Figure 15 which is a straight-line segmented approximation to Figure 8. The grid lines parallel to the t axis are separated by distances Δx_i; they need not be equally spaced.

Increments Δt_j are chosen arbitrarily along the t axis and need not be equally spaced. The points so formed are the generating points for the C^+ characteristic lines.

The value of a variable at the i^{th} space point and on the j^{th} characteristic (C^+) will be denoted v_{ij}.

The characteristic curves shown in Figure 15 must be replaced by straight line segments whose slopes between points (i-1,j) and (i,j)

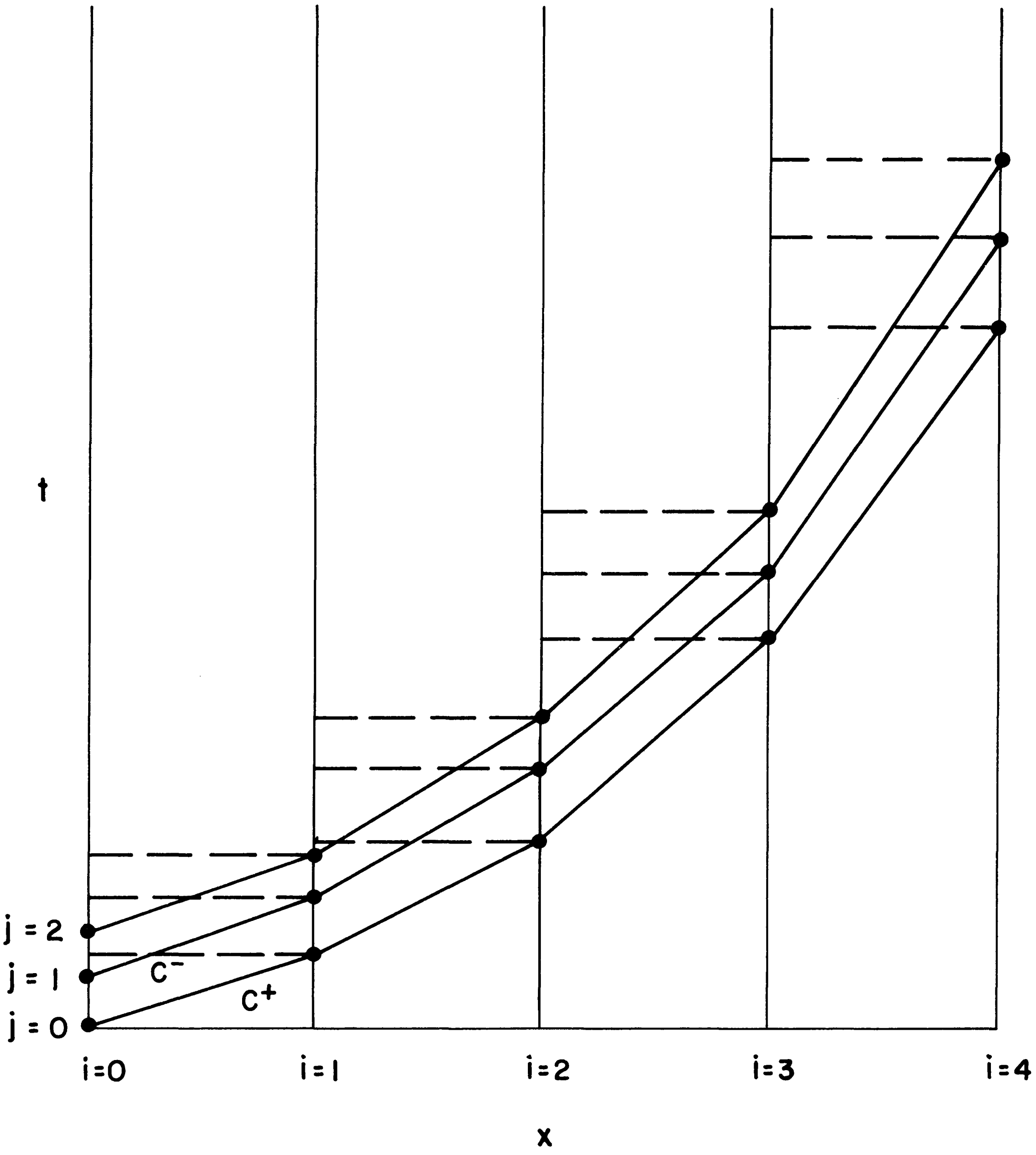


Figure 15. Finite Difference Grid with Characteristics Shown for Plug-Flow Equations.

are given by

$$\frac{dt}{dx} = \frac{2}{v_{i-1,j} + v_{i,j}} \tag{A62}$$

Define three rate functions appearing in the equations to follow:

$$R^1_{i,j} = -\frac{(1 - \psi y_{i,j})}{f v_{i,j} \rho} Q_{Ai,j} \tag{A63}$$

$$R^2_{i,j} = -\frac{\psi}{f\rho} Q_{Ai,j} \tag{A64}$$

$$R^3_{i,j} = \frac{r_0 \psi}{3D} Q_{Ai,j} \tag{A65}$$

1. Gas Phase Concentration

Equation (59) is used between point (i-1,j) and (i,j) to give the mole fraction $y_{i,j}$ in the form

$$y_{i,j} = y_{i-1,j} + \int_{x_{i-1}}^{x_i} R^1 dx \tag{A66}$$

A modified Euler method is employed here to approximate the integral. Thus an iterative scheme is set up, since the Euler method uses the average of the rate at point (i-1,j) which is known and that at point (i,j) which is unknown since it depends upon the variables at point (i,j)

$$y^k_{i,j} = y_{i-1,j} + \left(\frac{R^1_{i-1,j} + R^{1\,k}_{i,j}}{2}\right) \Delta x_i \tag{A67}$$

2. Velocity

Similarly, the velocity relation (60) is integrated along characteristic C^-. However, note from Figure 15 that it is in general necessary to interpolate to the velocity and the rate R^2 at the base point for integration along the characteristic to point (i,j). Linear interpolation is used.

$$v_{i,j} = v_{i-1}\ (t_{i,j}) + \int_{x_{i-1}}^{x_i} R^2 dx \qquad \text{(A68)}$$

where the notation $v_{i-1,(t_{i,j})}$ is intended to represent the velocity on x grid line i-1 and at the time point corresponding to the point (i,j).

The Euler formula for the velocity integration is then:

$$v^k_{i,j} = v_{i-1,(t_{i,j})} + \left(\frac{\overset{1}{R}_{i-1,(t_{i,j})} + \overset{2}{R}{}^k_{i,j}}{2}\right)\Delta x_i \qquad \text{(A69)}$$

3. Time

The time at point (i,j) where $i \neq 0$, is obtained iteratively from the following modification of Equation (A62):

$$t^k_{i,j} = t_{i-1,j} + \frac{2\Delta x_i}{v_{i-1,j} + v^k_{i,j}} \qquad \text{(A70)}$$

and $\Delta t^k_{i,j}$ is obtained from

$$\Delta t^k_{i,j} = t^k_{i,j} - t_{i,j-1} \qquad \text{(A71)}$$

4. Solid Phase Concentration

The diffusion equation was set up in a difference form for inclusion in the plug-flow model calculations. Choice of this scheme over the analytic solution employed in the data reduction step was made on two accounts.

Firstly, the rate function at grid point (i,j) is not known as it is in the data reduction scheme. The analytic solution requires knowledge of this rate function as an explicit function of time and it makes use of the derivatives of the function as well. In the Plug-Flow Model calculations the rate is an unknown at point (i,j) and in order to obtain it as a function of time, curve fitting would be required over several previous points and the assumed value at (i,j). In view of the linear interpolation used elsewhere in the finite difference solution, this does not seem justified. The finite difference approximation to the diffusion equation uses the equivalent of the function and its first derivative.

Secondly, the finite difference equations can be solved much more quickly than the infinite series of the analytic solution; especially where a method of solution described by Richtmyer(21) and developed below for this case is used. Since the plug-flow model calculations require a considerable amount of computer time for solution, this was an important consideration. Balanced against this, of course, is the question of the accuracy and stability of a finite difference approximation. The stability of this finite difference form of the diffusion equation is quite good as is shown by various authors.(10,21) By trial of several grid dimensions, one was chosen which gave a satisfactory compromise between accuracy and time for solution.

A difference approximation to Equation (22) arises from the use of backward time and space differences as follows:

$$\frac{s_{n,m} - s_{n,m-1}}{\Delta\tau} = D\left(\frac{2}{n\Delta r}\ \frac{s_{n,m} - s_{n-1}}{\Delta r} + \frac{s_{n+1,m} - 2s_{n,m} + s_{n-1,m}}{(\Delta r)^2}\right) \tag{A72}$$

The integration here extends along the i^{th} x-grid line from $t_{i-1,j}$ to $t_{i,j}$. Subscripts i and j will be omitted for the sake of clarity.

In place of the boundedness condition on s (24) we require that the gradient of s at the center of the particle be zero. The following set of difference equations then arises:

$$- s_{1,m} + s_{0,m} = 0 \qquad 0 < m < n\tau$$
$$n = 0$$

$$- \alpha s_{n+1,m} + \left\{2\left(\frac{n-1}{n}\right)\alpha + 1\right\} s_{n,m} - \left(\frac{n-2}{n}\right)\alpha s_{n-1,m} = s_{n,m-1}$$
$$0 < m < n_\tau$$
$$0 < n < n_r$$

$$s_{n_r,m} = s_{n_r-1,m} = \frac{r_0\psi}{3D} Q_A \left(t_{i-1,j} + m\,\Delta\tau\right)$$
$$0 < m < n_\tau$$
$$n = n_r \tag{A73}$$

where

$$\alpha = \frac{D\Delta\tau}{(\Delta r)^2} \tag{A74}$$

and

$$\Delta\tau = \frac{\Delta t_{i,j}}{n_\tau} \tag{A75}$$

Equation set (A70) may be written

$$-A_n s_{n-1,m} + B_n s_{n,m} - C_n s_{n-1,m} = D_n \tag{A76}$$

where

$$\begin{aligned} A_n &= 1 & n &= 0 \\ &= \alpha & 0 &< n < n_r \\ &= 0 & n &= n_r \end{aligned} \tag{A77}$$

$$\begin{aligned} B_n &= 1 & n &= 0 \\ &= 1 + 2\left(\frac{n-1}{n}\right) \alpha & 0 &< n < n_r \\ &= 1 & n &= n_r \end{aligned} \tag{A78}$$

$$\begin{aligned} C_n &= 0 & n &= 0 \\ &= \left(\frac{n-2}{n}\right)\alpha & 0 &< n < n_r \\ &= 1 & n &= n_r \end{aligned} \tag{A79}$$

$$\begin{aligned} D_n &= 0 & n &= 0 \\ &= s_{n,m-1} & 0 &< n < n_r \\ &= \frac{r_o\psi}{3D} Q_A(t_{i-1,j} + m\Delta\tau) & n &= n_r \end{aligned} \tag{A80}$$

Richtmyer(21) shows that because of the special form of this set of equations; i.e., the matrix of coefficients contains elements only on the major diagonal, on one diagonal immediately above and one immediately below the major diagonal; one can reduce the implicit dependency of $s_{n,m}$ upon $s_{n+1,m}$ and $s_{n-1,m}$ to an explicit form in which it depends only upon $s_{n+1,m}$. This relation is of the form

$$s_{n,m} = E_n s_{n-1,m} - F_n \qquad 0 \leq n < n_r \qquad \text{(A81)}$$

$$s_{n_r,m} = \frac{(R^3_{i,j-1} + m\Delta R^3)\Delta r + F_{n_r-1}}{1 + E_{n_r-1}} \qquad n = n_r$$

$$R^3_{i,j} = r_0\psi/(3D) \cdot Q_A(x_i,t_j) \qquad \text{(A82)}$$

where the coefficients E and F are obtained recursively from the following relations:

$$E_0 = 1$$

$$E_n = \frac{A_n}{B_n - C_n E_{n-1}} \qquad 0 < n \leq n_r \qquad \text{(A83)}$$

$$F_0 = 0 \qquad 0 < n \leq n_r \qquad \text{(A84)}$$

$$F_n = \frac{D_n + C_n F_{n-1}}{B_n - C_n E_{n-1}}$$

As is shown by Richtmyer,(21) use of these relations minimizes the number of arithmetic operations required and hence ensures the best possible solution scheme as regards round-off error and time.

D. Derivation of the Equilibrium Velocity Relation

From Equations (60) and (58) we get

$$\left(\frac{dv}{dx}\right)_{C^-} = -\frac{\psi\rho_s}{f\rho} Q_A \qquad \text{(A85)}$$

From (59) and (56), we get that

$$Q_A = -\frac{dv\rho}{\rho_s(1 - \psi y)} \left(\frac{dy}{dx}\right)_{C^+} \qquad \text{(A86)}$$

Now substitute for Q_A in (A85).

$$\left(\frac{dv}{dx}\right)_{C^-} = \frac{\psi v}{1 + \psi y}\left(\frac{dy}{dx}\right)_{C^+} \tag{A87}$$

This is now a separable expression which may be rewritten and integrated.

$$\int_{v_0}^{v} \frac{dv_{C^-}}{v} = \int_{y_0}^{y} \frac{\psi}{1 + \psi y}\, dy_{C_+} \tag{A88}$$

or

$$\log_e(v/v_0) = \log_e \frac{1 + \psi y_0}{1 + \psi y}$$

or

$$v = v_0\left(\frac{1 + \psi y_0}{1 + \psi y}\right)$$

If the density is constant this, of course, may be written

$$G = G_0\left(\frac{1 + \psi y_0}{1 + \psi y}\right) \tag{63}$$

It may be shown by somewhat more general derivation that Equation (63) holds even if the density is not constant. This is not developed here.

APPENDIX B

PHYSICAL PROPERTIES CORRELATIONS

A. Vapor Density

The volume-explicit form of the Beattie-Bridgeman$^{(2)}$ equation of state was used to obtain the specific volume of propane and propylene vapors

$$\underline{V} = \left[\frac{RT}{P} + B_0\left(1 - \frac{bP}{RT}\right)\right]\left[1 - \frac{cP}{RT^4}\right] - \left[\frac{A_0}{RT}\right]\left[1 - \frac{aP}{RT}\right] \qquad \text{(B1)}$$

Table IX contains the constants for propylene and propane

TABLE IX

	Propylene	Propane
A_0	12.25	11.92
B_0	.192	.181
a	.07	.0732
b	.06	.0429
c	1000000.	1198845.

Additivity of specific volumes was tested against the rules for mixture coefficients of the Beattie-Bridgeman equation as developed by and was found to be quite adequate in the range of temperature and pressure in question. The molar density ρ and mass density ρ_n were calculated from the following equations:

$$\rho = \frac{1}{y\underline{V}_A + (1 - y)\underline{V}_B} \qquad \text{(B2)}$$

$$\rho_n = \frac{yM_A + (1 - y)M_B}{y\underline{V}_A + (1 - y)\underline{V}_B} \qquad \text{(B3)}$$

B. Viscosity

The equation of Bromley and Wilke(20) for viscosity is rewritten in the form

$$\mu = \frac{0.00333(MT_c)^{1/2}\ f_1(1.33T_R)}{V_c^{2/3}} \qquad \text{(B4)}$$

The temperature function $f_1(1.33T_R)$ was correlated as a power series function of T_R from a tabulation given in Sherwood and Reid.

$$f_1(1.33T_R) = \sum_{i=0}^{3} e_i(T_R)^i \qquad \text{(B5)}$$

The correlation constants are given in Table X.

Table X

i	e
0	- .092678353
1	-1.0754612
2	- .1622960
3	- .014580901

After insertion of the appropriate critical constants and molecular weights into (B4) and rearrangement into the dimension system used; i.e., mg/cm sec, the following two relations were obtained and used for pure phase viscosity:

Propylene: $\mu_A = .12825\ f_1(1.33T_R)$ (B6)

Propane: $\mu_B = .12618\ f_1(1.33T_R)$ (B7)

Since the effect of pressure on viscosity over the range used was small, it was neglected.

The effect of composition was allowed for by means of Wilkė's equation in the form

$$\mu_{mixt} = \frac{\mu_A}{1 + (1 - y)\phi_{AB}/y} + \frac{\mu_B}{1 + y\phi_{BA}/(1 - y)} \qquad (B8)$$

where

$$\phi_{AB} = \frac{[1 + (\mu_A/\mu_B)^{1/2}(M_B/M_A)^{1/4}]^2}{2\sqrt{2}\ \ [1 + M_A/M_B]^{1/2}} \qquad (B9)$$

$$\phi_{BA} = \frac{[1 + (\mu_B/\mu_A)^{1/2}(M_A/M_B)^{1/4}]^2}{2\sqrt{2}\ \ [1 + M_B/M_A]^{1/2}} \qquad (B10)$$

C. Diffusivity(20)

The Gilliland semi-empirical equation was used in the form:

$$D_{AB} = \frac{0.0043\ T^{3/2}\ [(M_A + M_B)/M_AM_B]^{1/2}}{P(\underline{V}_{b_A}{}^{1/3} + \underline{V}_{b_B}{}^{1/3})} \qquad (B11)$$

where $\underline{V}_b$ is the molal volume of pure substance at the normal boiling temperature. This molal volume is estimated by Schroeder's method based upon the additivity of apparent atomic volumes. The values used here were obtained from a table given by Reid and Sherwood.(20)

Propylene: $\underline{V}_{b_A} = 66.6$

Propane $\underline{V}_{b_B} = 74.$

If these values and the appropriate molecular weights are substituted into (B11), the following expression for the diffusivity of propylene into propane or vice versa, in cm /sec is obtained.

$$D_{AB} = 0.00001364\, T^{3/2}/P \qquad \text{(B12)}$$

D. j Factor for Mass Transfer

From curves given by Treybal,(23) a correlation of j_D as a function of Reynolds number was made.

$$\log_e(j_D) = \sum_{i=0}^{3} h_i(\log_e \mathrm{Re})^i \qquad \text{(B13)}$$

Constants of the correlation are given in Table XI.

TABLE XI

i	h
0	.62562545
1	-.50637400
2	-.0070036931
3	.0011111660

E. Adsorptive Equilibrium Capacities

The isotherm data of Lewis *et al*(15) were reduced to Polanyi type distribution curves. See Appendix C for details of the Polanyi Adsorption Potential Theory from which this correlation method arises. These distribution curves were then correlated as power series fits - adsorption volume as a function of adsorption potential.

$$\phi_c = \sum_{i=0}^{5} b_{ci} \epsilon_c^{i} \qquad \begin{array}{l} c = A - \text{propylene} \\ \;\; = B - \text{propane} \end{array} \qquad (B14)$$

Coefficients of the correlation are given in Table XII.

TABLE XII

i	Propylene	Propane
0	4.0674661×10^{2}	3.7845195×10^{2}
1	$-2.6774164 \times 10^{-1}$	$-2.7165051 \times 10^{-1}$
2	7.4111129×10^{-5}	1.8987394×10^{-5}
3	$-1.1470834 \times 10^{-8}$	3.6440492×10^{-8}
4	$1.0611762 \times 10^{-12}$	$-1.2226315 \times 10^{-11}$
5	$-4.7175589 \times 10^{-17}$	$1.1776570 \times 10^{-15}$

F. Fugacity Ratio

Data for the correlation of the logarithm of the fugacity ratio were taken from Maxwell(18) and a curve-fit made in the form

$$\log_e\left(P \frac{f_s}{f}\right) = \sum_{i=0}^{3} a_i (1.8 \times 10^{-3}\, T)^{i-1} \qquad (B15)$$

$$a_i = \sum_{j=0}^{2} b_{ij} (P)^{j} \qquad (B16)$$

Coefficients b_{ij} are tabulated below in Table XIII and Table XIV.

TABLE XIII

		Propylene	
i	j 0	1	2
0	-3.1687540	.20078375	-.018708807
1	5.1288900	-1.0621171	.10345047
2	10.002484	1.9768422	-.18864216
3	-8.1783705	-1.2394364	.11365675

TABLE XIV

		Propane	
i	j 0	1	2
0	-1.1057091	- .61418538	.016313069
1	-6.1122970	3.2934058	-.083254437
2	29.151559	-5.6777008	.13939543
3	-18.863775	3.2003745	-.076787776

G. Liquid Specific Volume

Data for liquid specific volume of the two components was taken from Maxwell(18) and correlated in the form

$$\underline{V}_c = \sum_{i=0}^{3} c_{ci}(1.8T)^i \qquad \begin{array}{l} c = A \text{ - propylene} \\ \;\;= B \text{ - propane} \end{array} \qquad \text{(B17)}$$

TABLE XV

i	Propylene	Propane
0	-55.129320	-28.362340
1	873.32809	697.91541
2	-2179.3799	-1716.5041
3	1922.4285	1535.5613

H. Saturation Temperature

Data was taken from vapor pressure curves in Maxwell(18) and correlated according to the following equation:

$$(1/1.8T) = \sum_{i=0}^{3} d_{ci}(\log_e P)^i \qquad \begin{aligned} c &= A - \text{propylene} \\ &= B - \text{propane} \end{aligned} \qquad (B18)$$

Coefficients for this correlation are given in Table XVI.

TABLE XVI

i	Propylene	Propane
0	.24625632	.24071426
1	-.024189387	-.024266756
2	-.00016167607	-.0002237322
3	-.0000045771307	.0000059156969

I. Specific Area for Mass Transfer

The following chart (Figure 16) is constructed from a table given by Hougen and Watson,(12) Chemical Process Principles, Vol. 3, p. 987, Figure 194 for mass transfer to packed bed particles.

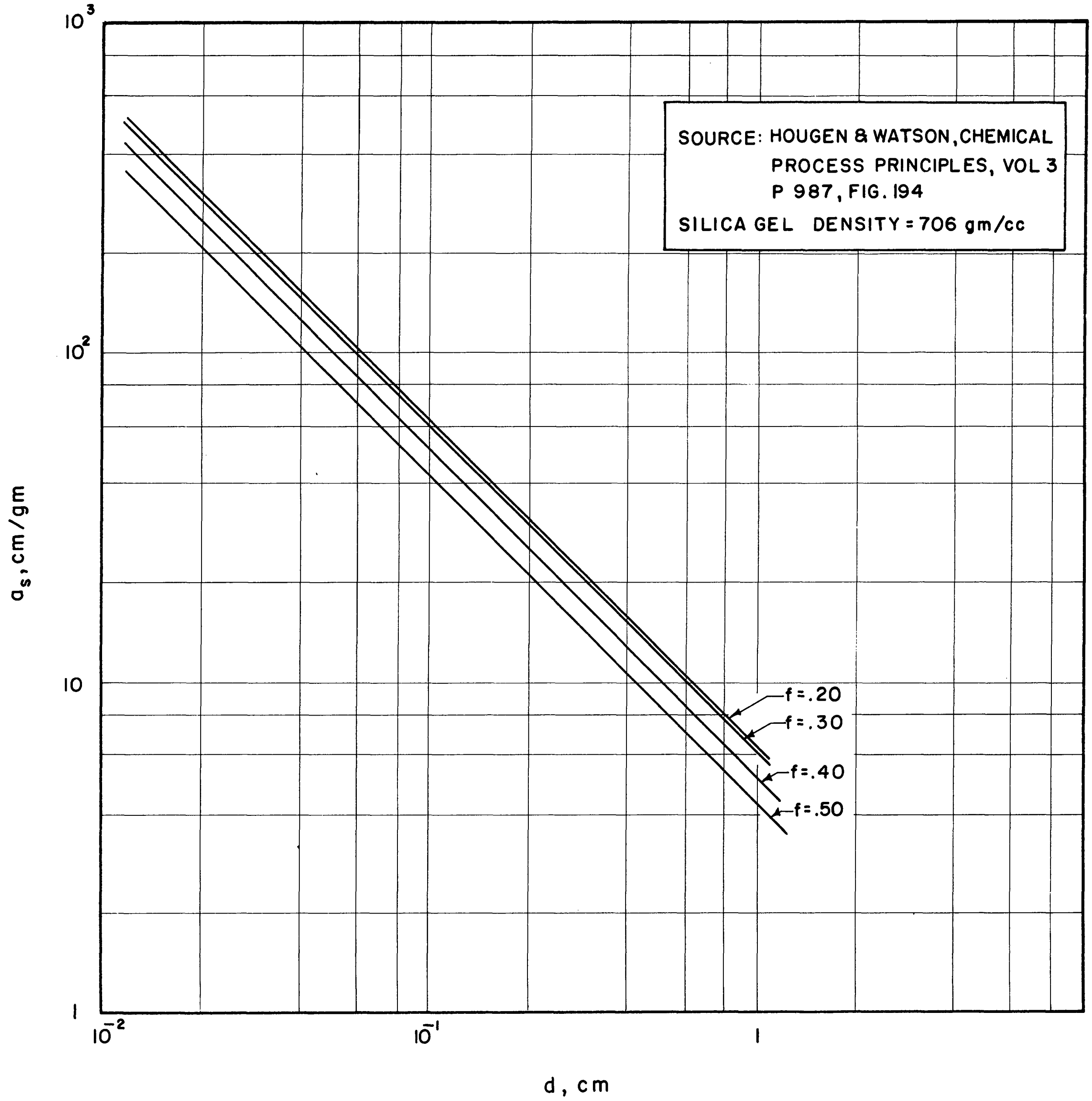


Figure 16. Specific Area for Mass Transfer.

APPENDIC C

THE POLANYI ADSORPTION POTENTIAL THEORY

A. Theory

According to Polanyi,(4,7,19) an adsorbent particle exerts a strong attractive force upon molecules of the surround fluid, this force giving rise to adsorption. Since succeeding depths of adsorbed material will contribute to the compression of underlying material, the density of this material will range from highest at the adsorbent surface to the bulk density at a sufficient distance from the particle.

Eucken was the first to describe the adsorptive force in terms of an intermolecular potential gradient and later Polanyi quantitatively described this potential at a point as the work done by the adsorptive force in bringing a molecule from the gas phase to that point.

For an isothermal system, the reversible work of compression is given by

$$\underline{W}_R = \int_{P_1}^{P_2} \underline{V}dP = \Delta\underline{F} \text{ between point 1 and point 2} \qquad (C1)$$

By definition the Polanyi adsorption potential at a point near the particle is this reversible isothermal work of compression or the difference in free energy $\underline{F}$ between that point and the adsorbent surface.

$$\epsilon_i = \int_{P_i}^{P_{surf}} \underline{V}dP \qquad (C2)$$

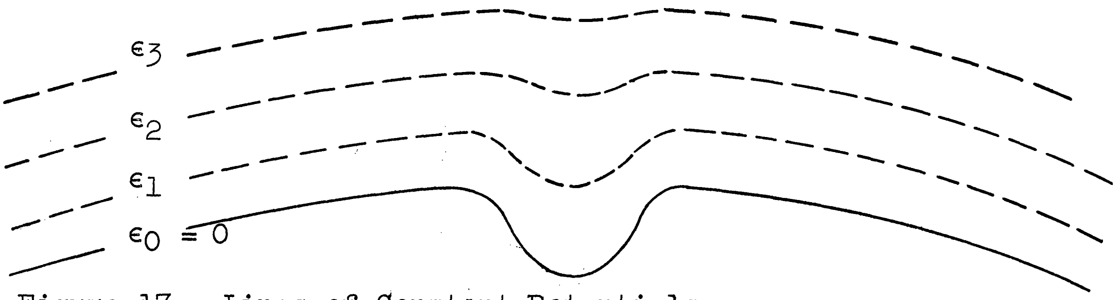


Figure 17. Lines of Constant Potentials.

Thus we can visualize shells of constant adsorption potential surrounding the adsorbent particle (Figure 17). The value of the potential on any one of these surfaces will be a function of the volume of material adsorbed and so we can find a relationship of the for $\epsilon = f(\phi)$. This is the so-called adsorption "characteristic" or distribution" curve.

Since the adsorption potential expresses the work of temperature-independent forces, the distribution curve should be independent of temperature.

Computation of the adsorption potential requires a knowledge of the equation of state for the fluid in question both in the gaseous and in the adsorbed (liquid) state.

As shown by Brunauer, we can visualize the variation of specific volume $\underline{V}$ for three typical systems as in the following Figure 18.

Case I represents a system far below the critical temperature and near saturation pressure so that practically all the adsorption volume i is filled with liquid.

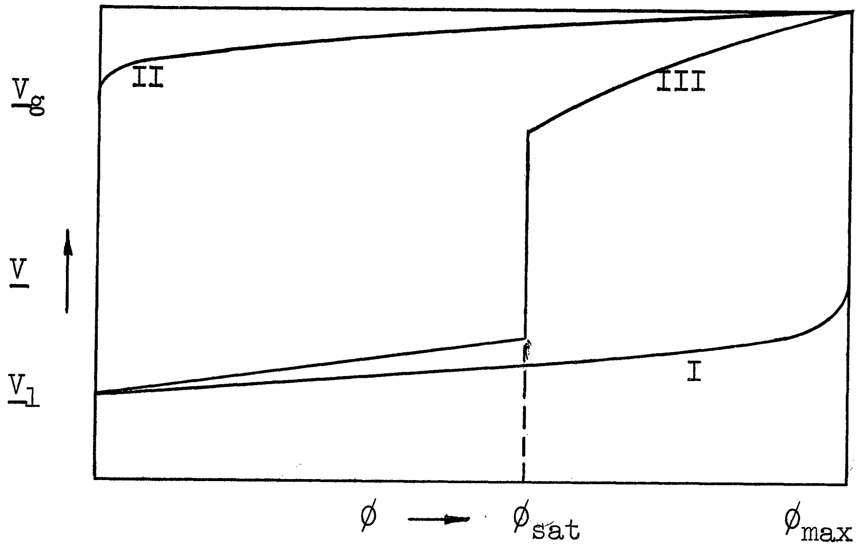


Figure 18. Variation of Adsorbed Specific Volume with Adsorbed Volume for Three Typical Cases.

Case II represents a gaseous system above the critical temperature so that practically all the adsorption volume contains material of high specific volume.

Case III represents a gas intermediate to the other two. In this case ϕ_{sat} contains adsorbed liquid and the volume $\phi_{max} - \phi_{sat}$ contains gas.

For case I, the integral $\int VdP$ is adequately represented if we consider only that part of the integral arising from compression of the gas to the point of condensation. That is, we consider the liquid to be incompressible.

Even for case II, it can be seen that if that part of the adsorption space containing gas is large compared to that containing liquid, the specific volume of the liquid is so much smaller that the largest mass of the adsorbed material is in the liquid phase and the same method of computing the adsorption potential may be useful.

B. Application to Propylene and Propane Isotherm Data

In this work, the gases are well described by case I and so the adsorption potential was taken as

$$\epsilon = RT \log_e(\frac{f_s}{f}) \qquad (C3)$$

where f_s is the fugacity of saturated liquid at adsorption temperature, f is the fugacity at adsorption pressure.

The adsorbed volume is computed from the following relation:

$$\phi = N\underline{V}_s$$

where N is the amount adsorbed in mg-mols per gm of adsorbent and $\underline{V}_s$ is the molal volume of saturated liquid at adsorption temperature.

The data of Lewis _et_ _al_. were recomputed to obtain the data on the distribution curve of Figures 19 and 20. A power series fit was then made of the two distribution curves as shown in Appendix B, section E. The resulting correlation was then tested by recomputing the isotherms shown in Figure 21 and Figure 22. Points plotted are the original Lewis data.

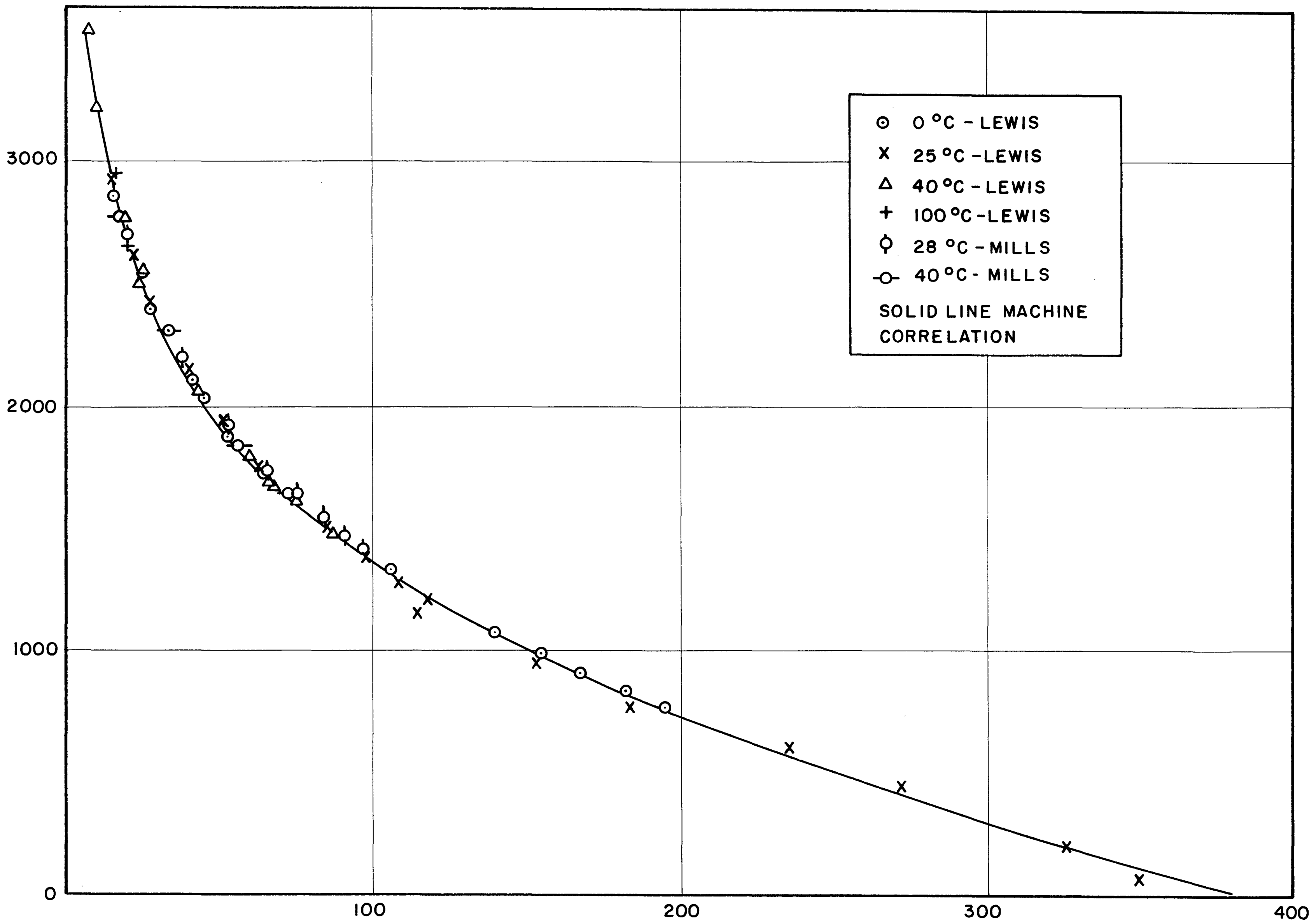


Figure 19. Polanyi Adsorption Potential Characteristic Curve for Propane on Silica Gel.

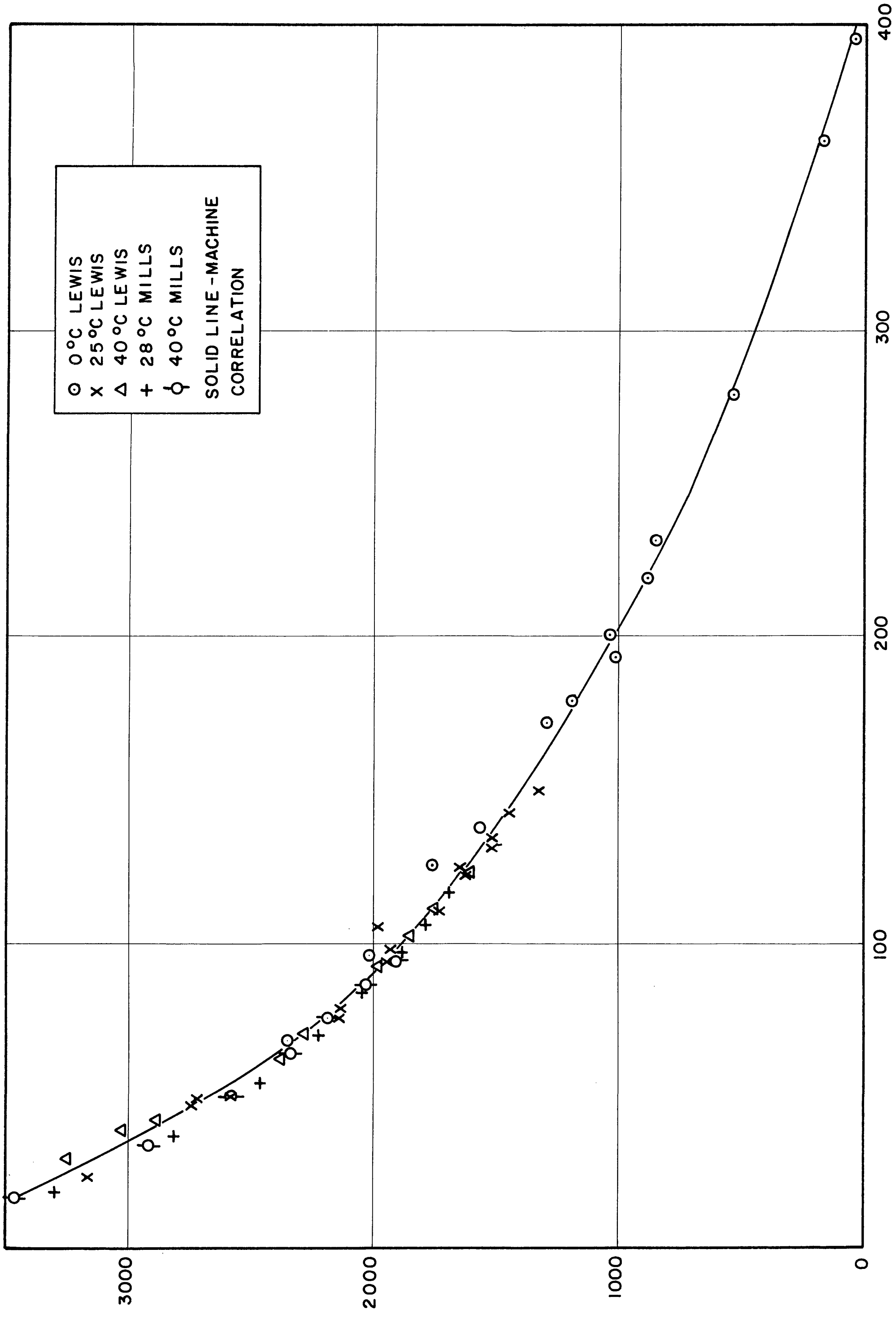


Figure 20. Polanyi Adsorption Potential Characteristic Curve for Propylene on Silica Gel.

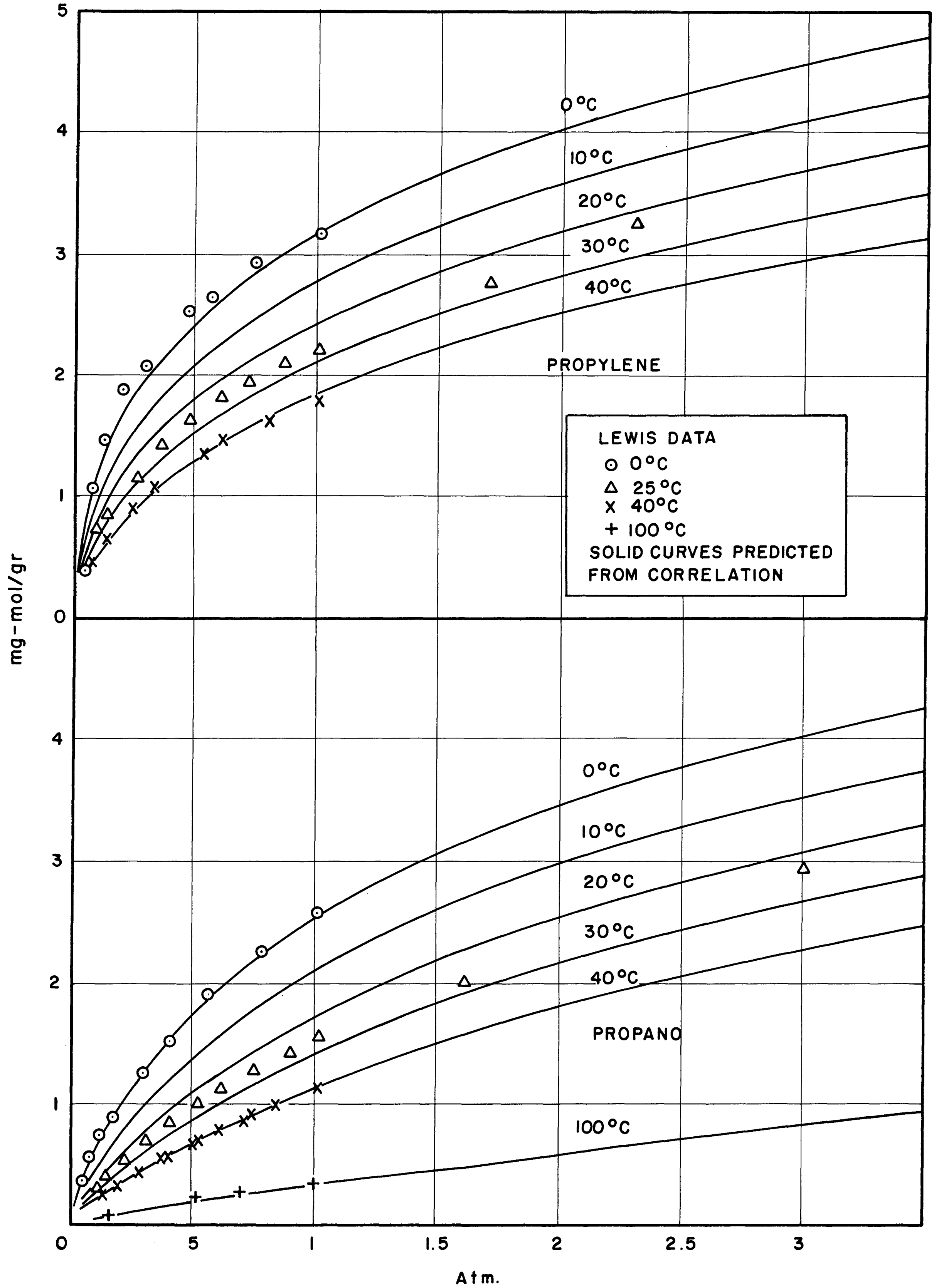


Figure 21. Predicted Isotherms with Experimental Points for Propane.

APPENDIX D

CALIBRATIONS

A. System Volumes

Total system plus one sampling manometer	1	1194 cc.
	2	1191.6
	ave.	1193 cc.
One sampling manometer and leads		37 cc.
Total volume of system		1156 cc.

TABLE XVII

DISTRIBUTION OF VOLUMES IN SYSTEM

1.	Inlet valve to bottom of bed in cell 1	300 cc.
2.	Top of bed 1 to sample point in cell 1	64 cc.
3.	Sample point 1 to bottom of bed 2	223 cc.
4.	Top of bed 2 to sample point in cell 2	64 cc.
5.	Sample point 2 to bottom of bed 3	223 cc.
6.	Top of bed 3 to sample	64 cc.
7.	Sample point 3 to outlet valve	104 cc.
8.	Volume of beds	150 cc.

B. Flowmeters

Flowmeters were calibrated by passing propane or propylene through the system, recording readings simultaneously from all four manometers and measuring the actual flowrate by downward displacement of water timed with an electric counter. The results of the calibration runs are given in Table XVIII. These results were correlated least squares to obtain the coefficients in the four equations following. The form of the equations comes from the orifice formula

$$W = K\sqrt{\rho}\,(\Delta P)^{a} \qquad \text{(D1)}$$

It is likely that the positioning of the pressure taps some distance from the orifice resulted in the exponent a differing from the theoretical value of 1/2.

Inlet manometer $W/\sqrt{\rho} = .1693(\Delta P)^{.5531}$ (D2)

Manometer #1 $W/\sqrt{\rho} = .1567(\Delta P)^{.5655}$ (D3)

Manometer #2 $W/\sqrt{\rho} = .1607(\Delta P)^{.5302}$ (D4)

Manometer #3 $W/\sqrt{\rho} = .1814(\Delta P)^{.5124}$ (D5)

C. System Pressure Drop

By actual measurement the pressure drop through the system was the sum of the orifice pressure drops within the experimental error. That is, the resistance of the beds was negligible at the flow rates used.

D. Analysis - Calibration of Chromatography Results

Since the gas mixtures to be analyzed are simple binaries containing only propylene and propane, and since these two gases are very similar in physical properties, a simple ratio of peak areas to total of the two peak areas was used as a measure of the mol fraction of each gas.

TABLE XVIII

FLOWMETER CALIBRATION DATA

Gas	Orifice Pressure Drops mm Acet. Tetrabromide				Bar. Press mm Hg	Sys Temp. °C	Coll Temp. °C		Vol. Coll. cc.	Elapsed Time sec.
	I	1	2	3						
C_3H_8	20.0	21.5	25.5	23.0	737.4	25.0	25.0	1	1860	168.4
								2	1855	168.9
								3	1860	169.5
C_3H_8	47.0	48.0	64.0	56.5	737.4	25.0	25.0	1	1866	102.4
								2	1933	104.5
								3	1882	101.8
C_3H_8	89.0	92.5	119.5	114.5	737.4	25.0	25.0	1	1815	69.7
								2	1840	70.7
								3	1840	71.0
C_3H_8	140.0	150.0	192.0	192.0	737.4	25.0	25.0	1	1840	54.3
								2	1840	54.2
C_3H_8	10.5	12.0	15.0	13.0	737.1	25.0	25.0	1	1825	221.5
								2	1830	227.0
C_3H_8	30.0	33.0	41.0	37.0	736.8	25.0	25.0	1	1820	127.5
								2	1835	129.0
C_3H_8	28.0	29.5	36.5	32.7	736.8	25.0	20.0	1	1980	144.4
								2	1980	142.4
								3	1965	140.3
C_3H_6	98.5	104.0	134.5	129.0	736.8	25.0	20.0	1	1940	70.1
								2	1960	70.2

Synthetic mixtures of known proportions were made up and analyzed. The comparison of the analysis and known composition is given in Table XIX for the calibration analyses.

TABLE XIX

CALIBRATION OF CHROMATOGRAPHY RESULTS

Mol Fraction Propylene			
Analysis	Known	Deviation	Percent Dev.
.558	.539	- .019	- 3.4
.374	.389	.015	4.0
.688	.703	.015	2.2
.568	.565	.003	- 0.5
.528	.557	.029	5.5
.256	.255	- .001	- 0.4
.867	.894	.027	3.1
.133	.142	.009	6.7
.427	.404	- .023	- 5.4
.149	.160	.011	7.0
.921	.924	.003	0.3
.457	.448	- .009	- 2.0
.268	.282	.016	6.0
.891	.921	.030	3.4
.275	.290	.015	5.5
.930	.938	.008	0.9
.786	.809	.023	2.9
.904	.898	- .006	- 0.6
.667	.690	.023	3.5
.0843	.094	.010	11.9
.933	.942	.011	1.2
.0658	.0624	- .0034	- 5.0

Average absolute percentage deviation 3.7%.

APPENDIX E

COMPUTER FLOWSHEETS

A. Data Reduction Routine

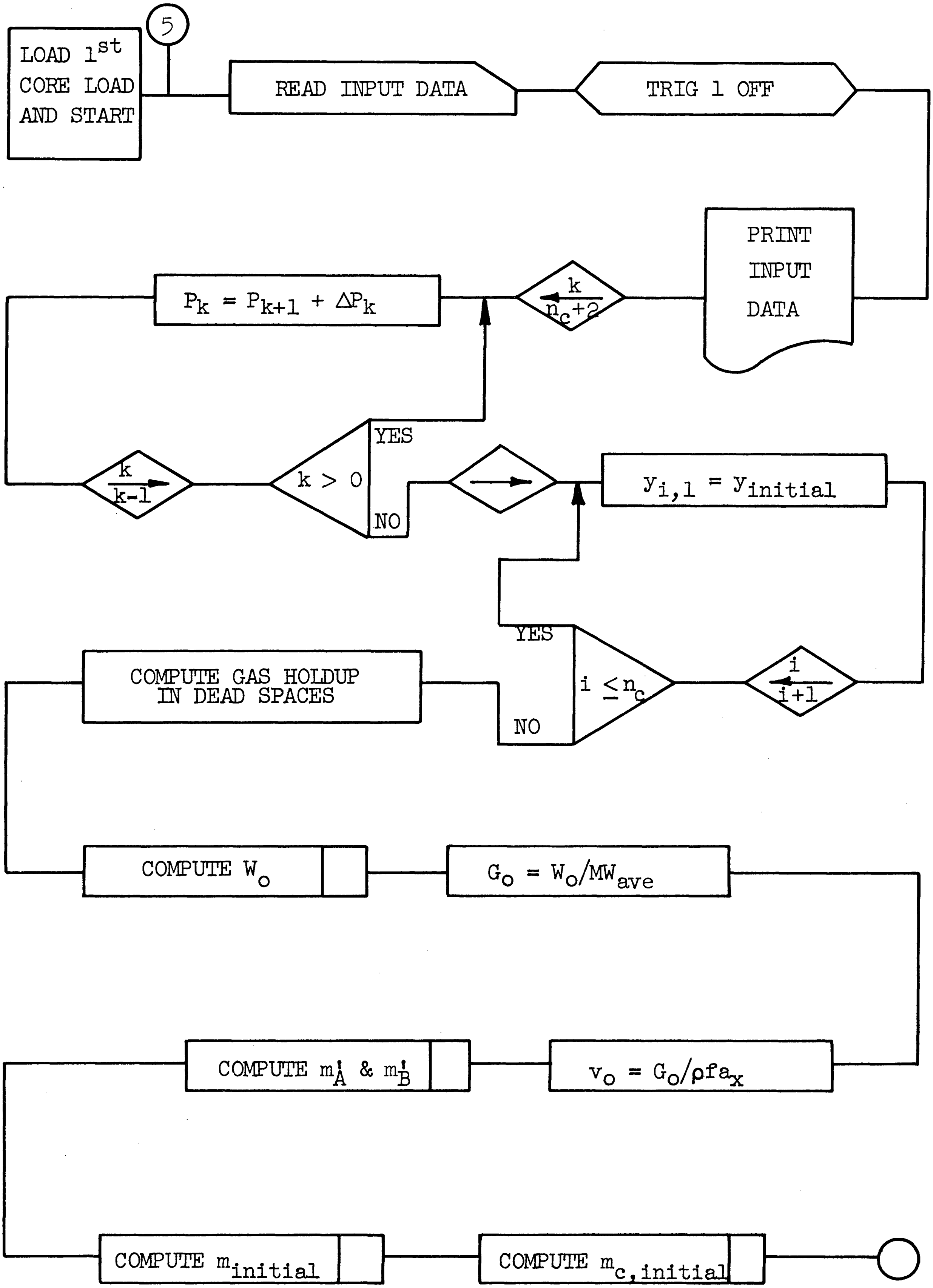
The detailed flowsheet for all calculations as performed by the IBM 704 in reducing the break-through curves to values of the diffusion coefficient D is here given.

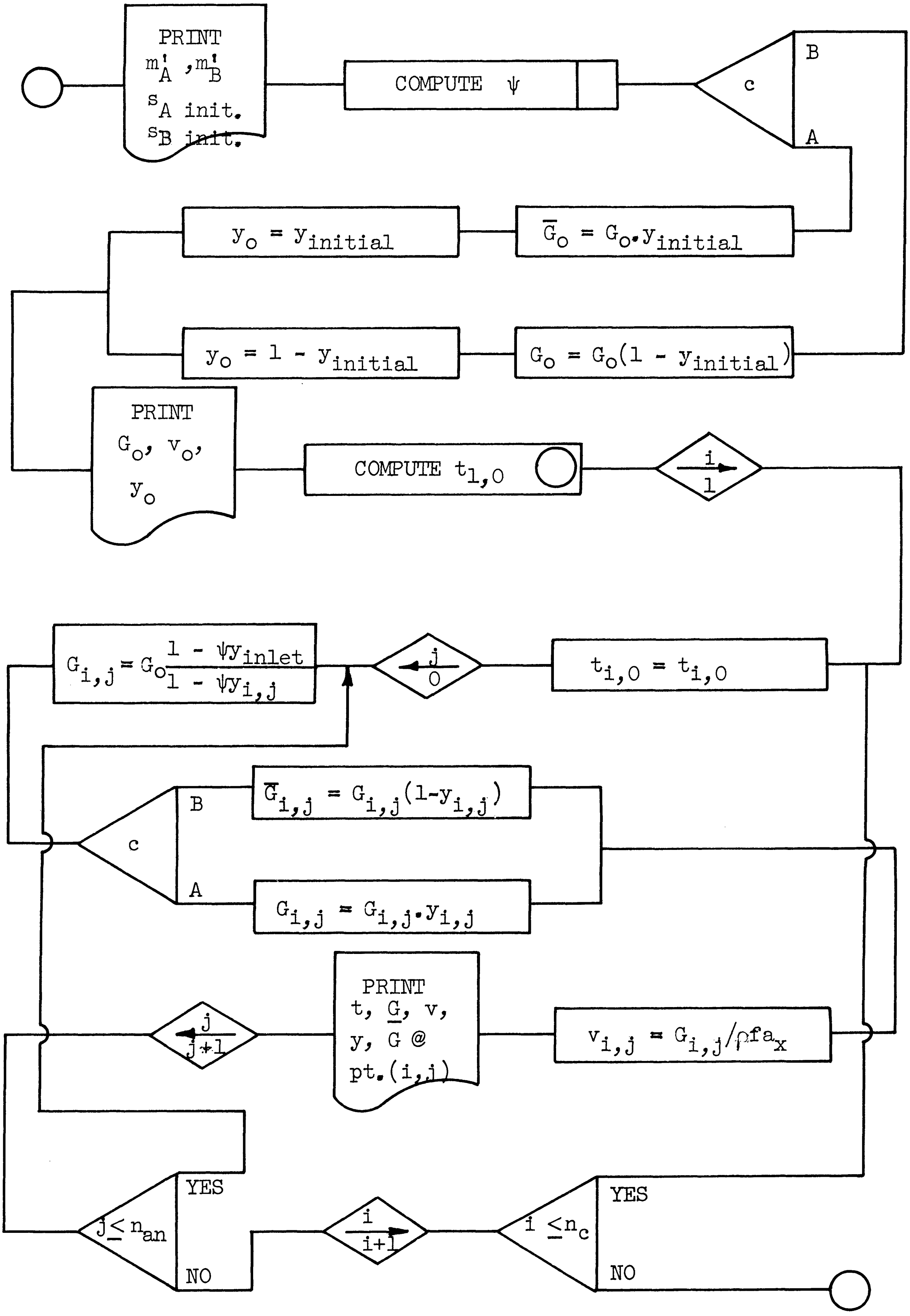
FIGURE 22

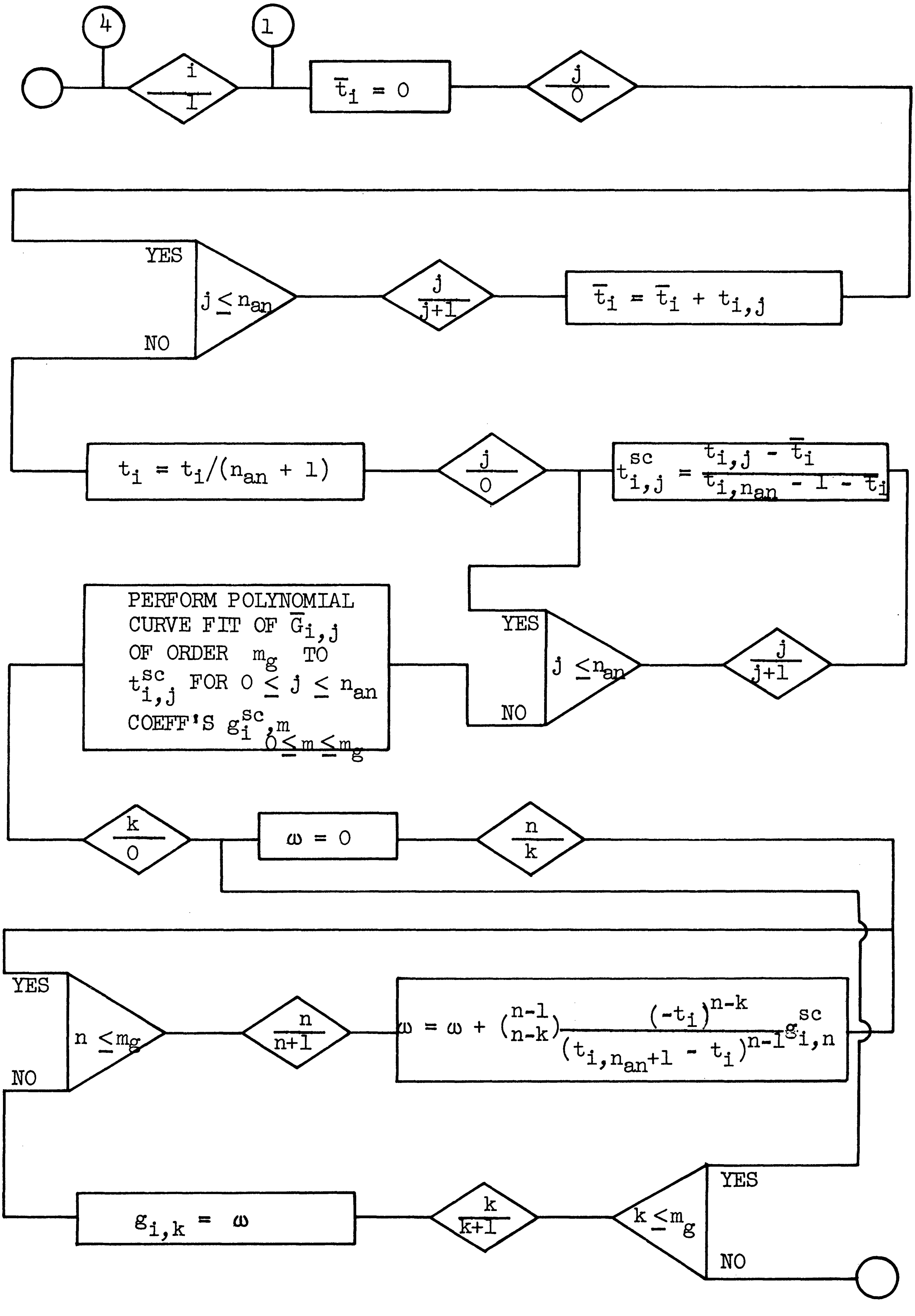
DATA PROCESSING CALCULATIONS

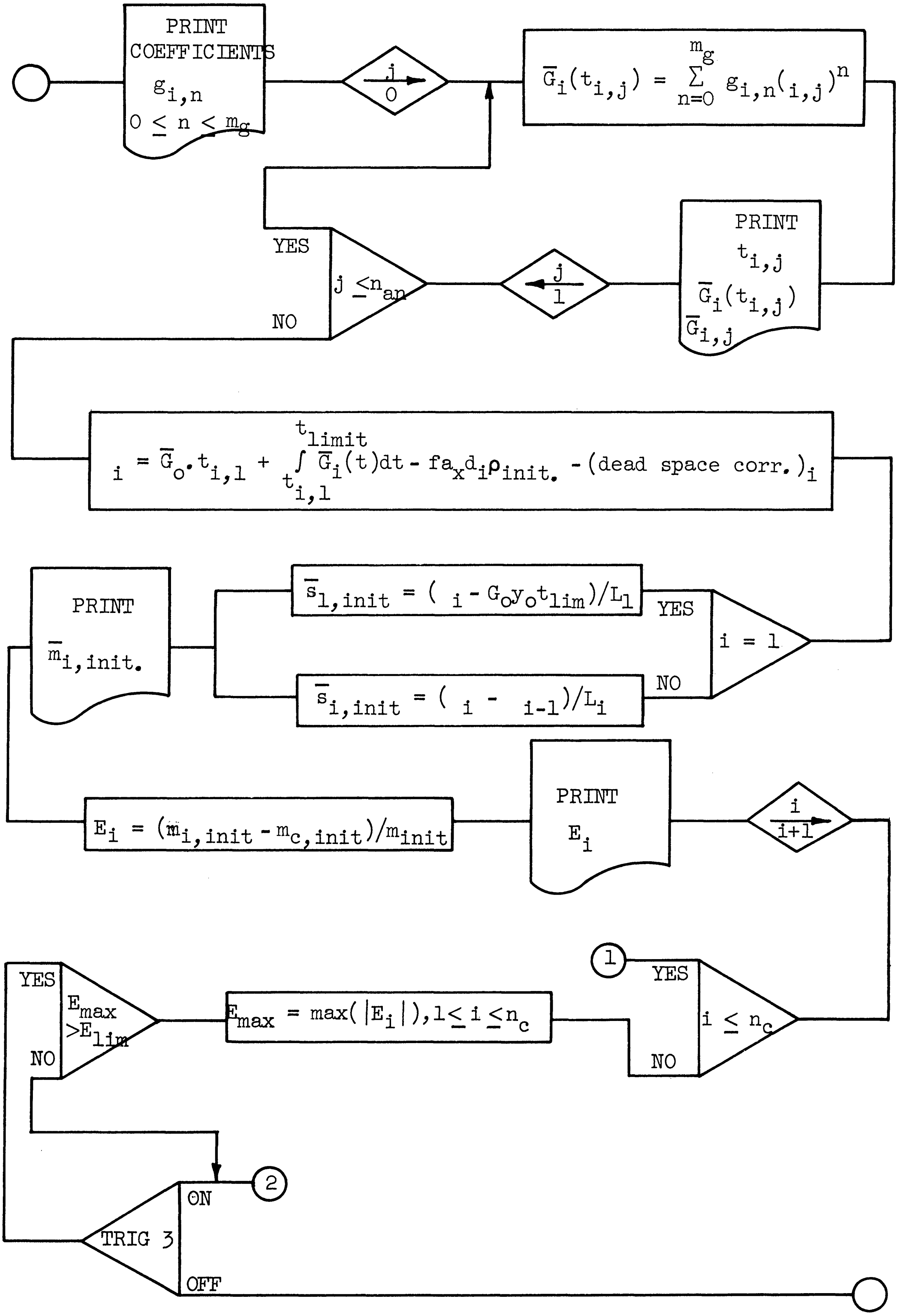
COMPUTER FLOW SHEETS

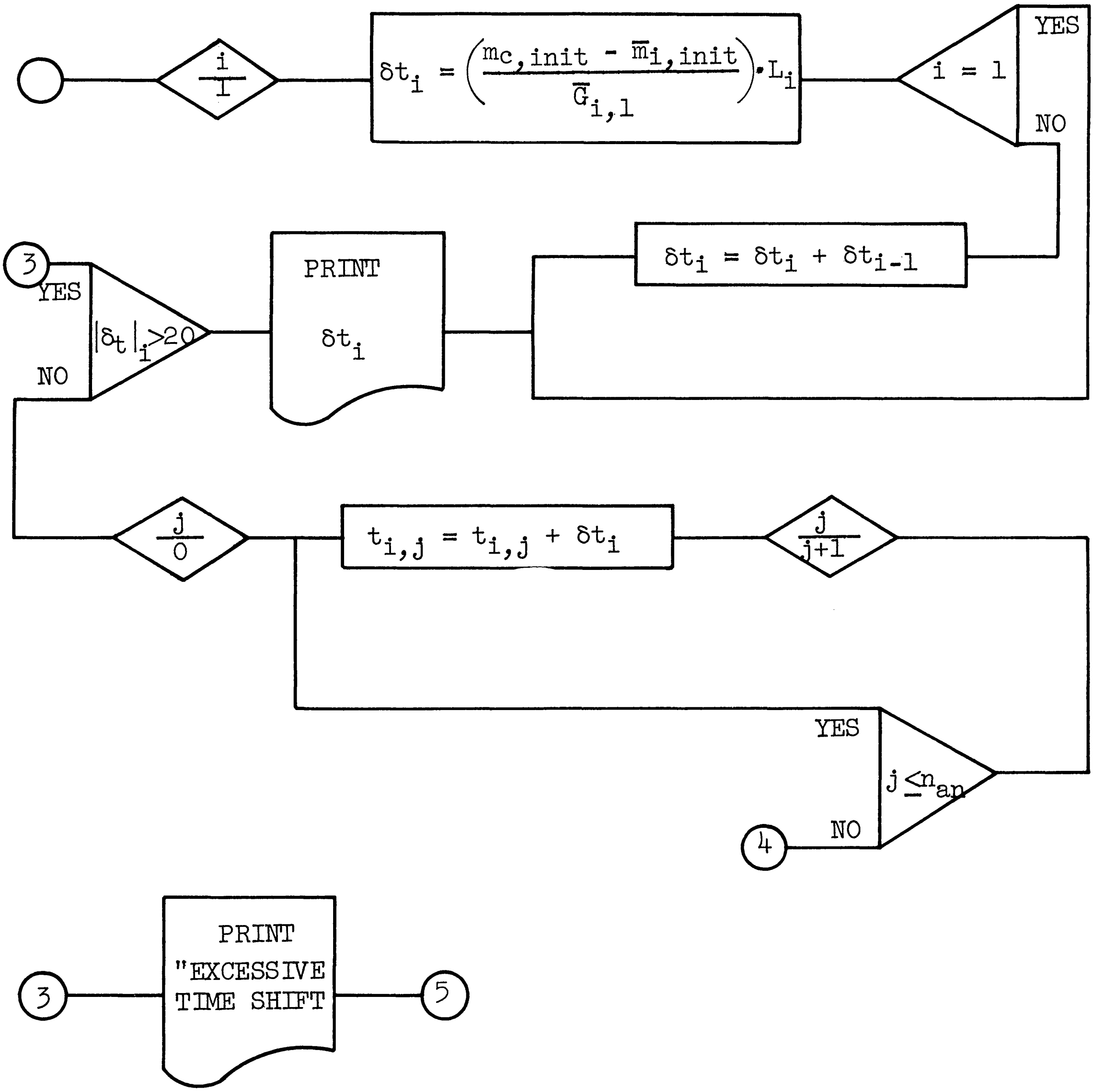
MASS BALANCE CLOSURE CALCULATIONS

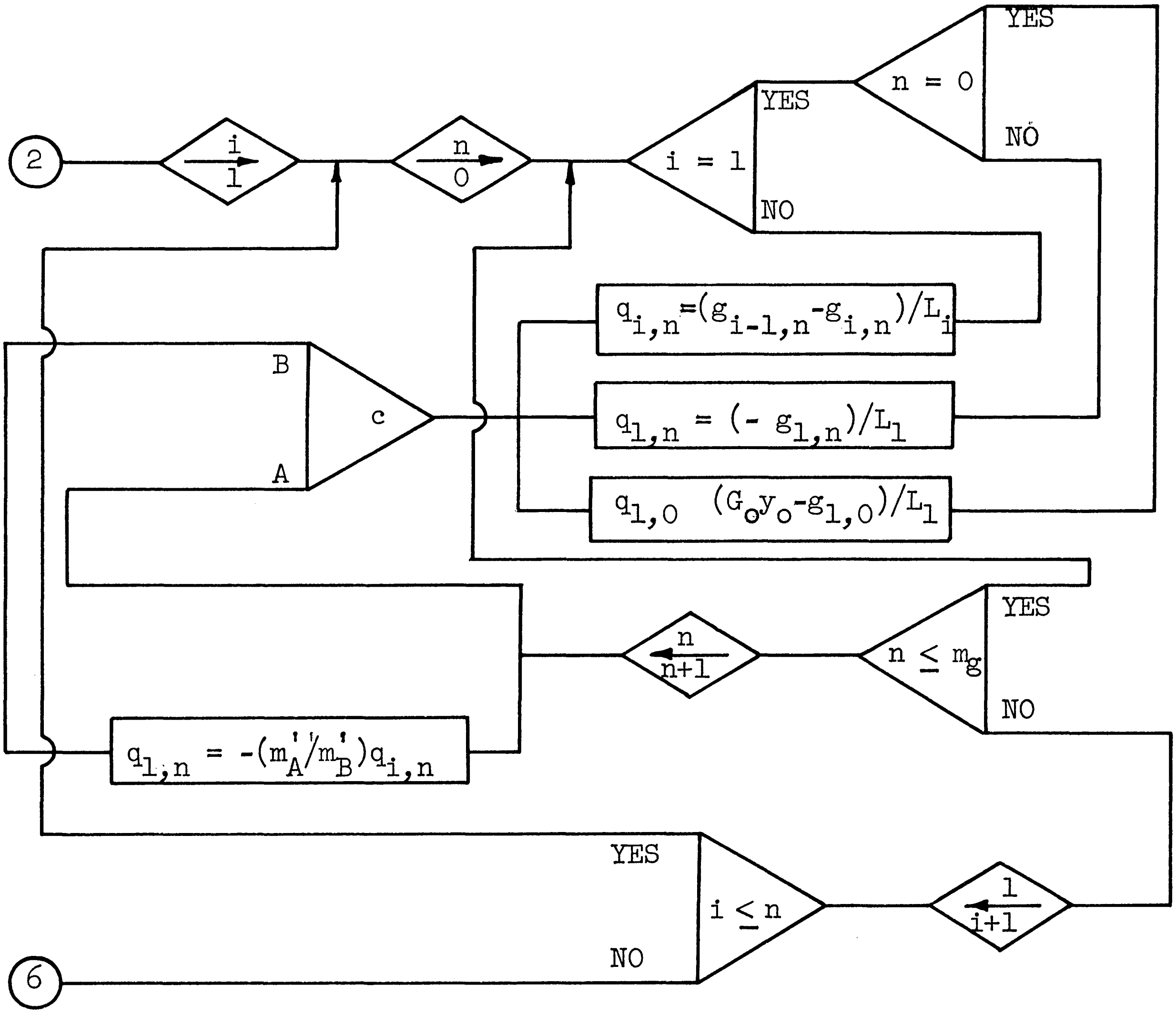


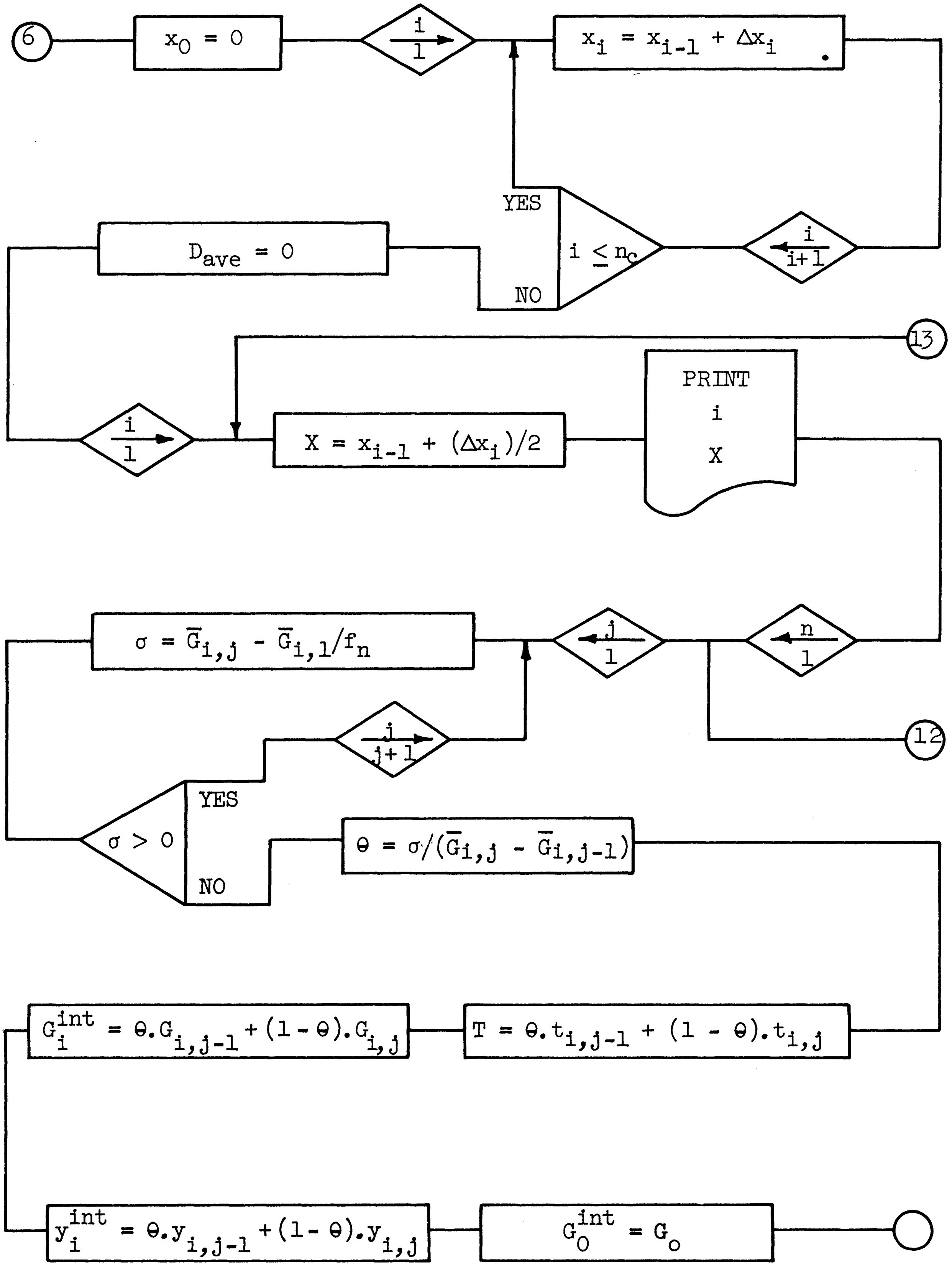

PRINT
m'A ,m'B
sA init.
sB init.
COMPUTE ψ
c
B
A
yo = yinitial
Ḡo = Go·yinitial
yo = 1 - yinitial
Go = Go(1 - yinitial)
PRINT
Go, vo,
yo
COMPUTE t1,0
i / 1
Gi,j = Go (1 - ψyinlet)/(1 - ψyi,j)
j / 0
ti,0 = ti,0
B
c
A
Ḡi,j = Gi,j(1-yi,j)
Gi,j = Gi,j·yi,j
j / j+1
PRINT
t, G, v,
y, G @
pt.(i,j)
vi,j = Gi,j/ρfax
j ≤ nan
YES
NO
i / i+1
i ≤ nc
YES
NO

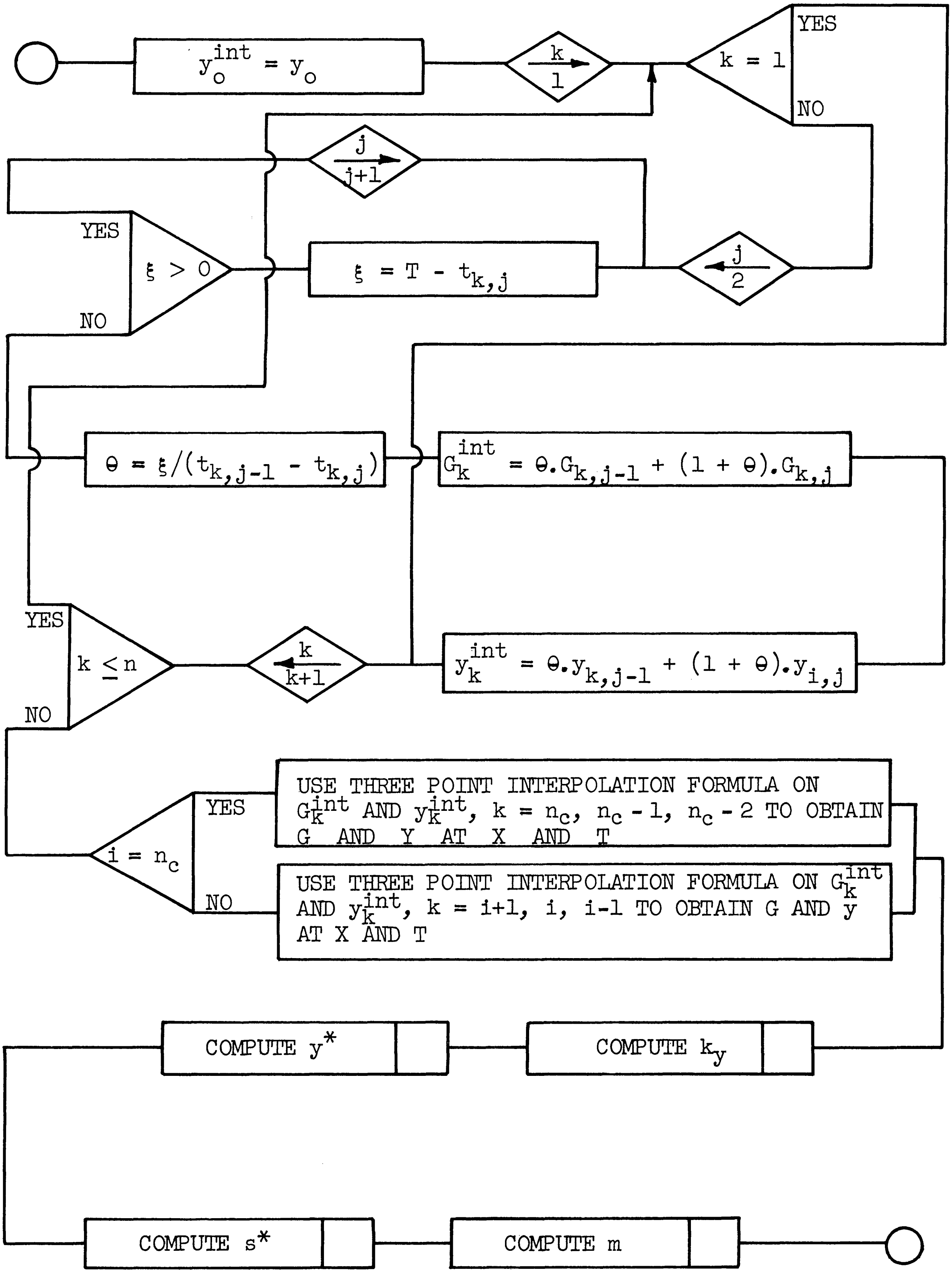

4
1
$\frac{i}{1}$
$\bar{t}_i = 0$
$\frac{j}{0}$
YES
$j \leq n_{an}$
NO
$\frac{j}{j+1}$
$\bar{t}_i = \bar{t}_i + t_{i,j}$
$t_i = t_i/(n_{an} + 1)$
$\frac{j}{0}$
$t^{sc}_{i,j} = \frac{t_{i,j} - \bar{t}_i}{t_{i,n_{an}} - 1 - \bar{t}_i}$
PERFORM POLYNOMIAL CURVE FIT OF $\bar{G}_{i,j}$ OF ORDER m_g TO $t^{sc}_{i,j}$ FOR $0 \leq j \leq n_{an}$ COEFF'S $g^{sc}_{i,m}$ $0 \leq m \leq m_g$
YES
$j \leq n_{an}$
NO
$\frac{j}{j+1}$
$\frac{k}{0}$
$\omega = 0$
$\frac{n}{k}$
YES
$n \leq m_g$
NO
$\frac{n}{n+1}$
$\omega = \omega + \binom{n-1}{n-k} \frac{(-t_i)^{n-k}}{(t_{i,n_{an}+1} - t_i)^{n-1}} g^{sc}_{i,n}$
$g_{i,k} = \omega$
$\frac{k}{k+1}$
$k \leq m_g$
YES
NO

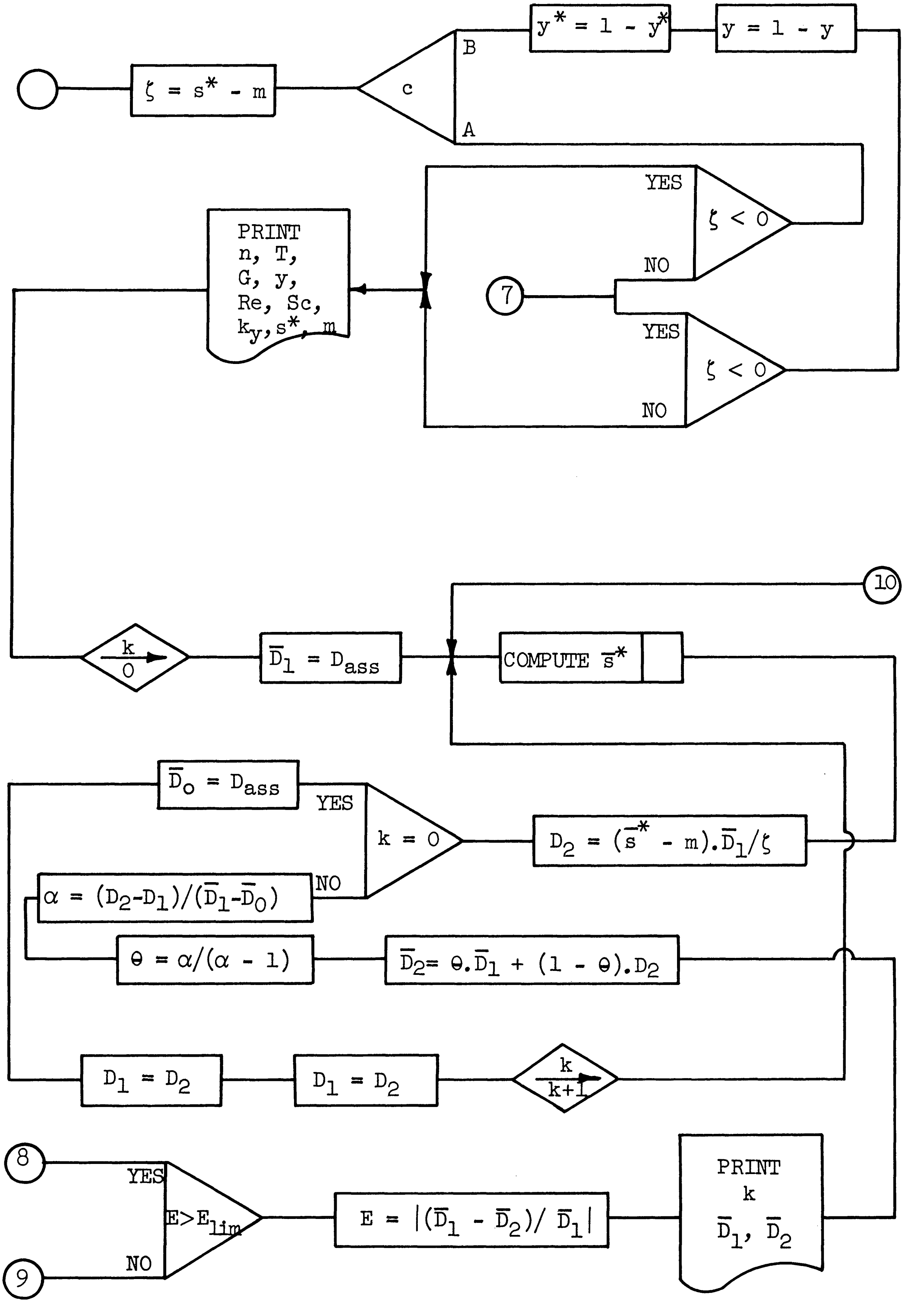

PRINT
COEFFICIENTS
$g_{i,n}$
$0 \le n \le m_g$
$\frac{j}{0}$
$\bar{G}_i(t_{i,j}) = \sum_{n=0}^{m_g} g_{i,n}(_{i,j})^n$
PRINT
$t_{i,j}$
$\bar{G}_i(t_{i,j})$
$\bar{G}_{i,j}$
$\frac{j}{1}$
YES
$j \le n_{an}$
NO
$_i = \bar{G}_o \cdot t_{i,1} + \int_{t_{i,1}}^{t_{limit}} \bar{G}_i(t)dt - fa_x d_i \rho_{init.} - (\text{dead space corr.})_i$
PRINT
$\bar{m}_{i,init.}$
$\bar{s}_{1,init} = (\ _i - G_o y_o t_{lim})/L_1$
$\bar{s}_{i,init} = (\ _i - \ _{i-1})/L_i$
YES
$i = 1$
NO
$E_i = (\bar{m}_{i,init} - m_{c,init})/m_{init}$
PRINT
E_i
$\frac{i}{i+1}$
1
YES
$i \le n_c$
NO
$E_{max} = \max(|E_i|), 1 \le i \le n_c$
YES
E_{max}
$>E_{lim}$
NO
2
ON
TRIG 3
OFF

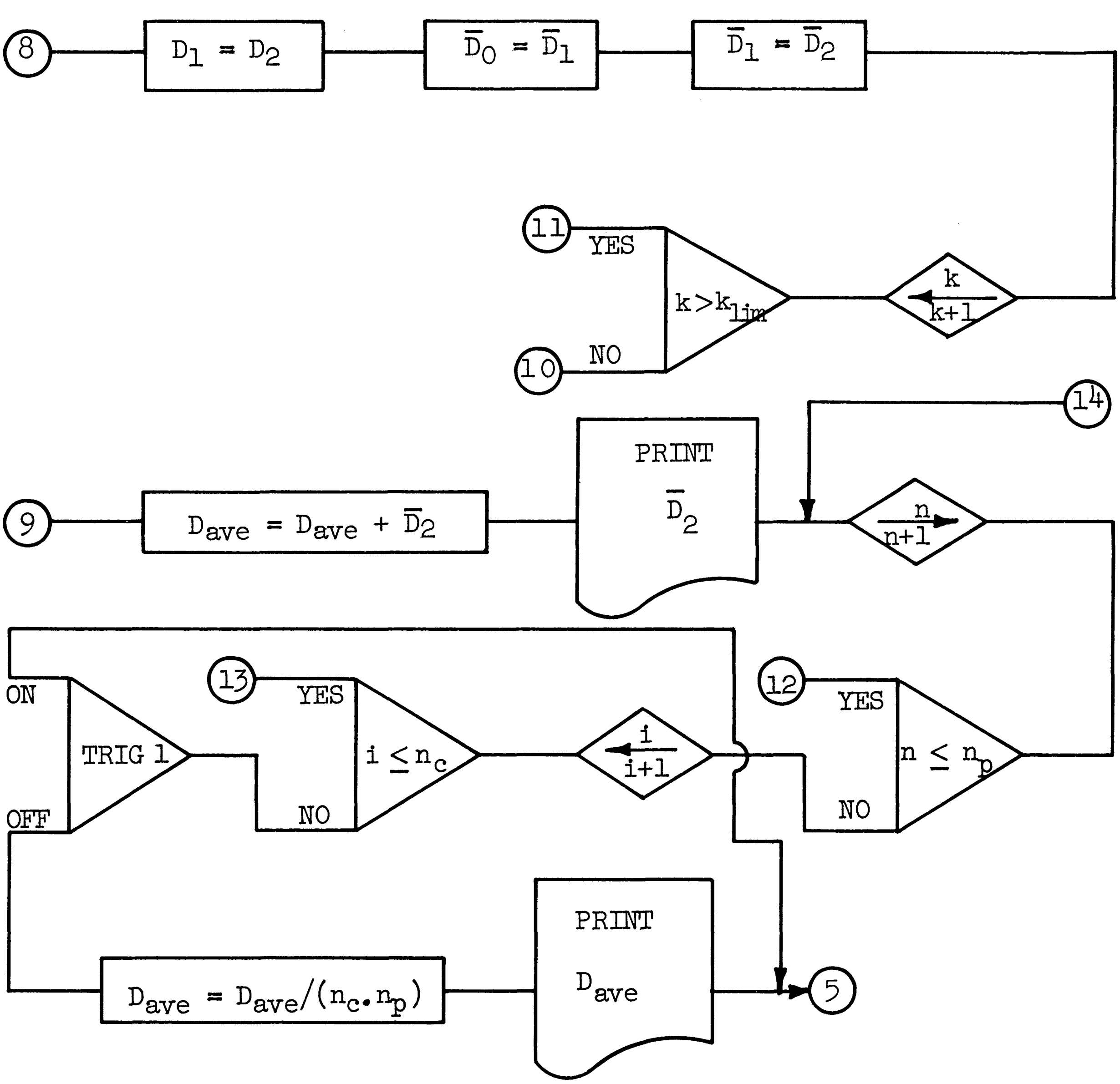

$\frac{i}{1}$
$\delta t_i = \left(\frac{m_{c,init} - \overline{m}_{i,init}}{\overline{G}_{i,1}}\right) \cdot L_i$
$i = 1$
YES
NO
$\delta t_i = \delta t_i + \delta t_{i-1}$
3
YES
$|\delta t|_i > 20$
NO
PRINT
δt_i
$\frac{j}{0}$
$t_{i,j} = t_{i,j} + \delta t_i$
$\frac{j}{j+1}$
YES
$j \leq n_{an}$
NO
4
3
PRINT
"EXCESSIVE
TIME SHIFT
5

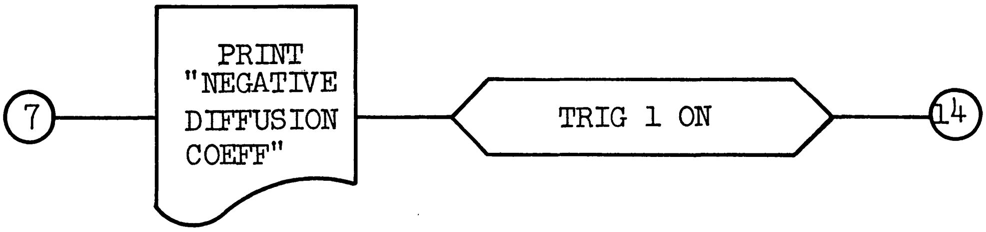

2
$i \leftarrow 1$
$n \leftarrow 0$
$i = 1$
YES
NO
$n = 0$
YES
NO
$q_{i,n} = (g_{i-1,n} - g_{i,n})/L_i$
$q_{1,n} = (- g_{1,n})/L_1$
$q_{1,0} \quad (G_o y_o - g_{1,0})/L_1$
B
c
A
YES
$n \leq m_g$
NO
$n \leftarrow n+1$
$q_{1,n} = -(m'_A/m'_B) q_{i,n}$
YES
$i \leq n$
NO
$1 \leftarrow i+1$
6

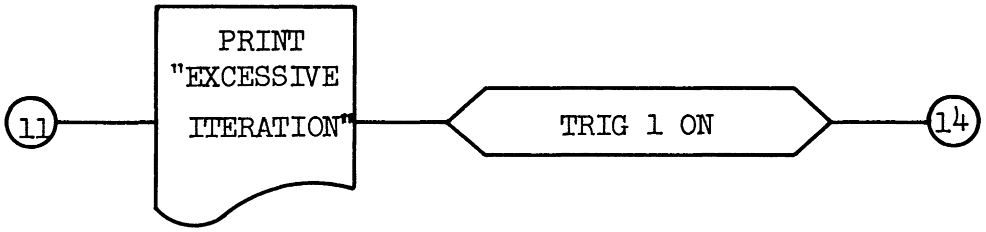

6
x₀ = 0
i / 1
xᵢ = xᵢ₋₁ + Δxᵢ
i / i+1
i ≤ n_c
YES
NO
D_ave = 0
13
i / 1
X = xᵢ₋₁ + (Δxᵢ)/2
PRINT
i
X
n / 1
j / 1
12
σ = Ḡᵢ,ⱼ - Ḡᵢ,₁/fₙ
j / j+1
σ > 0
YES
NO
Θ = σ/(Ḡᵢ,ⱼ - Ḡᵢ,ⱼ₋₁)
T = Θ.tᵢ,ⱼ₋₁ + (1 - Θ).tᵢ,ⱼ
Gᵢ^int = Θ.Gᵢ,ⱼ₋₁ + (1 - Θ).Gᵢ,ⱼ
yᵢ^int = Θ.yᵢ,ⱼ₋₁ + (1 - Θ).yᵢ,ⱼ
G₀^int = G₀


$y_o^{int} = y_o$
$k \xrightarrow{} 1$
$k = 1$
YES
NO
$j \xrightarrow{} j+1$
YES
$\xi > 0$
NO
$\xi = T - t_{k,j}$
$j \xleftarrow{} 2$
$\theta = \xi/(t_{k,j-1} - t_{k,j})$
$G_k^{int} = \theta . G_{k,j-1} + (1 + \theta) . G_{k,j}$
YES
$k \leq n$
NO
$k \xleftarrow{} k+1$
$y_k^{int} = \theta . y_{k,j-1} + (1 + \theta) . y_{i,j}$
$i = n_c$
YES
NO
USE THREE POINT INTERPOLATION FORMULA ON G_k^{int} AND y_k^{int}, $k = n_c$, $n_c - 1$, $n_c - 2$ TO OBTAIN G AND Y AT X AND T
USE THREE POINT INTERPOLATION FORMULA ON G_k^{int} AND y_k^{int}, $k = i+1$, i, $i-1$ TO OBTAIN G AND y AT X AND T
COMPUTE y^*
COMPUTE k_y
COMPUTE s^*
COMPUTE m


$\zeta = s^* - m$
c
B
A
$y^* = 1 - y^*$
$y = 1 - y$
YES
$\zeta < 0$
NO
7
YES
$\zeta < 0$
NO
PRINT
n, T,
G, y,
Re, Sc,
k_y, s^*, m
$\xrightarrow{k} 0$
$\bar{D}_1 = D_{ass}$
COMPUTE $\bar{s}^*$
10
$\bar{D}_0 = D_{ass}$
YES
$k = 0$
NO
$D_2 = (\bar{s}^* - m).\bar{D}_1/\zeta$
$\alpha = (D_2-D_1)/(\bar{D}_1-\bar{D}_0)$
$\theta = \alpha/(\alpha - 1)$
$\bar{D}_2 = \theta.\bar{D}_1 + (1 - \theta).D_2$
$D_1 = D_2$
$D_1 = D_2$
$\xrightarrow{k} k+1$
8
YES
$E > E_{lim}$
NO
9
$E = |(\bar{D}_1 - \bar{D}_2)/\bar{D}_1|$
PRINT
k
$\bar{D}_1, \bar{D}_2$


8
$D_1 = D_2$
$\bar{D}_0 = \bar{D}_1$
$\bar{D}_1 = \bar{D}_2$
11
YES
$k > k_{lim}$
$k \leftarrow k+1$
10
NO
14
PRINT $\bar{D}_2$
9
$D_{ave} = D_{ave} + \bar{D}_2$
$n \rightarrow n+1$
ON
TRIG 1
OFF
13
YES
$i \leq n_c$
NO
$i \leftarrow i+1$
12
YES
$n \leq n_p$
NO
$D_{ave} = D_{ave}/(n_c \cdot n_p)$
PRINT D_{ave}
5


7
PRINT "NEGATIVE DIFFUSION COEFF"
TRIG 1 ON
14


11
PRINT "EXCESSIVE ITERATION"
TRIG 1 ON
14

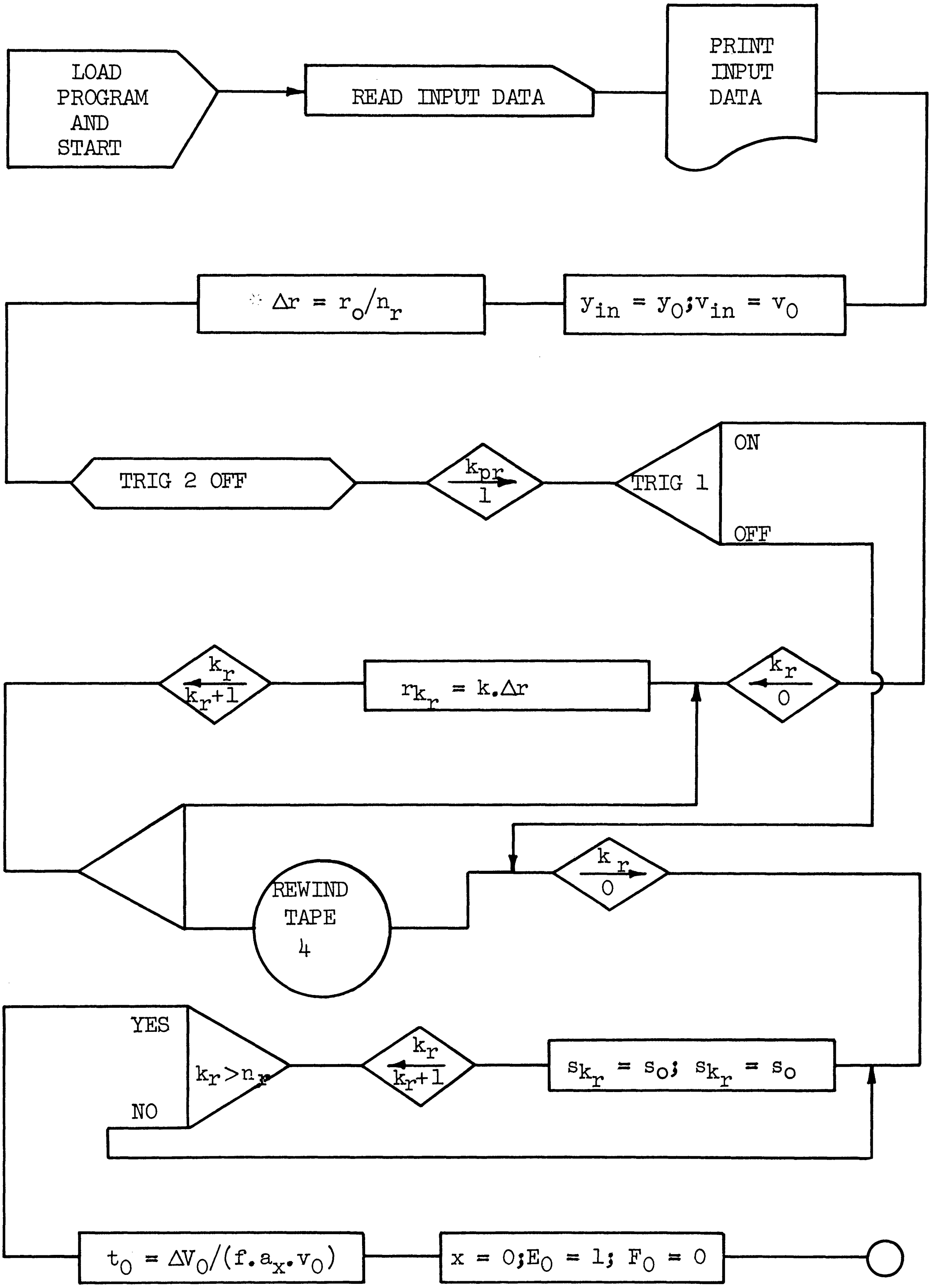
B. Plug-Flow Model Equation Solution

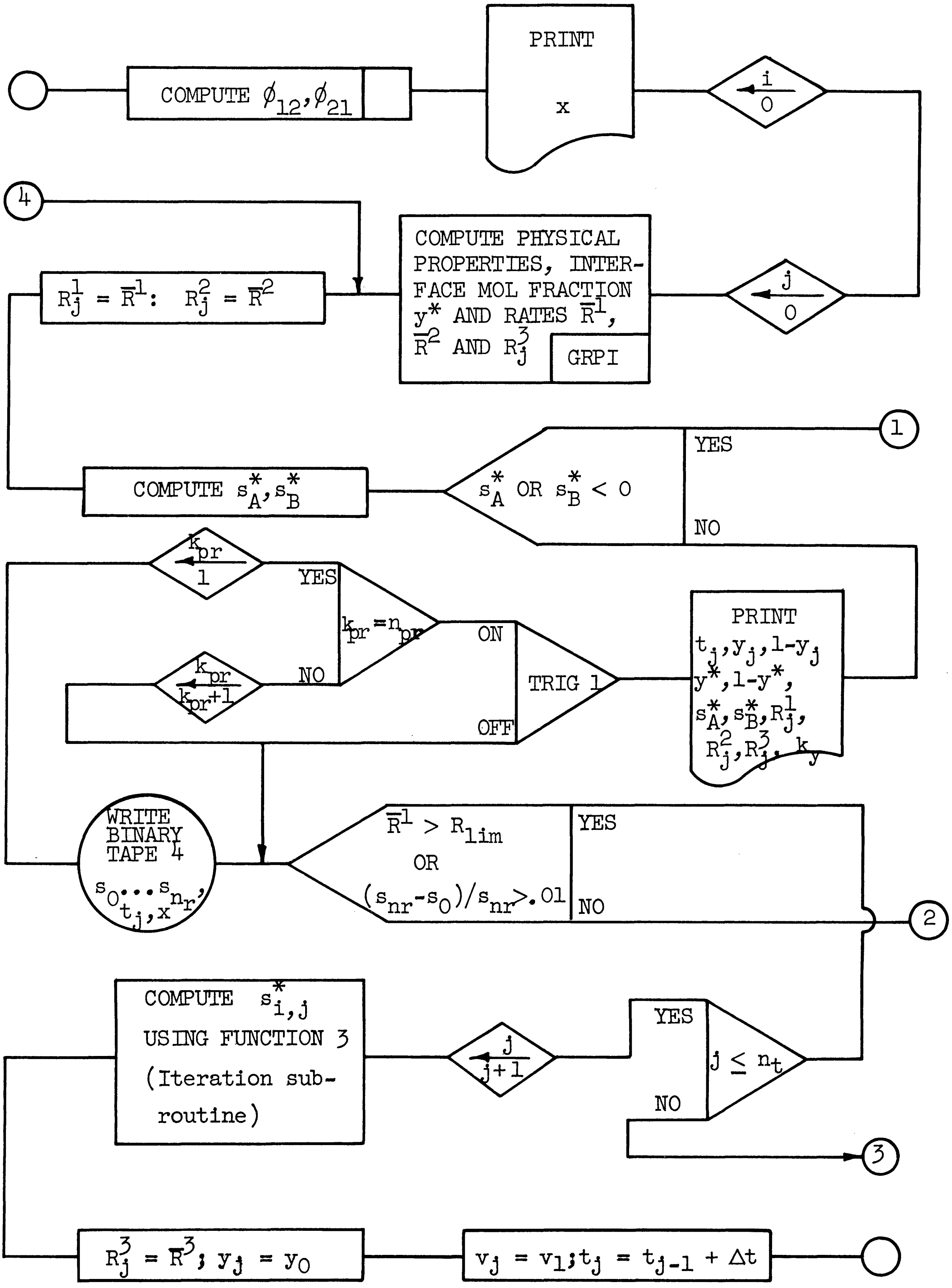
The following pages contain a detailed flowsheet of all calculation sequences used in the computer solution of the equations as detailed in the Theory section.

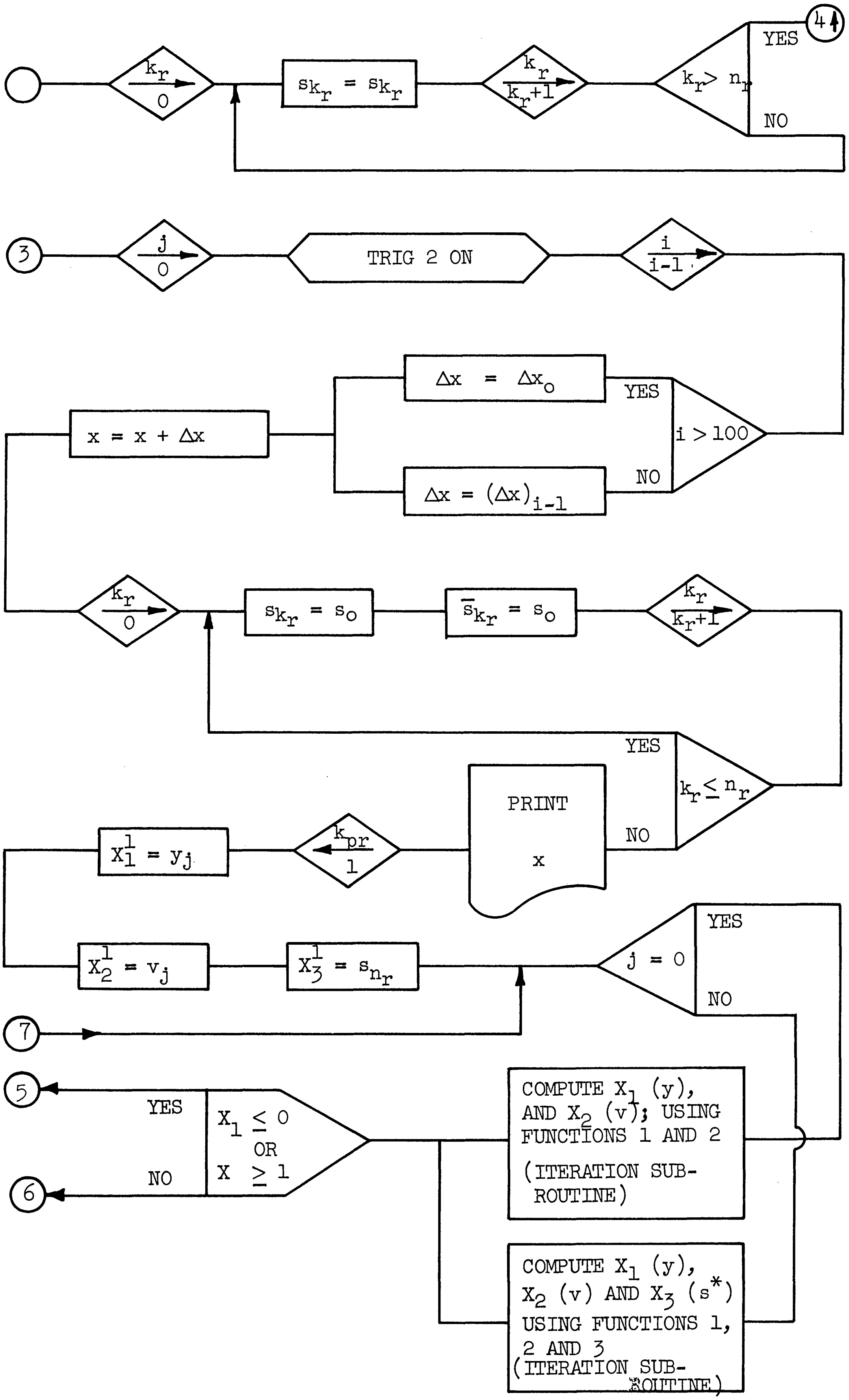
FIGURE 23

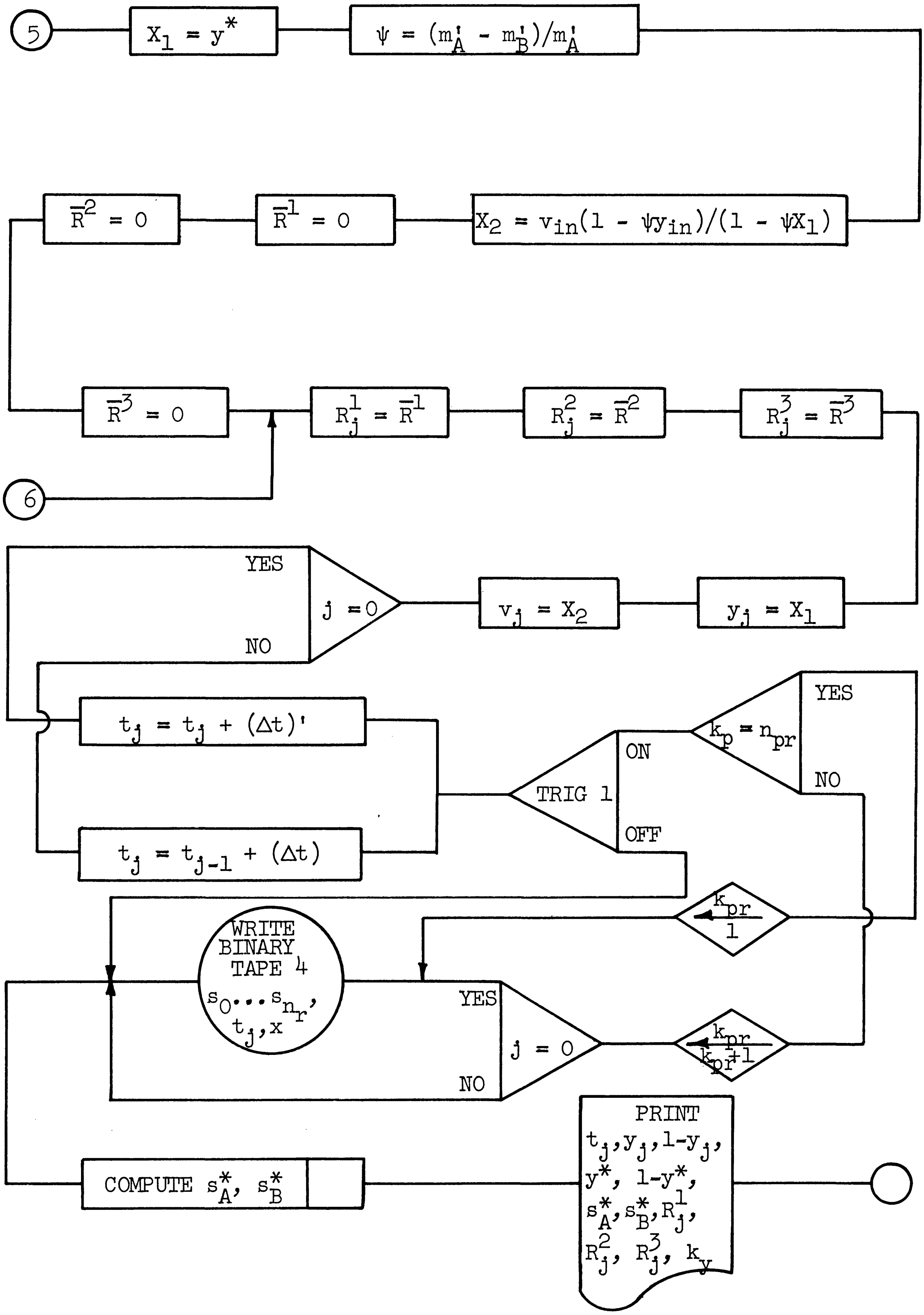
CONCENTRATION HISTORY CALCULATIONS

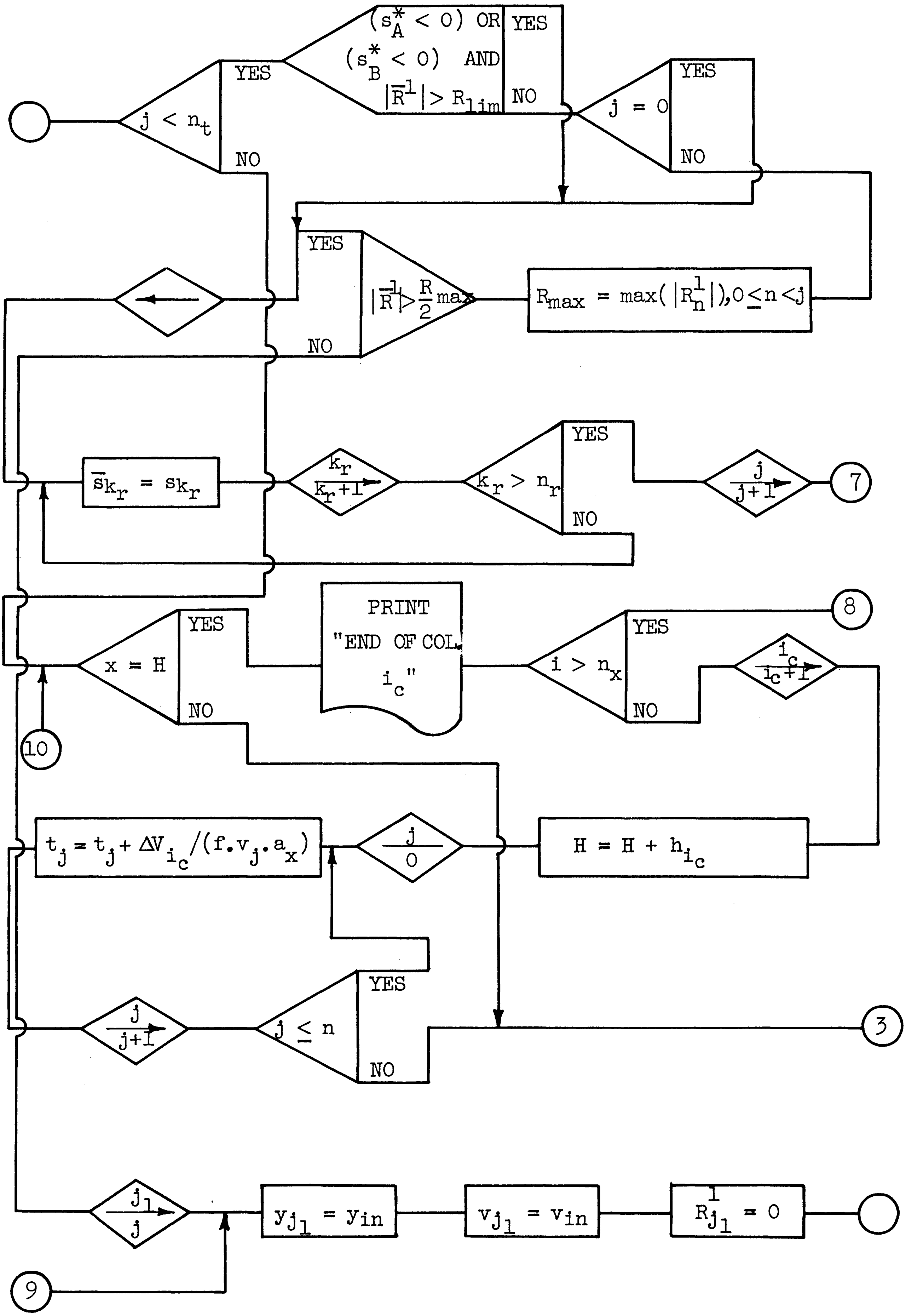
COMPUTER FLOW SHEETS

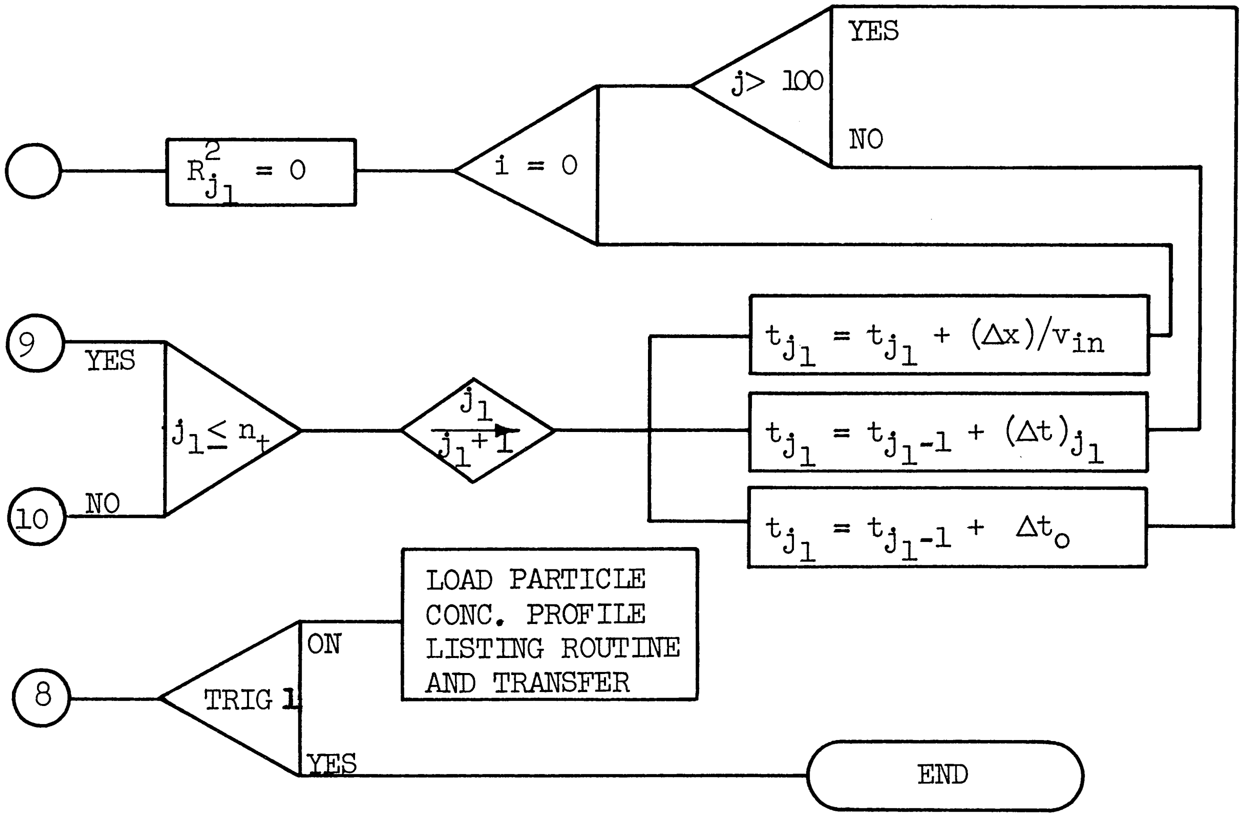

LOAD PROGRAM AND START
READ INPUT DATA
PRINT INPUT DATA
$y_{in} = y_0; v_{in} = v_0$
$\Delta r = r_0/n_r$
TRIG 2 OFF
$k_{pr} \leftarrow 1$
TRIG 1
ON
OFF
$k_r \leftarrow k_r+1$
$r_{k_r} = k.\Delta r$
$k_r \leftarrow 0$
REWIND TAPE 4
$k_r \leftarrow 0$
YES
$k_r > n_r$
NO
$k_r \leftarrow k_r+1$
$s_{k_r} = s_0; s_{k_r} = s_0$
$t_0 = \Delta V_0/(f.a_x.v_0)$
$x = 0; E_0 = 1; F_0 = 0$


COMPUTE ϕ_{12},ϕ_{21}
PRINT x
$\xleftarrow{i} 0$
4
$R_j^1 = \overline{R}^1$: $R_j^2 = \overline{R}^2$
COMPUTE PHYSICAL PROPERTIES, INTERFACE MOL FRACTION y^* AND RATES $\overline{R}^1$, $\overline{R}^2$ AND R_j^3
GRPI
$\xleftarrow{j} 0$
COMPUTE s_A^*, s_B^*
s_A^* OR $s_B^* < 0$
YES
1
NO
$\xleftarrow{k_{pr}} 1$
YES
$k_{pr} = n_{pr}$
NO
$\xleftarrow{k_{pr}} k_{pr}+1$
ON
TRIG 1
OFF
PRINT $t_j, y_j, 1-y_j$ $y^*, 1-y^*$, s_A^*, s_B^*, R_j^1, R_j^2, R_j^3, k_y
WRITE BINARY TAPE 4 $s_0 \ldots s_{n_r}$, t_j, x
$\overline{R}^1 > R_{lim}$ OR $(s_{nr}-s_0)/s_{nr} > .01$
YES
NO
2
COMPUTE $s_{i,j}^*$ USING FUNCTION 3 (Iteration subroutine)
$\xleftarrow{j} j+1$
YES
$j \leq n_t$
NO
3
$R_j^3 = \overline{R}^3$; $y_j = y_0$
$v_j = v_1$; $t_j = t_{j-1} + \Delta t$

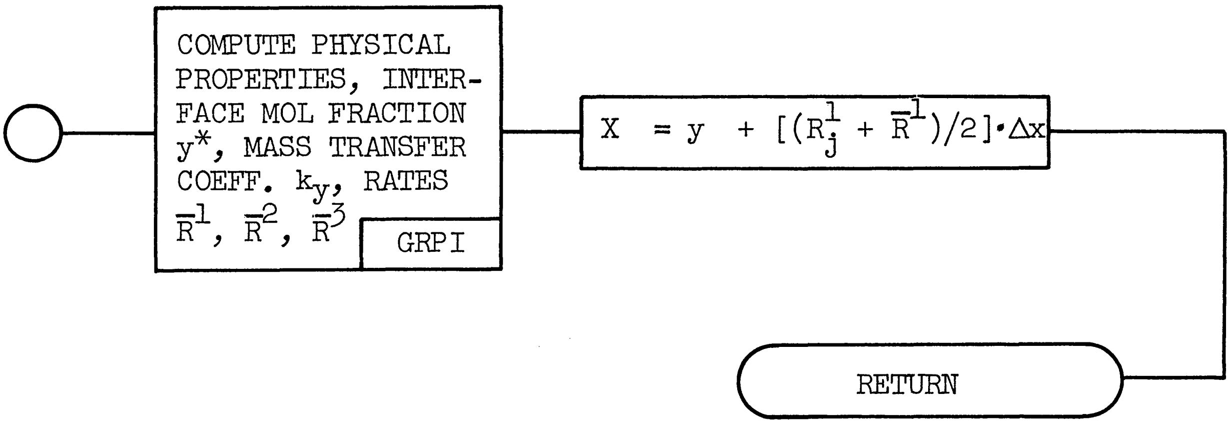

$k_r \rightarrow 0$
$s_{k_r} = s_{k_r}$
$k_r \rightarrow k_r+1$
$k_r > n_r$
YES
4
NO
3
$j \rightarrow 0$
TRIG 2 ON
$i \rightarrow i-1$
$i > 100$
YES
$\Delta x = \Delta x_o$
NO
$\Delta x = (\Delta x)_{i-1}$
$x = x + \Delta x$
$k_r \rightarrow 0$
$s_{k_r} = s_o$
$\bar{s}_{k_r} = s_o$
$k_r \rightarrow k_r+1$
$k_r \leq n_r$
YES
NO
PRINT x
$k_{pr} \leftarrow 1$
$X_1^1 = y_j$
$X_2^1 = v_j$
$X_3^1 = s_{n_r}$
$j = 0$
YES
NO
7
COMPUTE X_1 (y), AND X_2 (v); USING FUNCTIONS 1 AND 2 (ITERATION SUB-ROUTINE)
COMPUTE X_1 (y), X_2 (v) AND X_3 (s^*) USING FUNCTIONS 1, 2 AND 3 (ITERATION SUB-ROUTINE)
$X_1 \leq 0$ OR $X \geq 1$
YES
5
NO
6


5
$X_1 = y^*$
$\psi = (m_A' - m_B')/m_A'$
$X_2 = v_{in}(1 - \psi y_{in})/(1 - \psi X_1)$
$\bar{R}^1 = 0$
$\bar{R}^2 = 0$
$\bar{R}^3 = 0$
$R_j^1 = \bar{R}^1$
$R_j^2 = \bar{R}^2$
$R_j^3 = \bar{R}^3$
6
$y_j = X_1$
$v_j = X_2$
$j = 0$
YES
NO
$t_j = t_j + (\Delta t)'$
$t_j = t_{j-1} + (\Delta t)$
TRIG 1
ON
OFF
$k_p = n_{pr}$
YES
NO
$k_{pr} \leftarrow 1$
$k_{pr} \leftarrow k_{pr}+1$
WRITE BINARY TAPE 4
$s_0 \ldots s_{n_r}, t_j, x$
YES
$j = 0$
NO
COMPUTE s_A^*, s_B^*
PRINT
$t_j, y_j, 1-y_j,$
$y^*, 1-y^*,$
$s_A^*, s_B^*, R_j^1,$
R_j^2, R_j^3, k_y

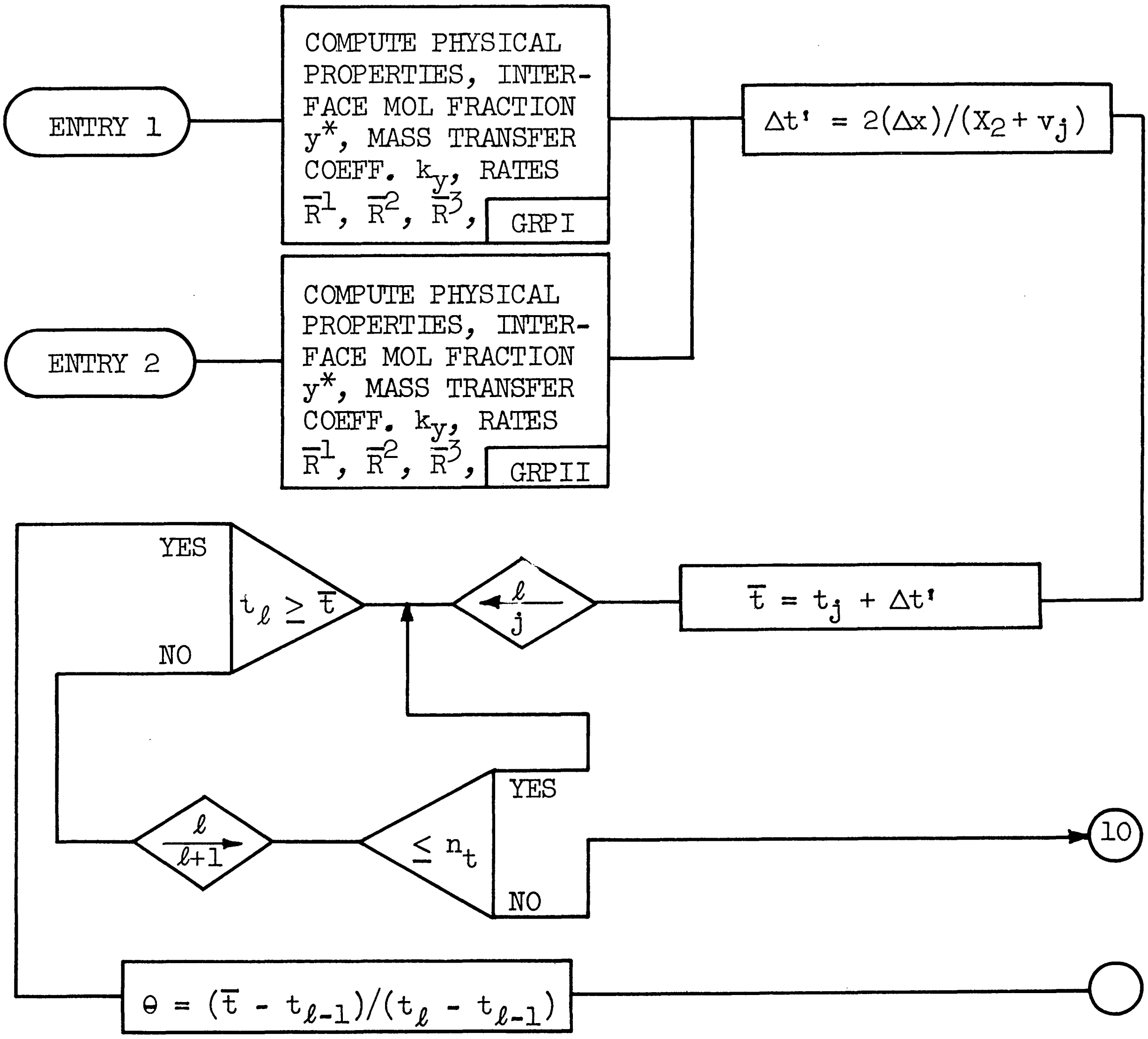

$j < n_t$
YES
NO
$(s_A^* < 0)$ OR
$(s_B^* < 0)$ AND
$|\bar{R}^1| > R_{1im}$
YES
NO
$j = 0$
YES
NO
YES
$|\bar{R}^1| > \frac{R}{2}\max$
NO
$R_{max} = \max(|R_n^1|), 0 \leq n < j$
$\bar{s}k_r = sk_r$
$\frac{k_r}{k_r+1}$
$k_r > n_r$
YES
NO
$\frac{j}{j+1}$
7
PRINT
"END OF COL.
i_c"
$x = H$
YES
NO
10
$i > n_x$
YES
NO
8
$\frac{i_c}{i_c+1}$
$t_j = t_j + \Delta V_{i_c}/(f.v_j.a_x)$
$\frac{j}{0}$
$H = H + h_{i_c}$
$\frac{j}{j+1}$
$j \leq n$
YES
NO
3
$\frac{j_1}{j}$
$y_{j_1} = y_{in}$
$v_{j_1} = v_{in}$
$R_{j_1}^1 = 0$
9

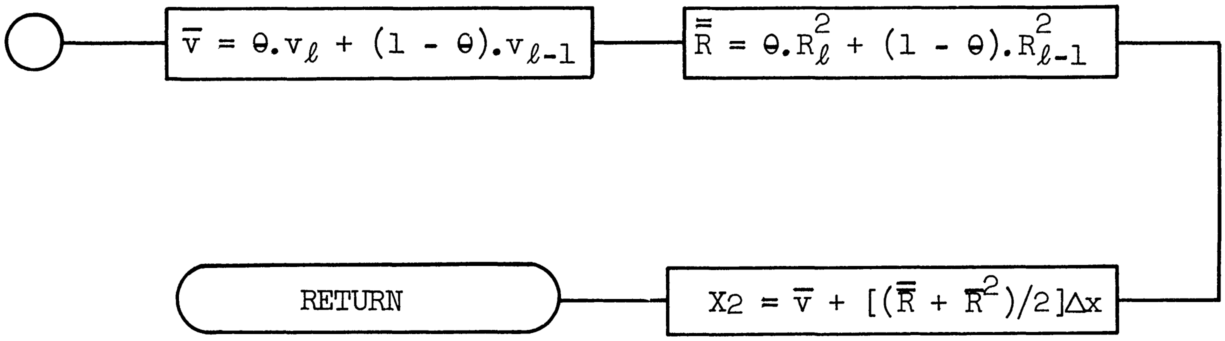

$R^2_{j_1} = 0$
$i = 0$
$j > 100$
YES
NO
9
YES
10
NO
$j_1 \leq n_t$
$j_1 \rightarrow j_1 + 1$
$t_{j_1} = t_{j_1} + (\Delta x)/v_{in}$
$t_{j_1} = t_{j_1 - 1} + (\Delta t)_{j_1}$
$t_{j_1} = t_{j_1 - 1} + \Delta t_o$
8
TRIG 1
ON
YES
LOAD PARTICLE CONC. PROFILE LISTING ROUTINE AND TRANSFER
END

Function 1

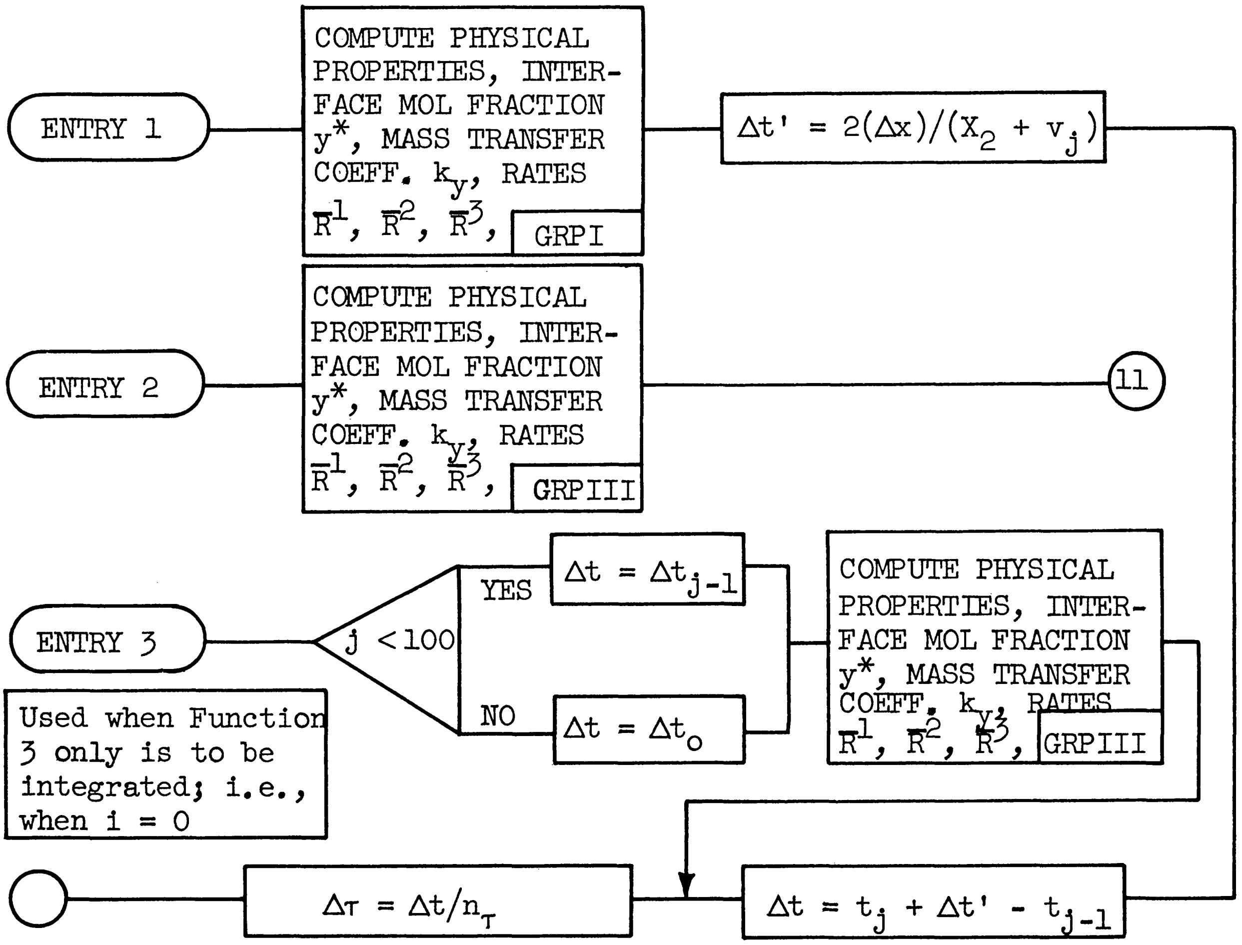


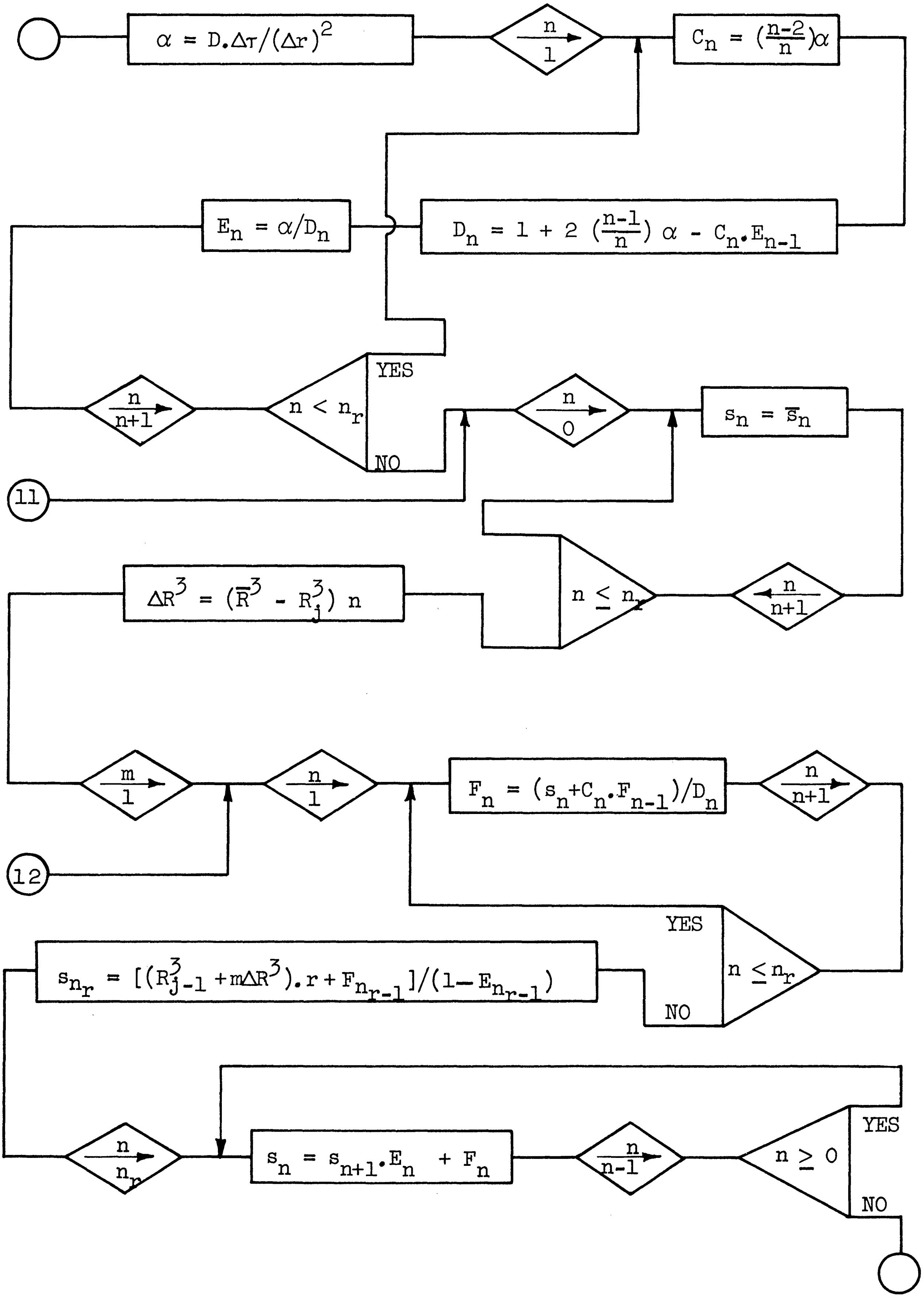
Function 2

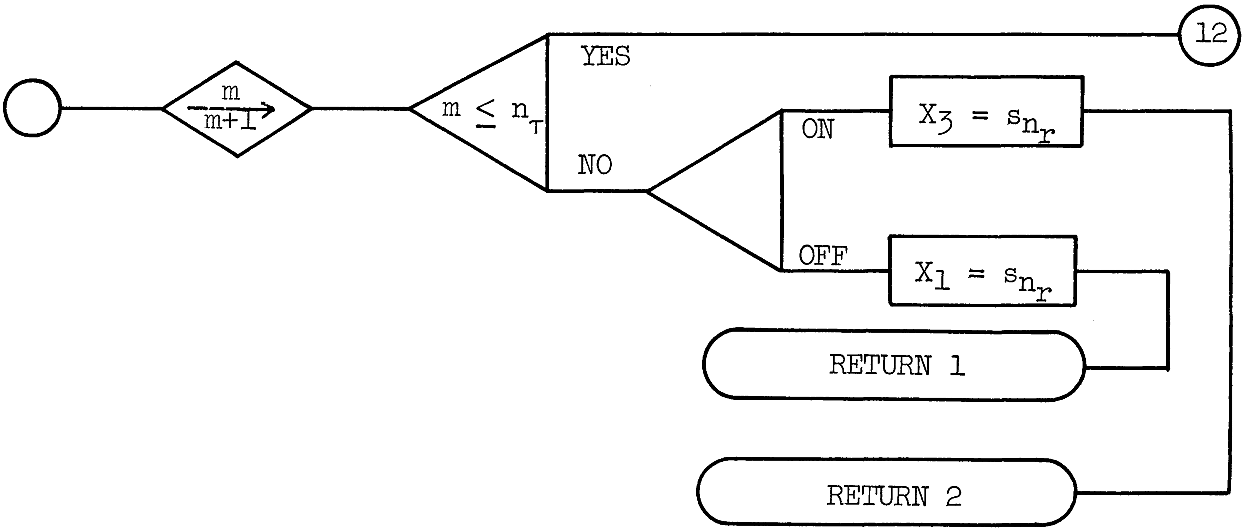



$\bar{v} = \theta . v_{\ell} + (1 - \theta) . v_{\ell-1}$
$\bar{\bar{R}} = \theta . R_{\ell}^2 + (1 - \theta) . R_{\ell-1}^2$
RETURN
$X2 = \bar{v} + [(\bar{\bar{R}} + \bar{R}^2)/2]\Delta x$

Function 3


ENTRY 1
COMPUTE PHYSICAL PROPERTIES, INTERFACE MOL FRACTION y^*, MASS TRANSFER COEFF. k_y, RATES $\bar{R}^1$, $\bar{R}^2$, $\bar{R}^3$,
GRPI
$\Delta t' = 2(\Delta x)/(X_2 + v_j)$
ENTRY 2
COMPUTE PHYSICAL PROPERTIES, INTERFACE MOL FRACTION y^*, MASS TRANSFER COEFF. k_y, RATES $\bar{R}^1$, $\bar{R}^2$, $\bar{R}^3$,
GRPIII
11
ENTRY 3
$j < 100$
YES
NO
$\Delta t = \Delta t_{j-1}$
$\Delta t = \Delta t_o$
COMPUTE PHYSICAL PROPERTIES, INTERFACE MOL FRACTION y^*, MASS TRANSFER COEFF. k_y, RATES $\bar{R}^1$, $\bar{R}^2$, $\bar{R}^3$,
GRPIII
Used when Function 3 only is to be integrated; i.e., when i = 0
$\Delta \tau = \Delta t/n_\tau$
$\Delta t = t_j + \Delta t' - t_{j-1}$


α = D.Δτ/(Δr)²
n → 1
Cn = ((n-2)/n)α
En = α/Dn
Dn = 1 + 2 ((n-1)/n) α - Cn.En-1
n → n+1
n < nr
YES
NO
n → 0
sn = s̄n
11
n ≤ nr
n ← n+1
ΔR³ = (R̄³ - Rj³) n
m → 1
n → 1
Fn = (sn+Cn.Fn-1)/Dn
n → n+1
12
YES
n ≤ nr
NO
snr = [(Rj-1³ +mΔR³).r + Fnr-1]/(1−Enr-1)
n → nr
sn = sn+1.En + Fn
n → n-1
n ≥ 0
YES
NO


m → m+1
m ≤ n_T
YES
NO
12
ON
OFF
X3 = s_{n_r}
X1 = s_{n_r}
RETURN 1
RETURN 2

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