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Effect of axial mixing in gas absorption

Sundareswaran Parameswaran Iyer

EFFECT OF AXIAL MIXING IN GAS ABSORPTION

By

SUNDARESWARAN PARAMESWARAN IYER - 1944

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THESIS

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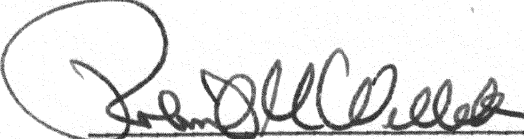in partial fulfillment of the requirements for the

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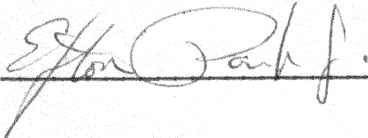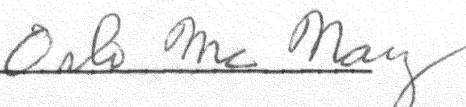MASTER OF SCIENCE IN CHEMICAL ENGINEERING

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TABLE OF CONTENTS

ABSTRACT

The effect of axial mixing in the liquid phase on the performance of a gas-absorption column was studied using the experimental data of Michael Brittan[1] for the carbon dioxide and water system. In this study, piston flow conditions were assumed for the gas phase.

A one-parameter mathematical model, which characterized the flow regimes in both the gas and the liquid phases undergoing plug flow conditions, was first curve fitted for its unknown parameter (i.e. the Number of Transfer Units) by a non-linear regression analysis procedure. The "AAPD" (i.e. the Average Absolute Percentage Deviation between the predicted value of the gas phase concentration and the experimental data) was also computed for each set of data.

An attempt was made to curve-fit a two-parameter mathematical model, which assumed plug flow in the gas phase but axial mixing in the water phase, by a similar non-linear regression analysis procedure. However, in the iterative technique used, the values of the unknown parameters (i.e., the water phase axial mixing parameter and the number of transfer units) failed to converge. As an alternate to this procedure a graphical method was used to study the effect of the axial mixing parameter on the value of the "AAPD".

The results obtained from the analysis of the two mathematical models were examined. A comparison showed that the "AAPD" computed for both the models were very close; hence, it was concluded that the effect of axial mixing in the water phase, for the nitrogen carbon dioxide-water system

based on the data obtained by Brittan and Woodburn[2] has little influence on

the gas-absorption column.

ACKNOWLEDGEMENT

A debt of gratitude is due Dr. R. M. Wellek for suggesting, guiding and encouraging this investigation and serving as the research advisor. Sincere appreciation is due Mr. V. K. Mathur for his assistance on the subject, to the Computer Science Center for the computational work carried out on IBM 360 Model and, for plotting the graphs on Calcomp Digital Incremental Plotter, and to Miss Barbara Burbank, for her cooperation in typing this thesis.

This work is dedicated to my mother Bhagirathi, for her invaluable encouragement and endurance, shown during the tennure of my entire education.

S. P. Iyer

LIST OF ILLUSTRATIONS

LIST OF TABLES

NOMENCLATURE

a = Interfacial area between two phases, per unit volume, (sq. ft.)/(cu. ft.)

A_c = Cross-section area of the column, sq. ft.

B = L/d, dimensionless, ft./ft.

$c_x o$ = Initial concentration of the incoming X phase, mole/cu. ft.

c_{x_o} = $(c_x)_{z--0}$, mole/cu. ft.

$c_y L$ = Initial concentration of the incoming Y phase, mole/cu. ft.

c_{y_L} = $(c_y)_{z--L}$, mole/cu. ft.

d = A representative length, ft.

E_i = Axial dispersion coefficient of i phase, in the direction of flow,

         sq. ft./hr.

F_i = Superficial mass flow rate of i phase, (lb.)/(hr.)(sq. ft.)

H = Henry's law solubility coefficient, atm./mole fraction.

H_{oi} = Apparent height of a transfer unit, ft.

$K_i a$ = Apparent capacity overall mass transfer coefficient based on i

         phase, (lb. mole)/(hr.)(cu. ft.)(lb. mole/cu. ft.)

L = Total height of the packing, ft.

m = Equilibrium distribution coefficient of a transfering component

         between X and Y phases, dimensionless.

n = Number of data points along the length of the column.

N_{oi} = Apparent number of overall transfer units.

P_i = Axial dispersion group, $(U_i \cdot L)/(E_i)$

P_T = Total pressure in the column, atm.

R $\quad$ = Liquid phase axial mixing parameter, $P_y B$.

U_i $\quad$ = Superficial velocity of the i phase, ft./hr.

X $\quad$ = Gas phase, (carbon dioxide and nitrogen)

Y $\quad$ = Liquid phase, (water)

z $\quad$ = Axial co-ordinate, distance between mean flow (X phase inlet is taken

$\quad\quad$ as the original point), ft.

Reduced co-ordinates:

C_x $\quad$ = $c_x/c_x o$, dimensionless, mole fraction.

C_y $\quad$ = $c_y/c_x o$, dimensionless, mole fraction.

Z $\quad$ = z/L, dimensionless, ft./ft.

C_x^* $\quad$ = Concentration of the solute in the X phase, predicted from the

$\quad\quad$ mathematical models, dimensionless, mole fraction.

Greek Letters:

ϵ_i $\quad$ = Void fraction of i phase, cu. ft./cu. ft.

$\bar{\epsilon}$ $\quad$ = $(C_{xi} - C_{xi}^*)$, deviation between experimental and predicted gas phase

$\quad\quad$ concentration

ρ_i $\quad$ = Density of i phase, lb. mole/cu. ft.

λ $\quad$ = $-N_{ox} (1 - \Lambda)$

Λ $\quad$ = Extraction factor, $(m\ F_x)/F_y$, dimensionless.

$\phi(c_i)$ $\quad$ = Volume rate of reaction, lb. mole/(cu. ft.)(hr.)

$\sigma^2_{(C_x)}$ $\quad$ = Variance on gas phase concentration.

$\sigma_{(C_x)}$ $\quad$ = Standard deviation on gas phase concentration.

Δt $\quad$ = Infinitesimal change in time, hr.

Δz $\quad$ = Infinitesimal change in height, ft.

I. INTRODUCTION

Packed columns are frequently selected as an effective and economical means of interphase contacting for gas-liquid absorption and stripping operations. The usual method of designing an absorption tower involves computing the number of transfer units (NTU) required to bring about a given separation and multiplying by a height factor (HTU) determined from previous experience on the subject. The NTU and the HTU concepts introduced by Colburn[4,5] have been applied successfully to absorption towers. In relating the NTU to stream composition Colburn uses a column material balance that inherently assumes a piston flow model for both of the immiscible phases. However, since the concept of plug flow is a hypothetical one, there is some backmixing in all packed towers which invalidates the piston flow assumption inherent in the existing design techniques. Further, Vermeulen[17] and his co-workers have shown that the effect of axial mixing, a deviation from piston flow, may be a significant factor for liquid-liquid extraction systems in packed columns.

The phenomenon of axial mixing arises from the fact that "packets" of fluid do not all move through a packed bed at a constant and uniform velocity. This non-uniform velocity may result from (a) velocity gradients as the fluid flows through the packing and/or (b) eddy motion of the fluid itself. The former is more characteristic of a laminar flow regime; whereas, the latter is probably more characteristic of turbulent flow. McHenry and Wilhelm[12] report that axial mixing is about six times as great as radial mixing in a packed bed. Axial mixing is, also, the consequence of more complex events such as local trapping, by-passing acceleration and deacceleration, than the

stream splitting or 'random walk' mechanism that has served well in explaining radial mixing.

Axial mixing tends to reduce the concentration driving force for interphase mass transfer from that which would exist for piston flow of both phases. This reduction is illustrated in Figure 1, where the concentration profiles for piston flow are represented by the dotted lines and the solid lines represent a typical axial mixing case[13]. Note that there is a discontinuity at the points where the countercurrent streams enter the column where axial mixing is present. (See appendix A). Attempts have been made recently to obtain "true" mass transfer coefficients by measuring concentration distributions within a column. This approach should be more accurate than the alternative of using a logarithmic mean driving force computed only from the end concentrations of the incoming and outgoing streams. In most of the reactor designs, axial diffusion is neglected because axial gradients are often not steep. This omission of axial diffusion may, in some cases be an unsafe assumption as even a small gradient multiplied by a large coefficient in a differential equation can lead to an important element in the solution of the equations.

Ogburn[15] in his studies has indicated that during the hydrogenation of ethylene in a fixed bed of catalyst with an isothermal wall, experimentally determined axial temperature profiles showed several departures from those calculated with all major effects except axial diffusion taken into account. The initial temperature gradient was not as steep as the predicted gradient. The measured peak temperature did not reach the calculated peak; the temperature downstream of the peak fell more rapidly than was anticipated
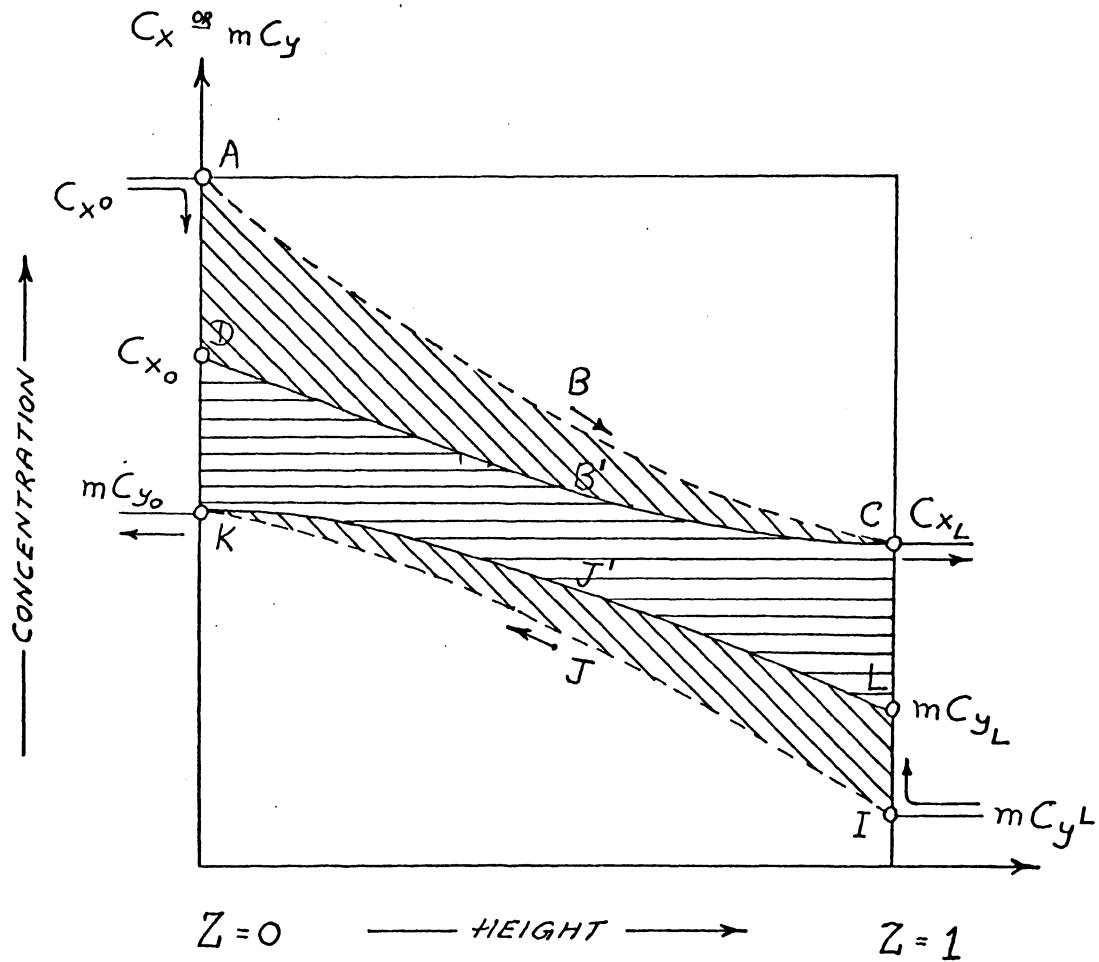
Figure I. 1   Concentration Profile, for Plug Flow and Axial Mixing Cases, in a Typical Absorption Column.

Curve IJK	= Apparent distribution of carbon dioxide in liquid phase assuming piston flow.
Curve ILJ'K	= Actual distribution of carbon dioxide in liquid phase.
Curve ABC	= Apparent distribution of carbon dioxide in gas phase assuming piston flow.
Curve ADB'C	= Actual distribution of carbon dioxide in gas phase.

from calculations. All three effects point to the presence of an important

heat leak away from the equipment from the temperature peak and hence

possibly to axial mixing.

Brittan and Woodburn[2] studied the absorption of carbon dioxide from

mixtures with nitrogen by countercurrent contact with water in an experimental

packed tower consisting of a single 3-5/8 inch i.d. glass section, with $\frac{1}{2}$-inch

raschig rings as the packings, packed to an overall height of 34.75 inches. In

the 110 experimental runs conducted, they varied the gas rate from 3.5 lb/(hr)

(sq. ft.) to 9.5 lb/(hr)(sq. ft.) and the liquid rate from 2,500 lb/(hr)(sq. ft.) to

9,500 lb/(hr)(sq. ft.). Radial and axial gas concentration profiles were

determined from measurements made within the packing. Substantial gas

phase channeling was observed. Characterizing the gas flow regime by both

piston flow and axial diffusion models yielded mass transfer values and

computed axial gas concentration profiles. In both the models, liquid flow

regime was characterized by plug flow. The differences between the gas phase

compositions predicted by the two models (solved by the Runge-Kutta method

of stepwise integration procedure) allowed Brittan to assess the influence of

axial dispersion and the applicability of the axial diffusion model.

Owing to the spread of fluid element residence time prevailing in an

absorption tower, the resulting longitudinal dispersion will in some measure

have an adverse influence on the performance. The magnitude of this effect

has not yet been determined, however. For carbon dioxide absorbers, in

particular, it has been speculated that the wide discrepancy between the actual

industrial scale performance and that predicted from standard mass transfer

correlations[9, 14, 16] is due to axial dispersion of the gas phase[2]. In two-phase operation of this nature, substantial gas phase mixing will be induced by the countercurrent liquid flow, particularly at the high water rate necessary to achieve satisfactory absorption of relatively insoluble gas such as carbon dioxide.

The purpose of this investigation is to consider the effect of axial dispersion in the water phase and to determine whether this axial mixing contribution is an important factor in the gas absorption column design for the carbon dioxide-water system. Hoffman[8] and Levenspiel and Bischoff[10] have postulated a number of mathematical models to describe the mixing characteristics prevailing in continuous flow columns. The mathematical models developed by Miyauchi[13] have been discussed and treated in this work to analyse the effects of liquid mixing for the carbon dioxide water system. To achieve a given separation, more transfer units and hence, a longer column is required for the axial mixing case owing to the reduced driving force. Likewise, for a given column under the conditions of axial mixing, HUT's reported on the basis of the Colburn equations are higher than the true HTU's that would be calculated from the actual mass transfer coefficients. By making use of the experimental data of the gas phase concentration at various heights along the length of the column, the two mathematical models are solved for the parameters in them. The deviation produced with these computed values of the parameters in predicting the gas phase concentrations along the length of the column from those gas phase concentrations experimentally determined should be a minimum. The solution of the mathematical model for the case

of plug flow in the gas phase and axial mixing in the liquid phase is compared with that for the case of plug flow in both the gas and the liquid phases, in fitting the mathematical model to the experimental curve. Depending upon the mathematical model which gives a better fit to the experimental curve, it may be possible to predict the effect of axial mixing in the liquid phase on the performance of the column.

The one-parameter mathematical model, suited for the plug flow conditions in the gas and the liquid phases (for the experimental data of Brittan) is curve fitted in this work, by the method of least square regression analysis; the value of the parameter N_{ox} (Number of Transfer Units) in the mathematical model that gives the best fit to the experimental curve is designated as the mass transfer parameter characteristic of the experimental system. The two parameter mathematical model which takes into consideration axial dispersion in the liquid phase and plug flow in the gas phase will be curve fitted in this study to the experimental data of Brittan by the method of least squares. Also, the extent to which the value of the gas phase concentration predicted from the mathematical model for the two parameter system deviates from that experimentally determined by changing the value of the axial mixing parameter R in the mathematical model (for the case of plug flow in the gas phase and axial mixing in the liquid phase) will be visually elucidated by plotting the graphs of the axial mixing parameter R against the average deviation produced in absolute terms using N_{ox} as the parameter.

II. PROPOSED MATHEMATICAL MODELS

In gas absorption column design, the values of the design parameters; namely, the overall mass transfer coefficient, the height of a transfer unit, the number of transfer units, etc., are computed from the mass transfer correlations which were evaluated by assuming piston flow conditions in the gas and liquid phases. Investigations by various workers, [1, 12, 15, 17], in the field of gas absorption and those related to it, show that the difference between the industrial scale performance and that predicted from the available mass transfer correlations may be due to the adverse effect caused by the axial mixing of the gas and the liquid phases during their flow through the column. In this chapter, an analysis of the mass transfer relations between the gas and the liquid phases, along the length of the column, is presented. This analysis takes into consideration the axial mixing in both the gas and the liquid phases which occur during their traverse across the packings in the absorption columns. The mathematical models and their respective boundary conditions for the different cases corresponding to the presence and/or absence of axial mixing in the gas and/or the liquid phases, also, have been presented.

For one-dimensional counter-current two phase mass transfer processes Danskohler's[7] equation of continuity for homogeneous continuous flow systems (see appendix B) may be modified and rearranged into a dimensionless form as follows:

$$\frac{d^2 C_x}{dZ^2} - P_x B \frac{dC_x}{dZ} - N_{ox} P_x B (C_x - mC_y) = 0 \qquad (2.1)$$

$$\frac{d^2C_y}{dZ^2} + P_yB \frac{dC_y}{dZ} + N_{oy} P_yB (C_x - mC_y) = 0 \tag{2.2}$$

The dimensionless boundary conditions as shown in appendix A are

a) $Z = 0$,   i) $-\left(\frac{dC_x}{dZ}\right) = P_xB (1 - C_x)$ $\tag{2.3}$

          ii) $-\left(\frac{dC_y}{dZ}\right) = 0$ $\tag{2.4}$

b) $Z = 1$,   i) $-\left(\frac{dC_x}{dZ}\right) = 0$ $\tag{2.5}$

          ii) $-\left(\frac{dC_y}{dZ}\right) = P_yB (C_{y_1} - C_y1)$ $\tag{2.6}$

In the mathematical models shown above, P_xB is the parameter for axial mixing in the gas phase, and P_yB is the parameter for axial mixing in the liquid phase. The parameters P_xB and P_yB are inversely proportional to the eddy diffusivities in the gas and the liquid phases, respectively; $P_xB = \dfrac{U_x L}{E_x}$ and $P_yB = \dfrac{U_y L}{E_y}$, where L is the effective height of the packing, E_x and E_y are the eddy diffusivities in the X and Y phases respectively, $U_x = \dfrac{F_x}{\epsilon_x}$, and $U_y = \dfrac{F_y}{\epsilon_y}$, where F_x and F_y are the superficial mass flow rate of the X and the Y phases, respectively. $N_{ox} = \dfrac{K_x a L}{F_x}$, and $N_{oy} = \dfrac{K_x a L}{F_y}$, where K_x is the overall mass transfer coefficient relative to the phase X, and a is the inter-facial area per unit volume.

Depending upon the presence and/or absence of the eddy diffusivities E_x and E_y in the individual phases, four different sets of mathematical models are derived from the equations (2.1) and (2.2). The various differential

equations and the boundary conditions which describe the various models are given as follows:

A.   Case 1: (One Parameter System)

Conditions of plug flow in the gas and the liquid phases are assumed, i.e. the eddy diffusivities $E_x \to 0$ and $E_y \to 0$, so that the axial mixing parameters $P_x B \to \infty$ and $P_y B \to \infty$, therefore, from equations (2.1) and (2.2)

$$\frac{dC_x}{dZ} + N_{ox} (C_x - mC_y) = 0 \tag{2.7}$$

and

$$\frac{dC_y}{dZ} + N_{oy} (C_x - mC_y) = 0 \tag{2.8}$$

The necessary boundary conditions are

a) $Z = 0$,   i) $C_x = 1$ $\tag{2.3a}$

$$\text{ii)} \quad -\left(\frac{dC_y}{dZ}\right) = 0 \tag{2.4}$$

b) $Z = 1$,   i) $-\left(\frac{dC_x}{dZ}\right) = 0$ $\tag{2.5}$

$$\text{ii)} \quad C_{y_1} = C_y 1 \tag{2.6a}$$

B.   Case 2: (Two Parameter System)

Conditions of axial mixing in the gas phase and plug flow in the liquid phase are assumed, i.e. the eddy diffusivities E_x is finite and $E_y \to 0$, so that $P_x B$ is finite and $P_y B \to \infty$; Therefore, equations (2.1) and (2.2) are reduced to

$$\frac{d^2 C_x}{dZ^2} - P_x B \frac{dC_x}{dZ} - N_{ox} P_x B (C_x - mC_y) = 0 \tag{2.1}$$

and

$$\frac{dC_y}{dZ} + N_{oy} (C_x - mC_y) = 0 \tag{2.8}$$

and the associated boundary conditions are,

a) $Z = 0$, i) $-(\frac{dC_x}{dZ}) = P_x B (1 - C_x)$ (2.3)

ii) $-(\frac{dC_y}{dZ}) = 0$ (2.4)

b) $Z = 1$, i) $-(\frac{dC_x}{dZ}) = 0$ (2.5)

ii) $C_{y_1} = C_y 1$ (2.6a)

C. Case 3: (Two Parameter System)

This case is the reverse of Case 2. Here the conditions assumed are

plug flow in the gas phase and axial mixing in the liquid phase, i.e. the eddy

diffusivities are given by $E_x \rightarrow 0$. E_y is finite so that the axial mixing parameters

reduce to $P_x B \rightarrow \infty$, and $P_y B$ is finite. Therefore, from equations (2.1) and (2.2)

$$\frac{dC_x}{dZ} + N_{ox} (C_x - mC_y) = 0 \tag{2.7}$$

and

$$\frac{d^2 C_y}{dZ^2} + P_y B \frac{dC_y}{dZ} + N_{oy} P_y B (C_x - mC_y) = 0 \tag{2.2}$$

where the necessary and sufficient boundary conditions are

a) $Z = 0$, i) $C_x = 1$ (2.3a)

ii) $-(\frac{dC_y}{dZ}) = 0$ (2.4)

b) $Z = 1$,   i) $-(\dfrac{dC_x}{dZ}) = 0$ (2.5)

ii) $-(\dfrac{dC_y}{dZ}) = P_y B (C_{y_1} - C_y 1)$ (2.6)

D. Case 4: (Three Parameter System)

This case represents the extreme case where conditions of axial mixing is

assumed in both the gas and the liquid phases, i.e. the eddy diffusivities E_x

and E_y in the gas and the liquid phases, respectively, are finite which means

that the axial parameters $P_x B$ and $P_y B$ in the respective phases are finite.

This case is represented by equations (2.1) and (2.2), and the boundary condi-

tions incorporated herein are as given by equations (2.3), (2.4), (2.5), and

(2.6).

Brittan has analysed Case 2 and has compared the results with those

obtained from Case 1; he has employed a numerical integration method for

analysing the aforesaid cases and thereby has predicted the effect of axial

mixing in the gas phase on the performance of the absorption column for the

carbon dioxide-water system. In this study, Case 3 is analysed, and the

results are compared with those computed for Case 1; a non-linear regression

analysis method and a graphical technique are used to predict the effect of

axial mixing in the liquid phase on the performance of the column. In the

following section, the foresaid methods are employed for computing the values

of the axial mixing parameter, $P_y B$, and the number of transfer units, N_{ox}

in the mathematical models represented by the Cases 1 and 3.

Depending upon the definition of the concentration driving force there should be three kinds of HTU (i.e. height of transfer unit):

i. "True" values:

By the original definition of HTU[3], "true" HTU is the ratio of volumetric flow rates across a unit cross-section to the true over-all coefficient of mass transfer.

$$H_{oxT} = \frac{F_x}{K_x a} \qquad (2.9)$$

Likewise, the true number of overall transfer units (NTU) is

$$N_{oxT} = \frac{K_x a L}{F_x} \qquad (2.10)$$

ii. "Measured" values:

When an absorber behaves in the same manner as the proposed model, the actual concentration distribution for the X phase in the absorber is given by curve ADB'C and for the Y phase by curve ILJ'K in Figure 1. These two curves can be obtained by measuring the concentration distribution in the absorber.

$$N_{oxM} = \int_{C_{xo}}^{C_{xl}} \frac{dC_x}{C_x - mC_y} \qquad (2.11)$$

and from this definition of NTU, an apparent HTU is derived as;

$$H_{oxM} = \frac{L}{N_{oxM}} \qquad (2.12)$$

iii. "Piston Flow" vlaues:

Another apparent NTU is defined in terms of the logarithmic-mean driving force computed from the exterior incoming and outgoing concentrations at both ends of the absorber:

$$N_{oxP} = \int_{1.0}^{C_{xl}} \frac{dC_x}{C_{xP} - mC_y}$$

(2.13)

Integration of the right-hand side of this equation (2.13) gives equations (3.1) and (3.2) for $\Lambda \neq 1$.

The corresponding apparent HTU is defined as

$$H_{oxP} = \frac{L}{N_{oxP}}$$

(2.14)

H_{oiM} and H_{oiP} should include the effect of longitudinal dispersion of the transfering material. In general one will find

$$H_{oiP} \geq H_{oiM} \geq H_{oiT}$$

$$N_{oiP} \leq N_{oiM} \leq N_{oiT}$$

Relations between H_{oxT}, H_{oxM} and H_{oxP} have been discussed elsewhere[13].

III. SOLUTION OF THE MATHEMATICAL MODELS

The mathematical models developed in the preceding section for the conditions of plug flow in both the gas and the liquid phases, represented by case 1 and for the conditions of plug flow in the gas phase but axial mixing in the liquid phase represented by case 3 are treated in this section; the normal equations are derived from the respective differential equations (2.7), (2.8), and (2.7), (2.2) for the two cases and are then solved for the parameters N_{ox} and R & N_{ox} by making use of the IBM 360 Computer. Also, a deviation between the values of the gas phase concentration predicted by the computed parameters and the values experimentally determined is calculated. Further a variance on the parameter N_{ox}, and on the concentration of carbon dioxide in the gas phase c_x, is also shown here:

A. Derivation of Normal Equations:

1. Case 1:

Conditions of plug flow in the gas phase and in the liquid phase are prevalent in this case. The differential equations describing the subject case are,

$$\frac{dC_x}{dZ} + N_{ox} (C_x - mC_y) = 0 \tag{2.7}$$

and

$$\frac{dC_y}{dZ} + N_{oy} (C_x - mC_y) = 0 \tag{2.8}$$

and the boundary conditions are,

a) Z = 0,   i) C_x = 1   (2.3a)

$$\text{ii)} \quad -\left(\frac{dC_y}{dZ}\right) = 0 \qquad\qquad (2.4)$$

$$\text{b)} \quad Z = 1 \qquad\qquad \text{i)} \quad -\left(\frac{dC_x}{dZ}\right) = 0 \qquad\qquad (2.5)$$

$$\text{ii)} \quad C_{y_1} = C_y 1 \qquad\qquad (2.6a)$$

The solutions of the above equations given elsewhere[13] are as follows:

$$\frac{C_x - mC_y 1}{1 - mC_y 1} = \frac{e^{\lambda Z} - \Lambda e^{\lambda}}{1 - \Lambda e^{\lambda}} \qquad\qquad (3.1)$$

and

$$\frac{m(C_y - mC_y 1)}{1 - mC_y 1} = \frac{(e^{\lambda Z} - e^{\lambda})\Lambda}{1 - \Lambda e^{\lambda}} \qquad\qquad (3.2)$$

Since the concentration in the available nitrogen-carbon dioxide-water experimental data are in the gas phase, equation (3.1) is used as the mathematical model for evaluating the value of the parameter N_{ox}. The carbon dioxide present in the inlet water at the top of the column is negligible, and $C_y 1 = 0$; hence equation (3.1) reduces to

$$\overset{*}{C}_x = \frac{e^{\lambda Z} - \Lambda e^{\lambda}}{1 - \Lambda e^{\lambda}} \qquad\qquad (3.3)$$

where

$$\Lambda = m\frac{F_x}{F_y} \qquad\qquad (3.4)$$

$$\lambda = -N_{ox}(1 - \Lambda) \qquad\qquad (3.5)$$

and

$\overset{*}{C}_x$ is predicted value of gas phase concentration.

The mathematical model represented by the equation (3.3) is curve-fitted by a non-linear least square technique for the parameter λ and hence N_{ox}. The "normal equation" as derived by the least square procedure in appendix C is given as follows:

$$\sum_{i=1}^{n} C_{xi} \left[\frac{Z_i e^{\lambda o Z_i} (1 - \Lambda e^{\lambda o}) + \Lambda e^{\lambda o} (e^{\lambda o Z_i} - 1)}{(1 - \Lambda e^{\lambda o})^2} \right]$$

$$-\sum_{i=1}^{n} \left[\frac{e^{\lambda o Z_i} - \Lambda e^{\lambda o}}{1 - \Lambda e^{\lambda o}} \right] \left[\frac{Z_i e^{\lambda o Z_i} (1 - \Lambda e^{\lambda o}) + \Lambda e^{\lambda o} (e^{\lambda o Z_i} - 1)}{(1 - \Lambda e^{\lambda o})^2} \right]$$

$$= \sum_{i=1}^{n} \left[\frac{Z_i e^{\lambda o Z_i} (1 - \Lambda e^{\lambda o}) + \Lambda e^{\lambda o} (e^{\lambda o Z_i} - 1)}{(1 - \Lambda e^{\lambda o})^2} \right]^2 (\lambda - \lambda o) \tag{3.6}$$

where λo is the starting value of λ, in the foreshown normal equation, assumed such that the iterated values of λ converges within an allowable error; the error value allowed in this study is of the order of 10^{-8}. By solving for the converged value of λ, it is possible to compute the value of the parameter N_{ox}. A computer program for solving the above shown normal equation is discussed in the next section.

2. Case 3:

Conditions of plug flow in the gas phase but axial mixing in the liquid phase are prevalent in this case. The differential equations for this case are,

$$\frac{dC_x}{dZ} + N_{ox} (C_x - mC_y) = 0 \tag{2.7}$$

and

$$\frac{d^2 C_y}{dZ^2} + P_y B \frac{dC_y}{dZ} + N_{oy} P_y B (C_x - mC_y) = 0 \qquad (2.2)$$

and the associated boundary conditions are,

a) $Z = 0$,   i) $C_x = 1$ (2.3a)

                     ii) $-\left(\frac{dC_y}{dZ}\right) = 0$ (2.4)

b) $Z = 1$,   i) $-\left(\frac{dC_x}{dZ}\right) = 0$ (2.5)

                     ii) $-\left(\frac{dC_y}{dZ}\right) = P_x B (C_{y_1} - C_y 1)$ (2.6)

The above basic differential equations are combined to give,

$$\frac{d^3 C_x}{dZ^3} + h \frac{d^2 C_x}{dZ^2} + k \frac{dC_x}{dZ} = 0 \qquad (3.7)$$

The solution of the above equation given elsewhere[13] for the value of $\Lambda \neq 1$

is shown below:

$$\frac{C_x - mC_y 1}{1 - mC_y 1} = H_1 e^{\lambda_1 Z} + H_2 e^{\lambda_2 Z} + H_3 e^{\lambda_3 Z} \qquad (3.8)$$

and

$$\frac{m(C_y - mC_y 1)}{1 - mC_y 1} = h_1 H_1 e^{\lambda_1 Z} + h_2 H_2 e^{\lambda_2 Z} + h_3 H_3 e^{\lambda_3 Z} \qquad (3.8a)$$

where as shown in appendix D

$$H_1 = \frac{DH_1}{DH} \qquad (D.7a)$$

$$H_2 = \frac{DH_2}{DH} \tag{D.7b}$$

$$H_3 = \frac{DH_3}{DH} \tag{D.7c}$$

$$DH = DH_1 + (h_3\lambda_3 - h_2\lambda_2) \tag{D.15}$$

$$DH_1 = \begin{vmatrix} h_2\lambda_2 & h_3\lambda_3 \\ \\ (1 + \frac{\lambda_2}{P_yB})\, e^{\lambda_2}\, h_2 & (1 + \frac{\lambda_3}{P_yB})\, e^{\lambda_3}\, h_3 \end{vmatrix} \tag{D.9a}$$

$$DH_2 = + h_3\lambda_3 \tag{D.9b}$$

$$DH_3 = - h_2\lambda_2 \tag{D.9c}$$

$$h_1 = 1 + \lambda_1\, N_{ox} \tag{D.17a}$$

$$h_2 = 1 + \lambda_2\, N_{ox} \tag{D.17b}$$

$$h_3 = 1 + \lambda_3\, N_{ox} \tag{D.17c}$$

$$\lambda_1 = 0 \tag{D.11a}$$

$$\lambda_2 = -(\tfrac{h}{2}) + \sqrt{(\tfrac{h}{2})^2 - k} \tag{D.11b}$$

$$\lambda_3 = -(\tfrac{h}{2}) - \sqrt{(\tfrac{h}{2})^2 - k} \tag{D.11c}$$

$$h = N_{ox} + P_yB \tag{D.12a}$$

and

$$k = N_{ox}\, P_yB\, (1 - \Lambda) \tag{D.12b}$$

Similar to case 1, equation (3.8) is used as the mathematical model with $C_y1 = 0$.

Hence equation (3.8) reduces to

$$\overset{*}{C}_x = H_1\, e^{\lambda_1 Z} + H_2\, e^{\lambda_2 Z} + H_3\, e^{\lambda_3 Z} \tag{3.9}$$

The above mathematical model was curve fitted for the parameter N_{ox} and the parameter $P_y B$. In the computer programs, the parameter N_{ox} will be denoted as 'X', and the parameter $P_y B$ will be denoted as 'R'.

The normal equations as derived in appendix D are as follows:

$$\sum_{i=1}^{n} C_{xi} \left[\frac{dC_{xi}^*}{dX}\right]_{Xo} - \sum_{i=1}^{n} C_{xo}^* \left[\frac{dC_{xi}^*}{dX}\right]_{Xo} + \sum_{i=1}^{n} \left[\frac{dC_{xi}^*}{dX}\right]_{Xo}^2 \cdot Xo + \sum_{i=1}^{n} \left[\frac{dC_{xi}^*}{dX}\right]_{Xo} \left[\frac{dC_{xi}^*}{dR}\right]_{Ro} \cdot Ro$$

$$= \sum_{i=1}^{n} \left[\frac{dC_{xi}^*}{dX}\right]_{Xo}^2 \cdot X + \sum_{i=1}^{n} \left[\frac{dC_{xi}^*}{dX}\right]_{Xo} \left[\frac{dC_{xi}^*}{dR}\right]_{Ro} \cdot R \qquad (3.10)$$

and

$$\sum_{i=1}^{n} C_{xi} \left[\frac{dC_{xi}^*}{dR}\right]_{Ro} - \sum_{i=1}^{n} C_{xo}^* \left[\frac{dC_{xi}^*}{dR}\right]_{Ro} + \sum_{i=1}^{n} \left[\frac{dC_{xi}^*}{dX}\right]_{Xo} \left[\frac{dC_{xi}^*}{dR}\right]_{Ro} \cdot Xo$$

$$+ \sum_{i=1}^{n} \left[\frac{dC_{xi}^*}{dR}\right]_{Ro}^2 \cdot Ro = \sum_{i=1}^{n} \left[\frac{dC_{xi}^*}{dX}\right]_{Xo} \left[\frac{dC_{xi}^*}{dR}\right]_{Ro} \cdot X + \sum_{i=1}^{n} \left[\frac{dC_{xi}^*}{dR}\right]_{Ro}^2 \cdot R \qquad (3.11)$$

where Xo and Ro are the starting values of the parameters X (i.e. N_{ox}) and R (i.e. $P_y B$) assumed, in the above normal equation, such that the iterated values of X and R converge as the process of iteration is continued.

B. Solution of the Normal Equations:

The normal equations, as derived in the preceding section for the case of plug flow in both the gas and the liquid phases and for the case of plug flow in the gas phase and axial mixing in the liquid phase, are solved here for their unknown parameters N_{ox} (for case 1) and the parameters N_{ox} and R (for case 3), respectively.

1. Case 1: (Plug flow in both the gas and the liquid phases)

The normal equation represented by the equation (3.6) is solved for the parameter λ by an iterative technique. (See appendix E.) λ is given by the

following equations: $\lambda = -N_{ox}(1 - \Lambda)$, where $\Lambda = m(\dfrac{F_x}{F_y})$. From the iterated

value of λ, the number of transfer units N_{ox} is calculated.

(i) Calculation of Average Absolute Percentage Deviation:

AAPD is a form of representing the deviation between the predicted value

of the gas phase concentration and the experimental data. By substituting the

iterated value of the parameter λ in the mathematical model, equation (3.3),

the gas phase concentration $\overset{*}{C}_{xi}$ is predicted at the point 'i' along the lenght of

the column. This value of $\overset{*}{C}_{xi}$ is compared with the experimentally determined

gas phase concentration C_{xi}, and their absolute percentage difference divided

by the experimental value, C_{xi} is summed up for all the 'n' number of data

points along the length of the column. The Average Absolute Percentage

Deviation is given by;

$$AAPD = \frac{100}{n} \sum_{i=1}^{n} \left[\left| \frac{C_{xi} - \overset{*}{C}_{xi}}{C_{xi}} \right| \right] \tag{3.12}$$

The AAPD gives a measure as to how close a given mathematical model,

with its computed parameters, fits the experimental curve--the lower the AAPD,

the better the fit.

(ii) The "Variance" on gas phase concentration: $\sigma^2_{(cx)}$

An estimate of the probability that the predicted value of the gas phase

concentration differs from the experimentally measured value is obtained in

terms of 'Variance' or alternatively, as the 'Standard Deviation' as follows:

$$\text{Sample Variance} = \sigma^2_{(cx)} = \frac{1}{D.F} \sum_{i=1}^{n} (c_{xi} - \overset{*}{c}_{xi})^2 \tag{3.13}$$

Where D.F. (Degree of Freedom) = n - m $\tag{3.13a}$

n = total number of data points

m = total number of parameters to be determined.

The sample variance is simply the mean square deviation of the 'n' predicted values from the experimental values. In this definition, positive and negative fluctuations between the predicted and experimental values do not 'cancel' one another.

The standard deviation is given by the following:

$$\sigma_{(cx)} = \text{sample standard deviation} = \sigma^2_{(cx)} \tag{3.14}$$

This value of the variance becomes more reliable as more experimental data are obtained. The true precision of the procedure of prediction of the gas phase concentration by the mathematical model is indicated by the value of variance calculated from a very large amount of data.

(iii) The "Variance" on the Number of Transfer Units: $\sigma^2_{(N_{ox})}$

The value of λ and hence N_{ox} as calculated from the mathematical model, equation (3.3), is subject to error. This error is a direct consequence of the error in the measured values of C_x. Estimates of the error variance of λ are given by the expression

$$\sigma^2_{(\lambda)} = \sum_{i=1}^{n} \left[\frac{\sigma^2_{(c_{xi})}}{\left[\dfrac{\partial \overset{*}{C}_{xi}}{\partial \lambda}\right]^2} \right] \tag{3.15}$$

$$= \left(\frac{1}{D.F}\right) \sum_{i=1}^{n} \frac{(c_{xi} - \overset{*}{c}_{xi})^2}{\left[\dfrac{Z_i\, e^{\lambda\, Z_i}\,(1-\Lambda\, e^{\lambda}) + \Lambda\, e^{\lambda}(e^{\lambda\, Z_i}-1)^2}{(1-\Lambda\, e^{\lambda})^2}\right]^2} \tag{3.16}$$

The sample standard deviation on λ is given by

$$\sigma_{(\lambda)} = \sqrt{\sigma_\lambda^2}$$

(3.17)

The sample standard deviation on N_{ox} is given by

$$\sigma_{(N_{ox})} = \frac{\sigma_{(\lambda)}}{(\Lambda - 1)}$$

(3.18)

where $\Lambda = m\dfrac{F_x}{F_y}$

(3.4)

A computer program was written (See appendix E) for calculating the following quantities:

The number of transfer units N_{ox}; to predict the value of the gas phase concetration, C_{xi}^*, along the length of the column, in comparison with the experimental data C_{xi}; the average absolute percentage deviation, between the predicted and the experimental values of the gas phase concentration, AAPD; the variance and the standard deviation, on c_x, $\sigma_{(cx)}^2$ and $\sigma_{(cx)}$; the standard deviation, on N_{ox}, $\sigma_{(N_{ox})}$.

The above values and results for all the 110 runs are tabulated and kept elsewhere[18].

2. Case 3: (Plug flow in the gas phase and axial mixing in the liquid phase)

The normal equations for this case are as given by equations (3.10) and (3.11). For solving the normal equations for the parameter N_{ox} (Number of Transfer Units) and the axial mixing parameter R, an iterativ. technique is used with the IBM/360 computer system. (See appendix F for the flow chart). But unlike the case of a one parameter model, in the two parameter model the values of the parameters N_{ox} and R failed to converge. In order to predict

the effect of introducing the axial mixing parameter R in the mathematical

model, equation (3.8), an alternate method is used. For the various values

of the parameter N_{ox}, the gas phase concentration is predicted by substituting

in increments of the value of the axial mixing parameter R in the two

parameter model. The average of the percentage deviation between this

predicted value of the gas phase concentration and the experimentally determined

gas phase concentration, (i.e. the AAPD), is plotted against the axial mixing

term R with N_{ox} as the parameter. A program for plotting the graphs by the

IBM/360 computer is shown in appendix F. The AAPD vs. R graphs with N_{ox}

as the parameter are presented for all the 110 runs and displayed elsewhere[18].

Of the 110 runs, the graphs and the computed values of 18 runs are presented

here and are tabulated elsewhere in this work. (See appendix G, and table D.)

IV. RESULTS AND DISCUSSION

This investigation allows one to ascertain and study the influence of axial dispersion in the liquid phase on the performance of a counter-current gas absorption column used for the carbon dioxide-water system. The conclusions arrived at are tentative, of course, since only set of data was available for analysis.

A. One-Parameter Model: (Piston flow in both the phases)

(i) In his experimental work, Brittan[2] measured the concentration of carbon dioxide in the gas phase, at various points, along the length of the column. Using a Runge-Kutta method of step-wise integration, Brittan[2] computed the concentration of carbon dioxide in the liquid phase. He calculated the NTU, HTU, and K_L a values from the following equation:

$$NTU = \int_{y_0}^{y_1} \frac{dy}{(y^* - y)} = \frac{K_L a. \rho y. L}{F_y} = \frac{L}{HTU}$$

where

y   = Solute concentration in liquid phase, (lb. mole solute/lb. mole solvent)

y^* = Equilibrium solute concentration in liquid phase, (lb. mole solute/lb. mole solvent)

0   = Lower terminal conditions

1   = Upper terminal conditions

F_y = Superficial mass liquid rate, (lb.)/(hr.)(sq. ft.)

ρ_y = Density of liquid, (lb./cu. ft.)

L   = Total height of packing, (ft.)

HTU = Apparant height of an overall transfer unit (ft.)

$K_L a$ = Apparant capacity overall transfer coefficient (lb. mole)/(hr.)(cu. ft.)

(lb. mole/cu. ft.)

(ii) In this work, the concentration of carbon dioxide in the gas phase

(Brittan's data) is substituted in the mathematical model, equation (3.3), and

the model is curve-fitted by the method of least squares. Using this non-

linear iterative procedure, the value of the parameter N_{ox} (i.e. the number of

transfer units) does converge for all the 110 runs.

The values of NTU and HTU obtained by this method are very close to

those obtained by Brittan in his work on the one-parameter system.

B. Two-Parameter Model:

(i) Brittan, also, investigated the effect of axial mixing in the gas phase

(with plug flow in the liquid phase) on the performance of the gas absorption

column. Upon analysing the results, he found that the influence of the gas

phase dispersion on the performance is only moderately adverse and that in

his opinion it is improbable that the effect is large enough to account for the

differences between industrial scale performance and that predicted from

available mass transfer correlations based upon small diameter columns.

(ii) Proceeding further in this work, the effect of axial mixing in the

liquid phase and plug flow in the gas phase for the carbon dioxide water

system was investigated. The two parameter mathematical model which

takes into consideration axial dispersion in the liquid phase is curve-fitted

to the experimental data of Brittan by the method of least squares. A

non-linear, iterative procedure is used. Unlike the case of the one-parameter

mathematical model, when using the two-parameter model, the values of the

parameter N_{ox} (i.e. the number of transfer units) and the parameter R (i.e.

water phase axial mixing term) obtained in the iterative search fail to converge.

When the value of R in the 'normal equations', equations (3.10) and (3.11),

derived from the two-parameter mathematical model, equation (3.9), exceeds

167, the exponential values in the 'normal equations' "overflow" beyond the

maximum magnitude which the IBM computer 360 can operate.

As an alternate approach to this non-converging iterative procedure,

computer plotting is employed to plot AAPD for the two parameter mathe-

matical model as a function of the curve-fitting parameters N_{ox} and R which

serves to visually elucidate the effect of the axial mixing parameter on the

performance of the column. These plots are prepared for each of the 110

runs. As speculated by Brittan, examination of these graphs for the various

experimental runs depicted little significance of the axial mixing parameter

R upon the performance of the tower.

C. Applicability of the Models:

From the figures shown (i.e. from G 1 to G 18), it is possible to obtain

the values of average absolute percentage deviation for each value of N_{ox}

corresponding to various values of R. For each value of N_{ox}, it is noted

that as the value of R is increased from 1 to 100 the value of AAPD remains

almost constant for the values of R greater than about 20. (i.e. when the

axial dispersion in the liquid phase reduces); note that when the value of R

tends to infinity, axial dispersion in the liquid phase disappears and the

liquid flow regime is characterised by the conditions of plug flow. For most of the runs, the value of AAPD increases when the value of R is decreased below 20. In the mathematical model studied here, equation (3.9), which considers the case of axial mixing in the liquid phase, the value of the AAPD decreases as the value of R increases and then remains constant, i.e. when the liquid phase axial mixing case tends towards the case of plug flow. The above-mentioned characteristics are seen in the Figures G 14, G 40, G 92, G 10, G 18, G 34, G 45, etc.

The minimum value of the AAPD obtained from the graph for each run is very close to the values of AAPD computed by the non-linear regression analysis of the mathematical model, equation (3.3), for the case of plug flow in both the gas and the liquid phases. As a result, the introduction of the liquid-phase, axial mixing parameter in the mathematical model, equation (3.8), has no effect in fitting the curve closer to the experimental data. Hence, the eddy diffusivity in the liquid pahse for the carbon dioxide water system, based on the data obtained by Brittan, has little significance as far as the performance of the gas-absorption column is concerned.

V. SUMMARY AND CONCLUSION

The purpose of the present work has been to investigate whether the axial

mixing in the liquid phase, for the carbon-dioxide water system, has any

adverse effect on the performance of the absorption tower. The conclusions

were drawn by comparing the results with that obtained by assuming plug flow

in the liquid phase. In both the cases piston flow was assumed in the gas

phase. Michael Brittan and Edward Woodburn[2] had considered the case of

axial mixing in the gas phase. This investigation lends further support to

Michael Brittan's prediction that the discrepancy between the acutal

absorption column performance and that predicted from standard mass trans-

fer correlations is due primarily to axial dispersion of the gas phase.

The experimental data for the present investigation were obtained from

Michael Brittan's[1] work on the absorption of carbon-dioxide by water in a

packed column. In this study, the gas rate was from 3.5 lb/(hr.)(sq. ft.) to

9.5 lb./(hr.)(sq. ft.) and the liquid rate from 2,500 lb./(hr.)(sq. ft.). The

absorption tower consisted of a single 3 5/8 inch I.D. glass section with

$\frac{1}{2}$ inch Raschig rings as the packings; the overall packed height was 34.75 inches.

The carbon dioxide concentration was measured at five different heights along

the length of the column in addition to the inlet and the outlet of the column.

The mathematical models used for the plug flow and the axial mixing

cases were obtained from the work of Miyauchi[13]. For the plug flow case,

the parameter N_{ox}, (i.e. the Number of Transfer Units) was obtained by the

use of the method of least squares. For the axial mixing case the axial mixing

parameter R and the number of transfer units parameter N_{ox} were obtained by

grpahical method. (A non-linear least square approach was attempted, but the solution did not converge.)

When analysing the data in terms of plug flow in the liquid phase, it was observed that the number of transfer units and the height equivalent to a transfer unit obtained for the various runs by the method of least squares were very close to those obtained by Brittan by a Runge-Kutta method of step-wise integration. At various heights along the length of the column, Brittan computed the concentration of carbon-dioxide in the liquid phase from which he obtained the NTU values. Whereas in this work, the concentration of carbon dioxide in the gas phase was employed to obtain the NTU values.

In the mathematical model for the case of axial mixing in the liquid phase, the value of the axial mixing parameter R was increased from 1 to 100, and that of the number of transfer units N_{ox}, from 0.27 to 1.43. Corresponding to these various permutations of R and N_{ox} the values of the carbon dioxide concentration in the gas phase were predicted along the length of the column. The percentage deviation of these predicted values of the gas phase concentration from the experimentally determined values was plotted against the liquid mixing term R with N_{ox} as the parameter for each of the 110 runs. All these plots exhibited a general trend; the value of the average absolute percentage deviation remained almost constant, irrespective of the value of the mixing parameter R, beyond the range of R equal to 20. For every individual value of N_{ox} the graph approached a minimum AAPD; and for every individual run, there was one unique value of N_{ox} and R where the value of AAPD was minimum. For the individual runs this value of the minimum AAPD remained close to the

value of the AAPD obtained from the plug flow case. This closeness between the values of AAPD meant that by introducing the axial mixing parameter R, in the mathematical model it was not possible to reduce the deviation between the predicted value and the experimental data. In other words, the axial mixing parameter R in the liquid phase had no significant effect in fitting the curve more closely to the experimental values. The above results lead to the conclusion that the effect of liquid mixing is negligible on the performance of the absorption column for the carbon-dioxide water system.

VI. APPENDICES

APPENDIX A

Derivation of the boundary conditions for the absorption column:

A. X Phase:

    1. Bottom of the column:

Taking a material balance at the section shown in Figure A.1

$$\text{input} \quad - \quad \text{output} \quad + \quad \text{generation} \quad = \quad \text{accumulation}$$

$$[U_x A_c \rho_x c_x \Delta t - E_x \frac{d(\rho_x c_x)}{dz} A_c \Delta t]_{-\frac{\Delta z}{2}}$$

$$-[U_x A_c \rho_x c_x \Delta t - E_x \frac{d(\rho_x c_x)}{dz} A_c \Delta t]_{+\frac{\Delta z}{2}} \qquad \qquad (A.1)$$

$$+[-K_x a A_c dz (c_x - c_x^*) \Delta t]_{+\frac{\Delta z}{4}} = 0$$

Since there is no absorption of the gas below the bed, (i.e. below z = 0), the

'generation' term is zero. Rearranging the equation (A.1),

$$[U_x c_x - E_x \frac{dc_x}{dz}]_{-\frac{\Delta z}{2}} \quad - \quad [U_x c_x - E_x \frac{dc_x}{dz}]_{+\frac{\Delta z}{2}} \quad = \quad 0 \qquad (A.2)$$

expanding the terms,

$$\left[U_x c_{x_{z<0}} - E_{x_{z<0}} \frac{dc_x}{dz}_{z<0} \right]_{\substack{z<0 \\ z \approx 0}} - \left[U_x c_x - E_{x_{0 \le z < L}} \frac{dc_x}{dz} \right]_{\substack{z<L \\ z \approx 0}} = 0 \qquad (A.3)$$

at z<0, $c_x = c_{xo}$; eddy diffusivity $E_x = 0$;

therefore

$$U_x c_{xo} - [U_x c_x - E_x \frac{dc_x}{dz}] = 0 \qquad \qquad (A.4)$$
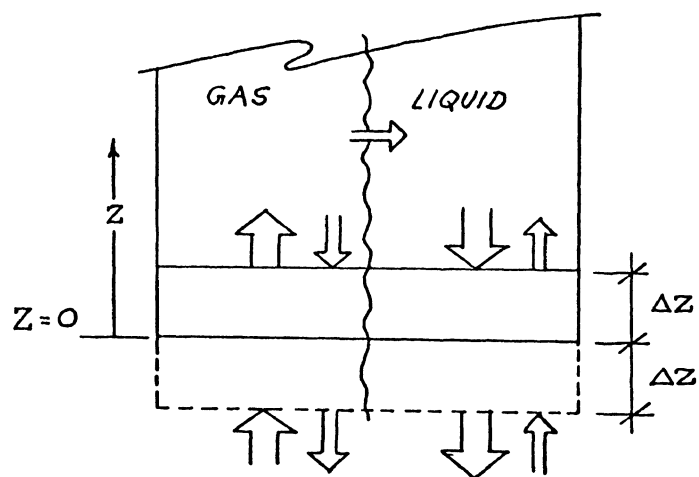
Figure A.1   Gas and Liquid Flow Regimes at the Bottom of an Absorption Tower.
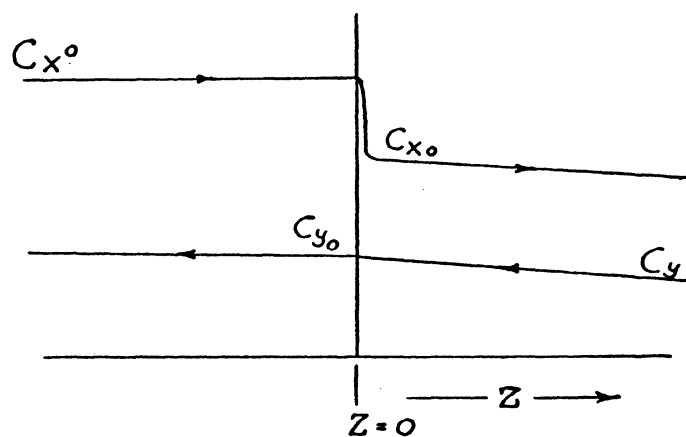
Figure A.2   Concentration Profile, of the Gas and the Liquid Phases, at the Bottom of the Absorption Tower.
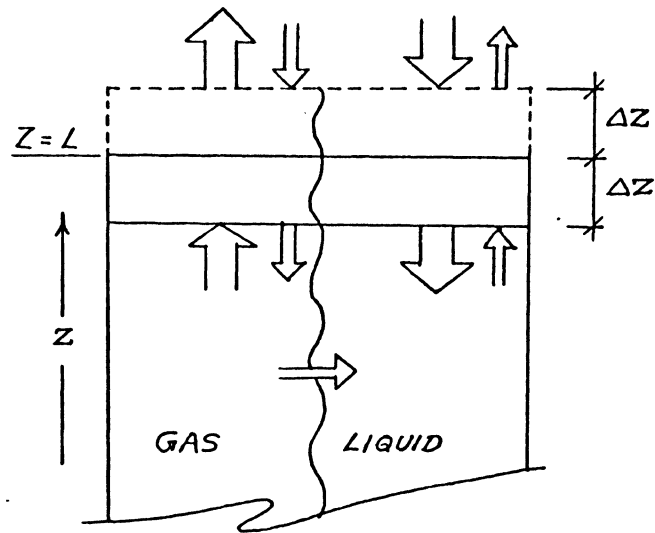
Figure A.3   Gas and liquid Flow Regimes at the Top of an Absorption Tower.
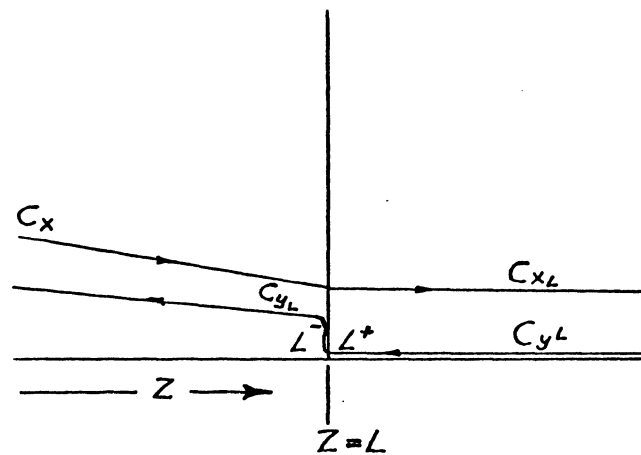
Figure A.4   Concentration Profile, of the Gas and the Liquid Phases, at
the Top of the Absorption Tower.

Rearranging the equation (A.4),

$$\frac{U_x}{E_x}(c_{xo} - c_x) = -\frac{dc_x}{dz} \tag{A.5}$$

Writing equation (A.5) into a dimensionless form by substituting $C_x = \dfrac{c_x}{c_{xo}}$

and $Z = \dfrac{z}{L}$

$$\frac{U_x L}{E_x}(1 - C_x) = -\frac{dC_x}{dZ} \tag{A.6}$$

But $\dfrac{U_x L}{E_x} = P_x B;$ $\tag{A.7}$

$$P_x B(1 - C_x) = -(\frac{dC_x}{dZ}) \tag{2.3}$$

Equation (2.3) is the boundary condition for the X phase at the bottom of the column.

2. Top of the column:

Taking a material balance at the section shown in the Figure A.3,

$$[U_x A_c \rho_x c_x \Delta t - E_x \rho_x \frac{dc_x}{dz} A_c \Delta t]_{L-\frac{\Delta z}{2}}$$

$$-[U_x A_c \rho_x c_x \Delta t - E_x \rho_x \frac{dc_x}{dz} A_c \Delta t]_{L+\frac{\Delta z}{2}}$$

$$+[-K_x a A_c dz(c_x - c_x^*) \Delta t]_{L-\frac{\Delta z}{4}} = 0 \tag{A.8}$$

Since there is no absorption of the gas above the bed, (i.e. above z = L), the generation term is zero. Rearranging the equation (A.8),

$$[U_x c_x - E_x \frac{dc_x}{dz}]_{L-\frac{\Delta z}{2}} - [U_x c_x - E_x \frac{dc_x}{dz}]_{L+\frac{\Delta z}{2}} = 0 \tag{A.9}$$

since for z>L, the eddy diffusivity $E_x = 0$,

Therefore,

$$\left[U_x c_x - E_x \frac{dc_x}{dz} \right]_{L - \frac{\Delta z}{2}} - \left[U_x c_x \right]_{L + \frac{\Delta z}{2}} = 0 \tag{A.10}$$

Rearranging the equation (A.10),

$$U_x \left[c_{x_{(L - \frac{\Delta z}{2})}} - c_{x_{(L + \frac{\Delta z}{2})}} \right] = E_x \left(\frac{dc_x}{dz} \right)_{L - \frac{\Delta z}{2}} \tag{A.11}$$

Now during the process of absorption the gas (i.e. X phase) concentration

decreases as the gas travels up the column, and so,

$$c_x \Big|_{L - \frac{\Delta z}{2}} \geq c_x \Big|_{L + \frac{\Delta z}{2}} \tag{A.12}$$

i.e.

$$c_x \Big|_{L - \frac{\Delta z}{2}} - c_x \Big|_{L + \frac{\Delta z}{2}} \geq 0 \tag{A.13}$$

From the Figure A.4 note that

$$\left(\frac{dc_x}{dz} \right)_{L - \frac{\Delta z}{2}} \leq 0 \tag{A.14}$$

To satisfy both (A.13) and (A.14), both must be equal to zero.

i.e.

$$c_x \Big|_{L^-} = c_x \Big|_{L^+} \tag{A.15}$$

and so $E_x = 0$ \hfill (A.16)

i.e. eddy diffusivity is zero at the top of the column.

B. Y Phase:

The process of absorption being counter-current the Y phase (i.e. water) enters at the top of the column and leaves from the bottom of the column. By reasonings similar to case of X Phase, the following results are obtained:

1. Bottom of the column: (exit end for Y phase)

$$E_y = 0 \qquad (A.17)$$

i.e. eddy diffusivity in the water phase at the bottom of the column is zero.

2. Top of the column: (inlet end for Y phase)

$$P_y B (C_{y_1} - C_y 1) = -\left[\frac{dC_y}{dZ}\right] \qquad (A.18)$$

where

$$C_{y_1} = \frac{c_{y_1}}{c_{xo}} \qquad (A.19)$$

and

$$C_y 1 = \frac{c_y 1}{c_{xo}} \qquad (A.20)$$

Equation (A.18) shows the presence of eddy diffusivity in the water phase at the top of the column.

APPENDIX B

Equation of Continuity for homogeneous flow systems:

For homogeneous continuous flow systems Damkohler[7] has given an equation of continuity as follows:

$$\frac{\partial c_i}{\partial \theta} = - \text{div} (-E_i \text{ grad } c_i) - \text{div} (U_i \ c_i) + \phi(c_i) \tag{B.1}$$

where U_i is the linear velocity of the fluid and c_i is the concentration of ith component at the point of interest. For one-dimensional steady state flow systems, in which a mean diffusivity and a mean velocity of the ith component are assumable, Damkohler's equation becomes

$$E_i \frac{d^2 c_i}{dz^2} - U_i \frac{dc_i}{dz} - \phi(c_i) = 0 \tag{B.2}$$

For one-dimensional countercurrent two-phase mass transfer process this equation is modified as follows, by introducing a void fraction ϵ for each phase and substituting the mass transfer term for $\phi(c_i)$;

$$\epsilon_x E_x \frac{d^2 c_x}{dz^2} - F_x \frac{dc_x}{dz} - K_x a(c_x - mc_y) = 0 \tag{B.3}$$

$$\epsilon_y E_y \frac{d^2 c_y}{dz^2} + F_y \frac{dc_y}{dz} + K_x a(c_x - mc_y) = 0 \tag{B.4}$$

where the direction of mass transfer is taken from phase x to phase y and a linear distribution equilibrium (with 'm' as the partition coefficient) is assumed. K_x represents the overall mass transfer coefficient relative to phase x; 'a' is the interfacial area per unit volume, and F is the superficial velocity of the designated phase. These equations are based on a simplified model which assumes the two phases flow in opposite directions,

with each phase undergoing longitudinal dispersion. Rearranging the

equation into dimensionless form we have,

$$\frac{d^2 C_x}{dZ^2} - P_x B \frac{dC_x}{dZ} - N_{ox} P_x B (C_x - mC_y) = 0 \tag{2.1}$$

and

$$\frac{d^2 C_y}{dZ^2} + P_y B \frac{dC_y}{dZ} + N_{oy} P_y B (C_x - mC_y) = 0 \tag{2.2}$$

where $C_x = \dfrac{c_x}{c_{xo}}$ (B.5)

$$C_y = \frac{c_y}{c_{xo}} \tag{B.6}$$

$$B = \frac{L}{d} \tag{B.7}$$

$$P_x = \frac{U_x d}{E_x} \tag{B.8}$$

$$P_y = \frac{U_y d}{E_y} \tag{B.9}$$

$$Z = \frac{z}{L} \tag{B.10}$$

$$N_{ox} = \frac{K_x a L}{F_x} \tag{B.11}$$

$$N_{oy} = \frac{K_x a L}{F_y} \tag{B.12}$$

$$U_x = \frac{F_x}{\epsilon_x} \tag{B.13}$$

$$U_y = \frac{F_y}{\epsilon_y} \qquad (B.14)$$

The associated boundary conditions as derived in Appendix A are as follows:

a) $Z = 0$, i) $-\left[\frac{dC_x}{dZ}\right] = P_x B (1 - C_x)$ (2.3)

ii) $-\left[\frac{dC_y}{dZ}\right] = 0$ (2.4)

b) $Z = 1$, i) $-\left[\frac{dC_x}{dZ}\right] = 0$ (2.5)

ii) $-\left[\frac{dC_y}{dZ}\right] = P_y B (C_{y_1} - C_y 1)$ (2.6)

APPENDIX C

Normal Equation for Case 1:

Let $\overset{*}{C}_{xi} = \dfrac{e^{\lambda z_i} - \Lambda e^{\lambda}}{1 - \Lambda e^{\lambda}}$ (C.1)

be the mathematical model for the case of plug flow in both the gas and the liquid phases; $\overset{*}{C}_{xi}$ is the predicted value of the concentration of carbon dioxide in the gas phase, and C_{xi} is that experimentally determined.

Let the deviation between the experimental and the predicted values be $\bar{\epsilon}$

i.e. $\bar{\epsilon}_i = (C_{xi} - \overset{*}{C}_{xi})$ (C.2)

The best fitting curve through the data is the curve which makes the sum of the squares of deviations of the experimental C_x values from the predicted $\overset{*}{C}_x$ values a minimum;

i.e. $S = \sum\limits_{i=1}^{n} (\bar{\epsilon}_i)^2$ is a minimum. (C.3)

where

$i = 1, 2, ------, (n-1), n.$

n = total number of data points

C_{xi} = concentration of carbon dioxide in the gas phase at the point Z_i

Z_i = height of the point i from the base of the column.

The sum of the squares of deviation is a function of N_{ox} and hence of λ.

This deviation will be a minimum when

$\dfrac{dS}{d\lambda} = 0;$ (C.4)

i.e. $\dfrac{dS}{d\lambda} = -2 \sum\limits_{i=1}^{n} (C_{xi} - \overset{*}{C}_{xi}) \dfrac{\partial \overset{*}{C}_{xi}}{\partial \lambda} \equiv 0$ (C.5)

Expanding the non-linear mathematical model, equation (C.1), in Taylor series around the point $\lambda = \lambda o$,

$$\overset{*}{C}_{x(\lambda)} \doteq \frac{e^{\lambda o Z} - \Lambda e^{\lambda o}}{1 - \Lambda e^{\lambda o}} + \left[\frac{\partial \overset{*}{C}_x}{\partial \lambda}\right]_{\lambda = \lambda o} (\lambda - \lambda o) + \text{(neglect higher order} \qquad \text{(C.6)}$$
$$\text{derivatives)}$$

Now taking the partial derivative of $\overset{*}{C}_x$, represented by equation (C.6), with respect to λ at $\lambda = \lambda o$,

$$\left[\frac{\partial \overset{*}{C}_x}{\partial \lambda}\right]_{\lambda = \lambda o} = \frac{(1 - \Lambda e^{\lambda o})(Z e^{\lambda o Z} - \Lambda e^{\lambda o}) - (e^{\lambda o Z} - \Lambda e^{\lambda o})(-\Lambda e^{\lambda o})}{(1 - \Lambda e^{\lambda o})^2} \qquad \text{(C.7)}$$

Rearranging the terms,

$$\left[\frac{\partial \overset{*}{C}_x}{\partial \lambda}\right]_{\lambda = \lambda o} = \frac{Z e^{\lambda o Z}(1 - \Lambda e^{\lambda o}) + \Lambda e^{\lambda o}(e^{\lambda o Z} - 1)}{(1 - \Lambda e^{\lambda o})^2} \qquad \text{(C.8)}$$

Substituting the value of $\frac{\partial \overset{*}{C}_x}{\partial \lambda}$ at $\lambda = \lambda o$, i.e. equation (C.8) in equation (C.6),

$$\overset{*}{C}_{x(\lambda)} \doteq \frac{e^{\lambda o Z} - \Lambda e^{\lambda o}}{1 - \Lambda e^{\lambda o}} + \frac{Z e^{\lambda o Z}(1 - \Lambda e^{\lambda o}) + \Lambda e^{\lambda o}(e^{\lambda o Z} - 1)}{(1 - \Lambda e^{\lambda o})^2} (\lambda - \lambda o) \qquad \text{(C.9)}$$

Equation (C.9) shows the mathematical model expanded in Taylor series.

Differentiating partially the mathematical model, equation (C.9), with respect to λ,

$$\left[\frac{\partial \overset{*}{C}_x}{\partial \lambda}\right] = 0 + \frac{Z e^{\lambda o Z}(1 - \Lambda e^{\lambda o}) + \Lambda e^{\lambda o}(e^{\lambda o Z} - 1)}{(1 - \Lambda e^{\lambda o})^2} \cdot (1-0) \qquad \text{(C.10)}$$

Substituting equation (C.10) in equation (C.5) as follows:

$$\frac{ds}{d\lambda} = 0 \equiv 2 \sum_{i=1}^{\eta} \left\{ \left[Cx_i - \frac{e^{\lambda_o Z_i} - \Lambda e^{\lambda_o}}{(1 - \Lambda e^{\lambda_o})} - \frac{Z_i e^{\lambda_o Z_i}(1-\Lambda e^{\lambda_o}) + \Lambda e^{\lambda_o}(e^{\lambda_o Z_i}-1)}{(1 - \Lambda e^{\lambda_o})^2}(\lambda - \lambda_o) \right] \right.$$

$$\left. \left[\frac{Z_i e^{\lambda_o Z_i}(1 - \Lambda e^{\lambda_o}) + \Lambda e^{\lambda_o}(e^{\lambda_o Z_i} - 1)}{(1 - \Lambda e^{\lambda_o})^2} \right] \right\} \tag{C.11}$$

Rearranging the above-shown equation,

$$\sum_{i=1}^{\eta} Cx_i \left[\frac{Z_i e^{\lambda_o Z_i}(1 - \Lambda e^{\lambda_o}) + \Lambda e^{\lambda_o}(e^{\lambda_o Z_i} - 1)}{(1 - \Lambda e^{\lambda_o})^2} \right]$$

$$-\sum_{i=1}^{\eta} \left[\frac{e^{\lambda_o Z_i} - \Lambda e^{\lambda_o}}{1 - \Lambda e^{\lambda_o}} \right] \left[\frac{Z_i e^{\lambda_o Z_i}(1 - \Lambda e^{\lambda_o}) + \Lambda e^{\lambda_o}(e^{\lambda_o Z_i} - 1)}{(1 - \Lambda e^{\lambda_o})^2} \right]$$

$$= \sum_{i=1}^{\eta} \left[\frac{Z_i e^{\lambda_o Z_i}(1 - \Lambda e^{\lambda_o}) + \Lambda e^{\lambda_o}(e^{\lambda_o Z_i} - 1)}{(1 - \Lambda e^{\lambda_o})^2} \right]^2 (\lambda - \lambda_o) \tag{3.6}$$

Equation (3.6) represents the 'normal equation' with λ as the parameter for

the case of plug flow in both the gas and the liquid phases.

APPENDIX D

Normal Equations for Case 3:

Let the mathematical model be,

$$\overset{*}{C}_x = H_1\, e^{\lambda 1^Z} + H_2\, e^{\lambda 2^Z} + H_3\, e^{\lambda 3^Z} \tag{D.1}$$

Similar to Appendix C we have the sum of the squares of the deviation between the experimental and the predicted values of the concentration of carbon dioxide in the gas phase, as follows:

$$S = \sum_{i=1}^{n} (C_{xi} - \overset{*}{C}_{xi})^2 \tag{D.2}$$

The sum of the squares of deviation is a function of N_{ox} (will be denoted as 'X') and $P_y B$ (will be denoted as 'R'). This deviation will be a minimum when the following are satisfied:

$$i) \quad \frac{\partial S}{\partial X} = -2 \sum_{i=1}^{n} (C_{xi} - \overset{*}{C}_{xi}) \frac{\partial \overset{*}{C}_x}{\partial X} \equiv 0, \tag{D.3}$$

$$ii) \quad \frac{\partial S}{\partial R} = -2 \sum_{i=1}^{n} (C_{xi} - \overset{*}{C}_{xi}) \frac{\partial \overset{*}{C}_x}{\partial R} \equiv 0. \tag{D.4}$$

Expanding the non-linear mathematical model represented by the equation (D.1), in Taylor series around the points $X = Xo$ and $R = Ro$,

$$\overset{*}{C}_x = \overset{*}{C}_{xo} + \frac{\partial \overset{*}{C}_x}{\partial X}\Big|_{X=Xo} (X - Xo) + \frac{\partial \overset{*}{C}_x}{\partial R}\Big|_{R=Ro} (R - Ro) + \text{(neglect the} \tag{D.5}$$
$$\text{higher order derivatives)}$$

A.. Partial Derivatives with respect to the parameter X (i.e. N_{ox})

Differentiating partially equation (D.1) w.r.t. X,

$$\frac{\partial \overset{*}{C}_x}{\partial X} = \frac{\partial H_1}{\partial X} \cdot e^{\lambda 1^Z} + H_1 \cdot Z \cdot \frac{\partial \lambda_1}{\partial X} \cdot e^{\lambda 1^Z} + \frac{\partial H_2}{\partial X} \cdot e^{\lambda 2^Z}$$

$$+ H_2 \cdot Z \cdot \frac{\partial \lambda_2}{\partial X} \cdot e^{\lambda_2 Z} + \frac{\partial H_3}{\partial X} \cdot e^{\lambda_3 Z} + H_3 \cdot Z \cdot \frac{\partial \lambda_3}{\partial X} \cdot e^{\lambda_3 Z} \tag{D.6}$$

Now,

$$H_1 = \frac{DH_1}{DH} \tag{D.7a}$$

$$H_2 = \frac{DH_2}{DH} \tag{D.7b}$$

$$H_3 = \frac{DH_3}{DH} \tag{D.7c}$$

Taking the partial derivative of equation (D.7a) w.r.t. X,

$$\frac{\partial H_1}{\partial X} = \frac{DH \cdot \frac{\partial}{\partial X} \cdot DH_1 - DH_1 \cdot \frac{\partial}{\partial X} \cdot DH}{(DH)^2} \tag{D.8a}$$

Again,

$$DH_1 = h_2 h_3 \lambda_2 (1 + \frac{\lambda_3}{R}) e^{\lambda_3} - h_3 h_2 \lambda_3 (1 + \frac{\lambda_2}{R}) e^{\lambda_2} \tag{D.9a}$$

Differentiating equation (D.9a),

$$\frac{\partial DH_1}{\partial X} = h_2 h_3 \lambda_2 \left[(1 + \frac{\lambda_3}{R})(\frac{\partial \lambda_3}{\partial X}) e^{\lambda_3} + \frac{e^{\lambda_3}}{R} \cdot \frac{\partial \lambda_3}{\partial X} \right]$$

$$+ (1 + \frac{\lambda_3}{R}) e^{\lambda_3} \left[h_2 h_3 (\frac{\partial \lambda_2}{\partial X}) + \lambda_2 (h_2 \frac{\partial h_3}{\partial X} + h_3 \frac{\partial h_2}{\partial X}) \right]$$

$$- h_3 h_2 \lambda_3 \left[(1 + \frac{\lambda_2}{R})(\frac{\partial \lambda_2}{\partial X}) e^{\lambda_2} + \frac{e^{\lambda_2}}{R} (\frac{\partial \lambda_2}{\partial X}) \right]$$

$$- (1 + \frac{\lambda_2}{R}) e^{\lambda_2} \left[h_3 h_2 (\frac{\partial \lambda_3}{\partial X}) + \lambda_3 (h_3 \cdot \frac{\partial h_2}{\partial X} + h_2 \cdot \frac{\partial h_3}{\partial X}) \right] \tag{D.10a}$$

Now in equation (D.1),

$$\lambda_1 = 0 \tag{D.11a}$$

$$\lambda_2 = -(\frac{h}{2}) + \sqrt{(\frac{h}{2})^2 - k} \tag{D.11b}$$

and

$$\lambda_3 = -\left(\frac{h}{2}\right) - \sqrt{\left(\frac{h}{2}\right)^2 - k} \qquad (D.11c)$$

where,

$$h = N_{ox} + P_y B \equiv X + R = a \qquad (D.12a)$$

and

$$k = N_{ox} \cdot P_y B \cdot (1 - \Lambda) \equiv X.R. \ (1 - \Lambda) = b \qquad (D.12\ b)$$

Differentiating partially equations (D.11b) and (D.11c) w.r.t. X,

$$\frac{\partial \lambda_2}{\partial X} = -\frac{1}{2} \cdot \frac{\partial a}{\partial X} + \frac{1}{2}\left(\frac{a^2}{4} - b\right)^{-\frac{1}{2}} \cdot \left(\frac{1}{2} \cdot a \cdot \frac{\partial a}{\partial X} - \frac{\partial b}{\partial X}\right) \qquad (D.13a)$$

and

$$\frac{\partial \lambda_3}{\partial X} = -\frac{1}{2} \cdot \frac{\partial a}{\partial X} - \frac{1}{2} \cdot \left(\frac{a^2}{4} - b\right)^{-\frac{1}{2}} \cdot \left(\frac{1}{2} \cdot a \cdot \frac{\partial a}{\partial X} - \frac{\partial b}{\partial X}\right) \qquad (D.13b)$$

where,

$$\frac{\partial a}{\partial X} = 1 \qquad (D.14a)$$

$$\frac{\partial b}{\partial X} = (1 - \Lambda)R \qquad (D.14b)$$

Again,

$$DH = DH_1 + (h_3 \lambda_3 - h_2 \lambda_2) \qquad (D.15)$$

$$DH_2 = +h_3 \lambda_3 \qquad (D.9b)$$

and

$$DH_3 = -h_2 \lambda_2 \qquad (D.9c)$$

Now differentiating equation (D.15) partially w.r.t. X to get the following:

$$\frac{\partial DH}{\partial X} = \frac{\partial DH_1}{\partial X} + h_3 \frac{\partial \lambda_3}{\partial X} + \lambda_3 \frac{\partial h_3}{\partial X} - h_2 \frac{\partial \lambda_2}{\partial X} - \lambda_2 \frac{\partial h_2}{\partial X} \qquad (D.16)$$

Also,

$$h_1 = 1 + \lambda_1 X \qquad (D.17a)$$

$$h_2 = 1 + \lambda_2 X \qquad (D.17b)$$

and

$$h_3 = 1 + \lambda_3 X \qquad (D.17c)$$

The partial derivatives of the above equations i.e. (D.17a), (D.17b) and (D.17c),

each w.r.t. X are as shown below:

$$\frac{\partial h_1}{\partial X} = \lambda_1 + X \cdot \frac{\partial \lambda_1}{\partial X} \qquad (D.18a)$$

$$\frac{\partial h_2}{\partial X} = \lambda_2 + X \cdot \frac{\partial \lambda_2}{\partial X} \qquad (D.18b)$$

$$\frac{\partial h_3}{\partial X} = \lambda_3 + X \cdot \frac{\partial \lambda_3}{\partial X} \qquad (D.18c)$$

Partially differentiating equations (D.7b) and (D.7c),

$$\frac{\partial H_2}{\partial X} = \frac{DH \cdot \frac{\partial DH_2}{\partial X} - DH_2 \cdot \frac{\partial DH}{\partial X}}{(DH)^2} \qquad (D.8b)$$

and

$$\frac{\partial H_3}{\partial X} = \frac{DH \cdot \frac{\partial DH_3}{\partial X} - DH_3 \cdot \frac{\partial DH}{\partial X}}{(DH)^2} \qquad (D.8c)$$

The partial derivatives of the equations (D.9b) and (D.9c) w.r.t. X are as

follows:

$$\frac{\partial DH_2}{\partial X} = h_3 \frac{\partial \lambda_3}{\partial X} + \lambda_3 \frac{\partial h_3}{\partial X} \qquad \text{(D.10b)}$$

and

$$\frac{\partial DH_3}{\partial X} = - h_2 \frac{\partial \lambda_2}{\partial X} - \lambda_2 \frac{\partial h_2}{\partial X} \qquad \text{(D.10c)}$$

B. Partial Derivatives with respect to the parameter R   (i.e. $P_y B$)

Differentiating partially equation (D.1) w. r. t. R,

$$\frac{\partial \overset{*}{C}_x}{\partial R} = \frac{\partial H_1}{\partial R} \cdot e^{\lambda_1 Z} + H_1 \cdot Z \cdot \frac{\partial \lambda_1}{\partial R} e^{\lambda_1 Z} + \frac{\partial H_2}{\partial R} \cdot e^{\lambda_2 Z} + H_2 \cdot Z \frac{\partial \lambda_2}{\partial R} \cdot e^{\lambda_2 Z}$$

$$+ \frac{\partial H_3}{\partial R} \cdot e^{\lambda_3 Z} + H_3 Z \cdot \frac{\partial \lambda_3}{\partial R} \cdot e^{\lambda_3 Z} \qquad \text{(D.19)}$$

Taking the partial derivative of equation (D.7a) w. r. t. R,

$$\frac{\partial H_1}{\partial R} = \frac{DH \cdot \dfrac{\partial DH_1}{\partial R} - DH_1 \dfrac{\partial DH}{\partial R}}{(DH)^2} \qquad \text{(D.20a)}$$

Differentiating equation (D. 9a),

$$\frac{\partial DH_1}{\partial R} = h_2 h_3 \lambda_2 \left[(1 + \frac{\lambda_3}{R})(\frac{\partial \lambda_3}{\partial R}) e^{\lambda_3} + e^{\lambda_3} (\frac{R \cdot \frac{\partial \lambda_3}{\partial R} - \lambda_3}{R^2}) \right]$$

$$+ (1 + \frac{\lambda_3}{R}) e^{\lambda_3} \left[h_2 h_3 \frac{\partial \lambda_2}{\partial R} + \lambda_2 (h_2 \frac{\partial h_3}{\partial R} + h_3 \frac{\partial h_2}{\partial R}) \right]$$

$$- h_3 h_2 \lambda_3 \left[(1 + \frac{\lambda_2}{R})(\frac{\partial \lambda_2}{\partial R}) e^{\lambda_2} + e^{\lambda_2} (\frac{R \frac{\partial \lambda_2}{\partial R} - \lambda_2}{R^2}) \right]$$

$$- (1 + \frac{\lambda_2}{R}) e^{\lambda_2} \left[h_3 h_2 \frac{\partial \lambda_3}{\partial R} + \lambda_3 (h_3 \frac{\partial h_2}{\partial R} + h_2 \frac{\partial h_3}{\partial R}) \right] \qquad \text{(D.21a)}$$

Differentiating partially equations (D.11b) and (D.11c) w.r.t. R,

$$\frac{\partial \lambda_2}{\partial R} = -\frac{1}{2} \cdot \frac{\partial a}{\partial R} + \frac{1}{2}(\frac{a^2}{4} - b)^{-\frac{1}{2}} (\frac{1}{2} \cdot a \cdot \frac{\partial a}{\partial R} - \frac{\partial b}{\partial R})$$ (D.22a)

and

$$\frac{\partial \lambda_3}{\partial R} = -\frac{1}{2} \cdot \frac{\partial a}{\partial R} - \frac{1}{2}(\frac{a^2}{4} - b)^{-\frac{1}{2}} (\frac{1}{2} \cdot a \cdot \frac{\partial a}{\partial R} - \frac{\partial b}{\partial R})$$ (D.22b)

where,

$$\frac{\partial a}{\partial R} = 1$$ (D.23a)

$$\frac{\partial b}{\partial R} = (1 - \Lambda)X$$ (D.23b)

Now we differentiate equation (D.15) partially w.r.t. R to get the following,

$$\frac{\partial DH}{\partial R} = \frac{\partial DH_1}{\partial R} + h_3 \frac{\partial \lambda_3}{\partial R} + \lambda_3 \frac{\partial h_3}{\partial R} - h_2 \frac{\partial \lambda_2}{\partial R} - \lambda_2 \frac{\partial h_2}{\partial R}$$ (D.24)

The partial derivatives equations (D.17a), (D.17b) and (D.71c), each w.r.t. R are as shown below,

$$\frac{\partial h_1}{\partial R} = X \cdot \frac{\partial \lambda_1}{\partial R}$$ (D.25a)

$$\frac{\partial h_2}{\partial R} = X \cdot \frac{\partial \lambda_2}{\partial R}$$ (D.25b)

$$\frac{\partial h_3}{\partial R} = X \cdot \frac{\partial \lambda_3}{\partial R}$$ (D.25c)

Partially differentiating equations (D.7b) and (D.7c),

$$\frac{\partial H_2}{\partial R} = \frac{DH \cdot \frac{\partial DH_2}{\partial R} - DH_2 \frac{\partial DH}{\partial R}}{(DH)^2}$$ (D.20b)

and

$$\frac{\partial H_3}{\partial R} = \frac{DH \cdot \frac{\partial DH_3}{\partial R} - DH_3 \frac{\partial DH}{\partial R}}{(DH)^2}$$ (D.20c)

The partial derivatives of the equations (D.9b) and (D.9c) w.r.t. R are as follows:

$$\frac{\partial DH_2}{\partial R} = h_3 \frac{\partial \lambda_3}{\partial R} + \lambda_3 \frac{\partial h_3}{\partial R}$$ (D.21b)

and

$$\frac{\partial DH_3}{\partial R} = - h_2 \frac{\partial \lambda_2}{\partial R} - \lambda_2 \cdot \frac{\partial h_2}{\partial R}$$ (D.21c)

Now for minimum deviation from equation (D.3) and (D.4),

$$\sum_{i=1}^{n} (C_{xi} - \overset{*}{C}_{xi}) \frac{\partial \overset{*}{C}_{xi}}{\partial X} = 0$$ (D.3a)

and

$$\sum_{i=1}^{n} (C_{xi} - \overset{*}{C}_{xi}) \frac{\partial \overset{*}{C}_{xi}}{\partial R} = 0$$ (D.4a)

Substituting equation (D.5) in the above equations,

$$\sum_{i=1}^{n} \left[C_{xi} - \overset{*}{C}_{xo} - (\frac{\partial \overset{*}{C}_{xi}}{\partial X})_{X=Xo} (X - Xo) - (\frac{\partial \overset{*}{C}_{xi}}{\partial R})_{R=Ro} (R - Ro) \right] (\frac{\partial \overset{*}{C}_{xi}}{\partial X})_{X=Xo} = 0$$ (D.26)

and

$$\sum_{i=1}^{n} \left[C_{xi} - \overset{*}{C}_{xo} - (\frac{\partial C_{xi}}{\partial X})_{X=Xo} (X - Xo) - (\frac{\partial \overset{*}{C}_{xi}}{\partial R})_{R=Ro} (R - Ro) \right] (\frac{\partial \overset{*}{C}_{xi}}{\partial R})_{R=Ro} = 0$$ (D.27)

Rearranging the above equations (D.26) and (D.27),

$$\Sigma\, C_{xi}\, \left(\frac{\partial C^*_{xi}}{\partial X}\right)_{Xo} - \Sigma\, C^*_{xo}\, \left(\frac{\partial C^*_{xi}}{\partial X}\right)_{Xo} + \Sigma\left(\frac{\partial C^*_{xi}}{\partial X}\right)^2_{Xo}\cdot Xo + \Sigma\left(\frac{\partial C^*_{xi}}{\partial R}\right)_{Ro}\left(\frac{\partial C^*_{xi}}{\partial X}\right)_{Xo}\cdot Ro$$

$$= \Sigma\left(\frac{\partial C^*_{xi}}{\partial X}\right)^2_{Ro}\, X + \Sigma\left(\frac{\partial C^*_{xi}}{\partial R}\right)_{Ro}\left(\frac{\partial C^*_{xi}}{\partial X}\right)_{Xo}\cdot R \qquad (3.10)$$

$$\Sigma\, C_{xi}\, \left(\frac{\partial C^*_{xi}}{\partial R}\right)_{Ro} - \Sigma\, C^*_{xo}\, \left(\frac{\partial C^*_{xi}}{\partial R}\right)_{Ro} + \Sigma\, \left(\frac{\partial C^*_{xi}}{\partial R}\right)^2_{Ro}\cdot Ro + \Sigma\, \left(\frac{\partial C^*_{xi}}{\partial R}\right)_{Ro}\left(\frac{\partial C^*_{xi}}{\partial X}\right)_{Xo}\cdot Xo$$

$$= \Sigma\, \left(\frac{\partial C^*_{xi}}{\partial R}\right)_{Ro}\left(\frac{\partial C^*_{xi}}{\partial X}\right)_{Xo}\cdot X + \Sigma\, \left(\frac{\partial C^*_{xi}}{\partial R}\right)^2_{Ro}\cdot R \qquad (3.11)$$

Equations (3.10) and (3.11) are the 'normal equations', for the case of plug

flow in the gas phase but axial mixing in the liquid phase, with X (i.e. N_{ox})

and R (i.e. $P_y B$) as the parameters.

APPENDIX E

Flow Chart for Case 1:

The 'normal equation' for the case of plug flow in both the gas and the

liquid phases as given by the equation (3.6) is given below:

$$C_{xi} [A] - \left[\frac{e^{\lambda o\, Z_i} - \Lambda e^{\lambda o}}{1 - \Lambda e^{\lambda o}} \right] [A] = [A]^2 (\lambda - \lambda_o) \qquad (3.6)$$

where

$$[A] = \frac{Z_i\, e^{\lambda o\, Z_i} (1 - \Lambda e^{\lambda o}) + \Lambda e^{\lambda o} (e^{\lambda o\, Z_i} - 1)}{(1 - \Lambda e^{\lambda o})^2} \qquad (E.1)$$

The values of the various terms in the above equation (3.6) are illustrated

below for run 30.

$$C_{xi} = \frac{c_{xi}}{c_{xo}} \quad \text{mole fraction} \qquad (B.5)$$

where

c_{xi} = concentration of carbon dioxide in the gas phase and the point i

along the length of the column

and

c_{xo} = concentration of carbon dioxide in the gas phase at the inlet end

of the column (i.e. 0.2 g mole/mole of $CO_2 + N_2$)

$$\Lambda = m \frac{F_x}{F_y} \qquad (3.4)$$

where

m = equilibrium distribution coefficient

= H/total pressure in atmosphere

H = Henry's constant

$$= 1767 \text{ atm/mole fraction}^{(11)}$$

$$\therefore \ m = 1767/(623.2/760) \ \text{--- for run 30}$$

$$F_x = \text{superficial gas flow rate (lb. mole/hr. sq. ft.)}$$

The molecular weight of 20% mixture of carbon dioxide in nitrogen is 31.2

$$\therefore \ F_x = 5.74/31.2 \ \text{(lb. mole/hr. sq. ft.)} \ \text{--- for run 30}$$

$$F_y = \text{superficial liquid flow rate (lb. mole/hr. sq. ft.)}$$

$$\therefore \ F_y = 7,356/18.0 \ \text{(lb. mole/hr. sq. ft.)} \ \text{--- for run 30}$$

$$Z_i = \frac{z_i}{L} \ \text{(dimensionless)} \tag{B.10}$$

where

$$z_i = \text{height of the packing from the base to the point i}$$

and

$$L = \text{total height of the packing (ft.)}$$

$$= 2.895 \text{ ft.}$$

$$\text{Variance on } c_x, \ \sigma^2_{(cx)} = \frac{1}{D.F.} \ \sum_{i=1}^{n} (c_{xi} - c_{xi}^*)^2 \tag{3.13}$$

where

$$D.F. = (6 - 1) \tag{3.13a}$$

$$\text{Variance on } \lambda, \ \sigma^2_{(\lambda)} = \sum_{i=1}^{n} \frac{1}{[A]^2} \ \sigma^2_{(cx)} \tag{3.16a}$$

$$\text{Standard deviation on } N_{ox}, \ \sigma N_{ox} = \frac{\sigma^2_{(\lambda)}}{(\Lambda - 1)} \tag{3.18)}$$

From equation (3.12),

$$AAPD = \frac{100}{n} \ \sum_{i=1}^{\eta} \left[\left| \frac{c_{xi} - c_{xi}^*}{c_{xi}} \right| \right] \tag{3.12}$$

$$K_G a = \frac{N_{ox} \cdot F_x}{L} \ \text{(lb. mole/hr. cu. ft. mole. fn.)} \tag{E.2}$$

```
C       SOLUTION OF NORMAL EQUATION
C       ONE PARAMETER NODEL; CASE 1
C       NON LINEAR REGRESSION ANALYSIS, NOX AS PARAMETER
1       DIMENSION CX(100), A(100), B(100), U(100), V(100),
        1W(100), CSX(100), Z(100), Z1(100), SX(100)
2       N=6
3       TR=110.
4       SOX=0.
5       SAAPD=0.
6       SVARI=0.
7       SSTDV=0.
8       SSDOX=0.
9       SAKGA=0.
10      SAZ=0.
11      READ(1,10)(Z1(1),I=1,N)
12      DO 60 K=1,110
13      READ(1,48)RUN
14      WRITE(3,49)RUN
15      READ(1,50)PT,FY,FX
16      WRITE(3,11)PT,FY,FX
17      READ(1,10)(SX(I),I=1,N)
18      WRITE(3,13)(SX(I),I=1,N)
19      WRITE(3,3)(Z1(I),I=1,N0
20      OX=2.
21      XO=.2000
22      PT=PT/760.
23      H=1767.0
24      D=H/PT
25      FY=FY/18.
26      FX=FX/31.2
27      E=2.895
```

```
28        CL=D*FX/FY
29        SL=-OX*(1.-CL)
30        DO 22 M=1,200
31        S1=0
32        S2=0
33        S3=0
34        DO 20 I=1,N
35        Z(I)=Z1(I)/E
36        CX(I)=SX(I)/XO
37        A(I)=EXP(SL*Z(I))
38        B(I)=EXP(SL)
39        U(I)=1.-CL*B(I)
40        V(I)=(Z(I)*A(I)*U(I)+CL*B(I)*(A(I)-1.))/U(I)**2
41        W(I)=(A(I)-CL*B(I))/(1.-CL*B(I))
42        S1=S1+CX(I)*V(I)
43        S2=S2+W(I)*V(I)
44     20 S3=S3+V(I)**2
45        SL1=SL+(S1-S2)/S3
46        IF (ABS(SL1**2-SL**2)-5.0E-08)30,30,31
47     31 SL=SL1
48     22 CONTINUE
49     30 OX=-SL/(1.-CL)
50        WRITE(3,12)OX
51        S5=0
52        S4=0
53        DO 23 I=1,N
54        CSX(I)=(A(I)-CL*B(I))/(1.-CL*B(I))
55        CSX(I)=CSX(I)*XO
56        S5=S5+(ABS(SX(I)-CSX(I)))/SX(I)
57     23 S4=S4+(SX(I)-CSX(I))**2
58        WRITE(3,14)(SX(I),I=1,N)
```

```
59          WRITE(3,88)(CSX(I),I=1,N)
60          VARI=S4/5.
61          AAPD=S5*100./6.
62          STDV=SQRT(VARI/S3)
63          SDOX=STDV/(CL-1.)
64          WRITE(3,15)VARI,AAPD,STDV,SDOX
65      10  FORMAT(3F18.8)
66      11  FORMAT(4X,'PT(MM HG)=',F10.4,//4X,'L(LB/HR.SQFT)='F10.4,//,4X,
            7'G(LB/HR.SQFT)='F10.4,///)
67      12  FORMAT(///,4X,'NOX='E18.8,///)
68      13  FORMAT(2X,'CX=',6F14.7)
69       3  FORMAT(2X,'7 =',6F14.7)
70      14  FORMAT(2X,'CX        ',2X,6F18.8)
71      88  FORMAT(2X,'CX(CAL)',2X,6E18.8)
72      15  FORMAT(///,4X,'VARIANCE**2='E18.8,//,4X,'AAPD        ='E18.8
            2//,4X,'S.DEVIATION='E18.8,//,4X,'S.DEV-NOX   ='E18.8//)
73      48  FORMAT(F10.4)
74      49  FORMAT('1',2OX,'RUN=',F5.0,/////)
75      50  FORMAT(3F18.8)
        C       CALCULATION OF HEIGHT OF THE TOWER
76          X1=0.2
77          READ(1,200)X2
78          Y2=0.
79          CIN=X1/(1-X1)
80          COUT=X2/(1-X2)
81          CABSOB=FX*(1-X1)*(CIN-COUT)
82          Y1=CABSOB/(FY+CABSOB)
83          Y1EQ=Y1*D
84          DBOT=X1-Y1EQ
85          DTOP=X2
86          DP=(DBOT-DTOP)/ALOG(DBOT/DTOP)
```

```
87        AKGA=OX*FX/E
88        AZ=CABSOB/(AKGA*DP)
89        WRITE(3,201)CABSOB
90        WRITE(3,202)Y1
91        WRITE(3,203)Y1EQ
92        WRITE(3,204)DP
93        WRITE(3,205)AKGA
94        WRITE(3,206)AZ
95        SOX=SOX+OX
96        AOX=SOX/TR
97        SVARI=SVARI+VARI
98        AVARI=SVARI/TR
99        SAAPD=SAAPD+AAPD
100       AAAPD=SAAPD/TR
101       SSTDV=SSTDV+STDV
102       ASTDV=SSTDV/TR
103       SSDOX=SSDOX+SDOX
104       ASDOX=SSDOX/TR
105       SAKGA=SAKGA+AKGA
106       AAKGA=SAKGA/TR
107       SAZ=SAZ+AZ
108       AAZ=SAZ/TR
109   200 FORMAT(F18.8)
110   201 FORMAT(//,4X,'CO2 ABSORBED(LBMOLE/HR.SQFT)     ='F18.8)
111   202 FORMAT(//,4X,'Y1(CO2 MOLE FN IN H2O AT BOTTOM)  ='F18.8)
112   203 FORMAT(//,4X,'EQUILIBRIUM MOLE FN AT BOTTOM     ='F18.8)
113   204 FORMAT(//,4X,'LOG MEAN DRIVING FORCE(MOLE FN)   ='F18.8)
114   205 FORMAT(//,4X,' KGA  LBMOLE/HR.CUFT. MOLE FN     ='F18.8)
115   206 FORMAT(//,4X,'ACTUAL HEIGHT OF COLUMN REQD      ='F18.8)
116    60 CONTINUE
117       WRITE(3,400)
```

```
118        WRITE(3,401)AOX,AVARI,AAAPD,ASTDV,ASDOX,AAKGA,AAZ
119   400  FORMAT('1',10X,'AVERAGE AVLUES',////)
120   401  FORMAT(//,4X,'NOX          =',E18.8,//,4X,'VARIANCE**2=',E18.8,//,
           24X,'AAPD         =',F18.8,//,4X,'S.DEVIATION='E18.8,//,4X,'S.DEV-NO
           3X  =',E18.8,4X,'KGA          ='.F18.8,//,4X,'HEIGHT       =',F18.8)
121        STOP
122        END
      /DATA
```

TABLE I

Data Selected for the Study

[The following table shows the experimental data of Brittan[1] that have been used in this work:]

RUN	GAS(LB./HR.SQ.FT.)	LIQUID(LB./HR.SQ.FT.)	TOTAL PRESSURE (M.M.HG.)
20	9.5830	9195.0000	623.5000
25	9.5780	7356.0000	623.0000
36	9.5750	5517.0000	623.0000
48	9.5880	3678.0000	623.8000
14	7.6680	9195.0000	623.6001
28	7.6770	7356.0000	624.3999
40	7.6420	5517.0000	621.5000
52	7.6700	3678.0000	623.8000
92	7.6610	2298.7500	623.1001
10	5.7470	9195.0000	623.2000
30	5.7470	7356.0000	623.2000
43	5.7550	5517.0000	624.1001
55	5.7550	3678.0000	624.1001
89	5.7490	2298.0000	623.3999

TABLE I (continued)

RUN	GAS(LB./HR.SQ.FT.)	LIQUID(LB./HR.SQ.FT.)	TOTAL PRESSURE (M.M.HG.)
18	3.8300	9195.0000	623.0000
34	3.8220	7356.0000	621.8000
45	3.8270	5517.0000	622.6001
57	3.8280	3678.0000	622.7000

TABLE II

Concentration of Carbon Dioxide in Gas Phase, Experimental Against Predicted

[The following table shows the concentration of carbon dioxide (mole fraction units), in the gas phase; those experimentally determined against those predicted from the one parameter mathematical model.] (Case 1)

RUN	HEIGHT (FT.)	0.26300000	0.91699990	1.40799900	1.87500000	2.56299900	2.89500000
20	CX(EXP)	0.19539990	0.17979990	0.17159990	0.15770000	0.13029990	0.12540000
	CX(CAL)	0.19386040	0.17812800	0.16586630	0.15383360	0.13542380	0.12623940
25	CX(EXP)	0.19379990	0.18370000	0.16970000	0.16060000	0.13840000	0.12919990
	CX(CAL)	0.19475100	0.18083170	0.16951410	0.15800570	0.13962380	0.13010160
36	CX(EXP)	0.19580000	0.18739990	0.17860000	0.16850000	0.15249990	0.14279990
	CX(CAL)	0.19618240	0.18573990	0.17691920	0.16765730	0.15227710	0.14403590
48	CX(EXP)	0.19520000	0.19040000	0.18500000	0.17599990	0.16439990	0.16019990
	CX(CAL)	0.19755570	0.19057600	0.18436240	0.17754350	0.16559410	0.15888730
14	CX(EXP)	0.19620000	0.17610000	0.15700000	0.14190000	0.11809990	0.11100000
	CX(CAL)	0.19196210	0.17187600	0.15670880	0.14220970	0.12072270	0.11029910
28	CX(EXP)	0.19270000	0.17869990	0.16409990	0.15079990	0.12879990	0.11830000
	CX(CAL)	0.19338670	0.17635040	0.16298500	0.14979610	0.12948190	0.11928850
40	CX(EXP)	0.19419990	0.18430000	0.17229990	0.15869990	0.13749990	0.12989990
	CX(CAL)	0.19495890	0.18137680	0.17011510	0.15847360	0.13950440	0.12950640

TABLE II (continued)

RUN	HEIGHT (FT.)	0.26300000	0.91699990	1.40799900	1.87500000	2.56299900	2.89500000
52	CX(EXP)	0.19520000	0.18739990	0.17849990	0.16990000	0.15920000	0.15299990
	CX(CAL)	0.19687650	0.18817470	0.18065750	0.17261430	0.15894780	0.15147870
92	CX(EXP)	0.19639990	0.19029990	0.18449990	0.17809990	0.17009990	0.16879990
	CX(CAL)	0.19815020	0.19272630	0.18774020	0.18211790	0.17193400	0.16605400
10	CX(EXP)	0.19129990	0.16530000	0.14380000	0.12300000	0.09840000	0.08399999
	CX(CAL)	0.18850080	0.16103290	0.14142470	0.12354420	0.09850448	0.08695251
30	CX(EXP)	0.19010000	0.16890000	0.15049990	0.13539990	0.10559990	0.09630001
	CX(CAL)	0.19048720	0.16694520	0.14937620	0.13274910	0.10840100	0.09671396
43	CX(EXP)	0.19349990	0.17519990	0.15869990	0.14380000	0.11919990	0.10799990
	CX(CAL)	0.19269690	0.17368100	0.15856480	0.14348230	0.11993900	0.10798530
55	CX(EXP)	0.19470000	0.18209990	0.16960000	0.15670000	0.14440000	0.13830000
	CX(CAL)	0.19557470	0.18344670	0.17317830	0.16237590	0.14439510	0.13474080
89	CX(EXP)	0.19620000	0.18879990	0.18110000	0.17119990	0.16089990	0.15729990
	CX(CAL)	0.19743930	0.19001280	0.18327520	0.17576240	0.16233930	0.15467880
18	CX(EXP)	0.18489990	0.15109990	0.12089990	0.09670001	0.06110000	0.04950000
	CX(CAL)	0.18167870	0.14151410	0.11580240	0.09439147	0.06749457	0.05624033

TABLE II (continued)

RUN	HEIGHT (FT.)	0.26300000	0.91699990	1.40799900	1.87500000	2.56299900	2.89500000
34	CX(EXP)	0.18580000	0.15170000	0.12790000	0.10699990	0.07560003	0.06200000
	CX(CAL)	0.18452750	0.14921700	0.12542340	0.10474610	0.07741290	0.06543744
45	CX(EXP)	0.18980000	0.16189990	0.13910000	0.12059990	0.09240001	0.07740003
	CX(CAL)	0.18810980	0.15940770	0.13864600	0.11950330	0.09233791	0.07965642
57	CX(EXP)	0.19120000	0.17269990	0.15619990	0.13959990	0.12199990	0.11479990
	CX(CAL)	0.19283120	0.17421180	0.15945570	0.14477050	0.12191770	0.11034630

TABLE III

Computed Values of One Parameter Model

[The following table shows the values of the Number of Transfer Units, AAPD, Variance, Standard Deviation, and the Overall Mass Transfer Coefficient Computed from the one parameter model;] (Case 1)

RUN	N_{ox}	AAPD	VARIANCE (c_x) $(\times 10^5)$	STD. DEVIATION (N_{ox}) $(\times 10^2)$	KGA (lb. mole)/(Hr.)(Cu. Ft.)(Mole Fn)
20	0.64130890	2.01874500	1.59893300	0.79402290	0.06804007
25	0.65309910	0.89318810	0.36413440	0.46694860	0.06925488
36	0.51620910	0.58807410	0.16027050	0.32095560	0.05472189
48	0.38662360	0.67776660	0.23036490	0.43980990	0.04104050
14	0.82541130	1.30241200	0.86703530	0.62930570	0.07007271
28	0.75470880	0.73024170	0.19366990	0.32332240	0.06414562
40	0.69280970	0.85805730	0.36236350	0.53385680	0.05861621
52	0.44776080	0.87189130	0.35624530	0.49784540	0.03802220
92	0.32735210	1.48060100	0.93000170	0.98988150	0.02776490
10	1.14163500	1.62664600	0.81416460	-0.68656980	0.07263821
30	1.05189800	1.19129000	0.40554690	-0.51932690	0.06692851
43	0.98137000	0.37025480	0.07347822	0.26370350	0.06252801
55	0.64686940	1.58296200	1.20536800	1.02715400	0.04121530
89	0.45609790	1.28357000	0.75002050	0.94917750	0.02902990

TABLE III (continuted)

RUN	N_{ox}	AAPD	VARIANCE (c_x) $(x\,10^5)$	STD. DEVIATION (N_{ox}) $(x\,10^2)$	KGA (lb.mole)/(Hr.)(Cu. Ft.)(Mole Fn)
18	1.66582400	6.46205900	4.39802100	-1.87906900	0.07063580
34	1.54640700	2.38441200	0.68198960	-0.76027170	0.06543511
45	1.37331100	1.10799700	0.31142800	-0.54791180	0.05818670
57	0.92883240	1.91058500	1.24244300	1.02477400	0.03936460

APPENDIX F

Flow Chart for Case 3:

The 'normal equations' for the case of plug flow in the gas phase and axial mixing in the liquid phase is as represented by the equations (3.10) and (3.11). These normal equations were programmed in the IBM computer 360, for solving the parameters N_{ox} and R by a method of iteration; but the values of N_{ox} and R failed to converge. The values of the terms like m, F_x, F_y, Z_i, C_{xi}, etc. used in the computer program were same as those shown in Appendix E: i.e.

m = Henry's constant/Total pressure in atmoshperes

F_x = superficial gas flow rate (lb. mole/hr. sq. ft.)

$\quad$ = 5.74/31.2 (lb. mole/hr. sq. ft.) --- for run 30

F_y = Superficial liquid flow rate (lb. mole/hr. sq. ft.)

$\quad$ = 7,356/18.0 (lb. mole/hr. sq. ft.) --- for run 30

$$Z_i = \frac{z_i}{L} \quad \text{(dimensionless)} \tag{B.10}$$

where

$\quad$ L = 2.895 (ft.)

$$C_{xi} = \frac{c_{xi}}{c_{xo}} \quad \text{(dimensionless mole fraction)} \tag{B.5}$$

where

$\quad c_{xo}$ = 0.2 mole CO_2/mole of ($CO_2 + N_2$)

$$\Lambda = m \frac{F_x}{F_y} \tag{3.4}$$

A computer program for the above method of iteration used, is as shown below:

```
C      SOLUTION OF NORMAL EQUATIONS
C      TWO PARAMETER MODEL; CASE 3
C      NON LINEAR REG. ANALYSIS, NOX AND PYB AS PARAMETERS
1      DIMENSION SX(100), Z(100),Z(100), Z1(100), CX(100), DXC(100), DRC(100), CHX(100
       1)
2      N=6
3      DO 60 K=1,110
4      READ(1,48)RUN
5      WRITE(3,49)RUN
6      READ(1,50)PT, FY, FX
7      WRITE(3,11)PT, FY, FX
8      READ(1,10)(SX(I), I=1, N)
9      READ(1,10)(Z1(I), I=1, N0
10     WRITE(3,3)(Z1(I), I=1, N)
11     WRITE(3,13)(SX(I), I=1, N)
12     XIN=.200
13     PT=PT/760.
14     H=1767.0
15     D=H/PT
16     FY=FY/18.
17     FX=FX/31.2
18     E=2.895
19     CL=D*FX/FY
20     X=.94
21     R=1.
22     DO 22 M=1,200
23      A=X+R
24      B=X*R*(1-CL)
25      SL1=0.
26      SL2=-A/2.+SQRT(A**2/4.-B)
27      SL3=-A/2.-SQRT(A**2/4.-B)
```

```
28      DXA=1.
29      DXB=(1-CL)*R
30      DXSL2=-DXA/2.+SQRT(1./(A**2/4.-B))*(A*DXA/2.-DXB)/2.
31      DXSL3=-DXA/2.-SQRT(1./(A**2/4.-B))*(A*DXA/2.-DXB)/2.
32      G2=1+SL2*X
33      G3=1+SL3*X
34      DXG2=SL2+X*DXSL2
35      DXG3=SL3+X*DXSL3
36      DH1=EXP(SL3/2.)*(G2*G3*SL2*(1+SL3/R)*EXP(SL3/2)-G3*G2*SL3*(1+SL2/R
        2)*EXP(SL2-SL3/2))
37      DH2=G3*SL3
38      DH3=-G2*SL2
39      DH=DH1+(G3*SL3-G2*SL2)
40      DXDH1=EXP(SL3/2)*(EXP(SL3/2)*G2*G3*SL2*((1+SL3/R)*DXSL3+DXSL3/R)
        2+EXP(SL3/2)*(1+SL3/R)*(G2*G3*DXSL2+SL2*(G2*DXG3+G3*DXG2))
        3-EXP(SL2-SL3/2)*(G3*G2*SL3*((1+SL2/R)*DXSL2+DXSL2/R))
        4-EXP(SL2-SL3/2)*(1+SL2/R)*(G3*G2*DXSL3+SL3*(G3*DXG2+G2*DXG3)))
41      DXDH2=G3*DXSL3+SL3*DXG3
42      DXDH3=-G2*DXSL2-SL2*DXG2
43      DXDH=DXDH1+G3*DXSL3+SL3*DXG3-G2*DXSL2-SL2*DXG2
44      H1=DH1/DH
45      H2=DH2/DH
46      H3=DH3/DH
47      DXH1=(DH*DXDG1-DH1*DXDH)/DH**2
48      DXH2=(DH*DXDH2-DH2*DXDH)/DH**2
49      DXH3=(DH*DXDH3-DH3*DXDH)/DH**2
50      DRA=1.
51      DRB=(1-CL)*X
52      DRSL2=-DRA/2.+SQRT(1./(A**2/4.-B))*(A*DRA/2.-DRB)/2.
53      DRSL3=-DRA/2.-SQRT(1./(A**2/4.-B))*(A*DRA/2.-DRB)/2.
54      DRG2=X*DRSL2
```

```
55        DRG3=X*DRSL3
56        DRDH1=EXP(SL3/2)*(EXP(SL3/2)*G2*G3*SL2*((1+SL3/R)*DRSL3+(RDRSL3-
          2SL3)/R**2)+EXP(SL3/2)*(1+SL3/R)*(G2*G3*DRSL2+SL2*(G2*DRG3+G3*DRG2)
          3)-EXP(SL2-SL3/2)*G3*G2*SL3*((1+SL2/R)*DRSL2+(R*DRSL2-SL2)/R**2)
          4-EXP(SL2-SL3/2)*(1+SL2/R)*(G3*G2*DRSL3+SL3*(G3*DRG2+G2*DRG3)))
57        DRDH2=G3*DRSL3+SL3*DRG3
58        DRDH3=-G2*DRSL2-SL2*DRG2
59        DRDH=DRDH1+G3*DRSL3+Sl3*DRG3-G2*DRSL2-SL2*DRG2
60        DRH1=(DH*DRDH1-DH1*DRDH)/DH**2
61        DRH2=(DH*DRDH2-DH2*DRDH)/DH**2
62        DRH3=(DH*DRDH3-DH3*DRDH)/DH**2
63        SUMX1=0.
64        SUMX2=0.
65        SUMX3=0.
66        SUMX4=0.
67        SUMX5=0.
68        SUMX6=0.
69        SUMR1=0.
70        SUMR2=0.
71        SUMR3=0.
72        SUMR4=0.
73        SUMR5=0.
74        SUMR6=0.
75        DO 20 I=1,N
76        Z(I)=Z1(I)/E
77        CX(I)=SX(I)/XIN
78        DXC(I)=EXP(SL3/2)*(DXH1*EXP(-SL3/2)+DXH2*EXP(SL2*Z(I)-SL3/2)+H2*
          2Z(I)*DXSL2*EXP(SL2*Z(I)-SL3/2)+DXH3*EXP(SL3*Z(I)-SL3/2)+H3*Z(I)*
          3DXSL3*EXP(SL3*7(I)-SL3/2))
79        DRC(I)=EXP(SL3/2)*(DRH1*EXP(-SL3/2)+DRH2*EXP(SL2*Z(I)-SL3/2)+H2*
```

```
        2Z(I)*DRSL2*EXP(SL2*Z(I)-SL3/2)+DRH3*EXP(SL3*Z(I)-SL3/2)+H3*Z(I)*
        3DRSL3*EXP(SL3*Z(I)-SL3/2))
80       CHX(I)=EXP(SL3/2)*(H1*EXP(-SL3/2)+H2*EXP(SL2*Z(I)-SL3/2)+H3*EXP
        2(SL3*Z(I)-SL3/2))
81       SUMX1=SUMX1+CX(I)*DXC(I)
82       SUMX2=SUMX2+CHX(I)*DXC(I)
83       SUMX3=SUMX3+DXC(I)**2*X
84       SUMX4=SUMX4DXC(I)*DRC(I)*R
85       SUMX5=SUMX5+DXC(I)**2
86       SUMX6=SUMX6+DXC(I)*DRC(I)
87       SUMR1=SUMR1+CX(I)*DRC(I)
88       SUMR2=SUMR2+CHX(I)*DRC(I)
89       SUMR3=SUMR3+DRC(I)**2*R
90       SUMR4=SUMR4+DRC(I)*DXC(I)*X
91       SUMR5=SUMR5+DRC(I)**2
92    20 SUMR6=SUMR6+DRC(I)*DXC(I)
93       S1=SUMX1-SUMX2+SUMX3+SUMX4
94       C1=SUMX5
95       C2=SUMX6
96       S2=SUMR1-SUMR2+SUMR3+SUMR4
97       C3=SUMR6
98       C4=SUMR5
      C
      C      NEWTONS METHOD OF ITERATION FOR 2 VARIABLES
      C
99       F(X,R)=C1*X+C2*R-S1
100      G(X,R)=C3*X+C4*R-S2
101      DFX=C1
102      DFR=C2
103      DGX=C3
104      DGR=C4
```

70

```
105        A1=-F(X,R)*DGR+G(X,R)*DFR
106        A2=-G(X,R)*DFX+F(X,R)*DGX
107        B1=DFX*DGR-DFR*DGX
108        DELTAX=A1/B1
109        DELTAR=A2/B1
110        WRITE(3,12)X,R
111        X=X+DELTAX/5.
112        R=R+DELTAR/10.
113        S4=0.
114        S5=0.
115        DO 23 I=1,N
116        CHX(I)=EXP(SL/2)*(H1*EXP(-SL3/2)+H2*EXP(SL2*Z(I)-SL3/2)+H3*EXP
           2(SL3*Z(I)-SL3/2))
117        CHX(I)=CHX(I)*XIN
118        S5=S5+(ABS(SX(I)-CHX(I)))/SX(I)
119   23   S4=S4+(SX(I)-CHX(I))**2
120        WRITE(3,14)(SX(I),I=1,N)
121        WRITE(3,88)(CHX(I),I=1,N)
122        DF=6.-2.
123        SIGMSX=S4/DF
124        D=C1*C4-C2*C3
125        C11=C4/D
126        C22=C1/D
127        STDVX=SXRT(ABS(C11*SIGMSX))
128        STDVR=SQRT(ABS(C22*SIGMSX))
129        AAPD=S5*100./6.
130   22   WRITE(3,15)SIGMSX,AAPD,STDVR,STDVX
131   10   Format(3F18.8)
132   11   FORMAT(4X,'PT(MM HG)=',F10.4,//4X,'L(LB/HR.SQFT)='F10.4,//,4X,
           7'G(LB/HR.SQFT)='F10.4,///)
133   12   FORMAT(///,4X,'X=',E18.8,//,4X,'R=',E18.8.///)
```

```
134   13   FORMAT(2X,'CX=',6F14.7)
135    3   FORMAT(2X,'Z =',6F14.7)
136   14   FORMAT(2X,'CX      ',2X,6E18.8)
137   88   FORMAT(2X,'CX(CAL)',2X,6E18.8)
138   15   FORMAT(///,4X,'VARIANCE**2='E18.8,//,4X,'AAPD       ='E18.8
           2//,4X,'S.DEV  R    ='E18.8,//,4X,'S.DEV-NOX  ='E18.8//)
139   48   FORMAT(F10.4)
140   49   FORMAT('1',20X,'RUN=',F5.0,/////)
141   50   FORMAT(3F18.8)
142   60   CONTINUE
143        STOP
144        END
      /DATA
```

TABLE IV

Computed Values of Two Parameter Model

[The following table shows the value of minimum AAPD against R, with N_{ox} as the parameter, for the case 3, (i.e. plug flow in the gas phase and axial mixing in the liquid phase). These values have been obtained from the graphs plotted for the various runs.] (Figures G-1 to G-18)

RUN	N_{ox}	AAPD (minimum)	R
20	1.35	1.54	35.0
25	1.23	0.71	10.0
36	1.21	0.20	6.0
48	1.15	0.65	2.0
14	1.19	1.29	25.0
28	1.17	0.40	30.0
40	1.15	0.80	18.0
52	1.13	0.45	1.0
92	1.07	0.65	1.0
10	0.81	1.34	30.0
30	0.91	1.19	31.0
43	0.99	0.42	39.0
55	1.03	0.90	2.0
89	1.07	0.68	1.0
18	0.37	5.90	16.0
34	0.41	0.55	11.0
45	0.67	0.75	30.0
57	0.89	1.05	3.0

APPENDIX G

Computer program for the graphs:

Graphs of average absolute percentage deviation against, i.e. AAPD, against

the axial mixing parameter in the liquid phase, i.e. R, for the case of plug flow

in the gas phase and axial mixing in the liquid phase, for the carbon-dioxide

water system, have been plotted by using the UMR IBM 360 Model, 50 digital

computer system and the Calcomp Digital Incremental Plotter. The mathe-

matical model represented by the equation (3.9) was made use of for computing

the values of AAPD. For each of the 110 runs, R was increased, in steps of 1,

from 1 to 100. N_{ox}, which was used as the parameter for the above graphs,

was varied in the steps of 0.02, from 0.30 to 1.45. Besides the graphs, the

values of AAPD, R and N_{ox} were also printed in the computer output. A

program for the plotter made use of in this study, which includes the main

graphs of AAPD vs. R, and the printing of their values on their respective

axis together with the gas and the liquid flow rates is as given below:

```
C    AXIAL MIXING IN ABSORPTION COLUMN
C    MIXING IN THE LIQUID PHASE - PLUG FLOW IN GAS PHASE
C    NON LINEAR REG ANALYSIS  NOX AND PYB AS PARAMETERS
C
0001        DIMENSION SX(10), Z(10), Z1(10), CX(10), CHX(10), AAPD(110)
0002        CALL PENPOS('IYER.S.P.',9,1)
0003        N=6
0004        READ(1,10)(Z1(I), I=1,N)
0005        DO 700 NJ=1,2
0006        CALL NEWPLT(1.0,2.0,11.0)
0007        CALL ORIGIN(1.0,0.0)
0008        READ(1,48)RUN
0009        READ(1,50)PT, FY, FX
0010        READ(1,10)(SX(I), I=1,N)
0011        XIN=.200
0012        PT=PT/760.
0013        H=1767.0
0014        D=H/PT
0015        FY1=FY/18.
0016        FX1=FX/31.2
0017        E=2.895
0018        CL=D*FX1/FY1
0019        X=1.09
0020        DO 600 KN=1,18
0021        R=1.
0022        DO 601 KK=1,40
0023        A=X+R
0024        B=X*R*(1-CL)
0025        SL1=0.
0026        SL2=-A/2.+SQRT(A**2/4.-B)
0027        SL3=-A/2.-SQRT(A**2/4.-B)
```

```
0028        G2=1+SL2*X
0029        G3=1+SL3*X
0030        DH1=EXP(SL3/2.)*(G2*G3*SL2*(1+SL3/R)*EXP(SL3/2)-G3*G2*SL3*(1+SL2/R
           2)*EXP(SL2-SL3/2))
0031        DH2=G3*SL3
0032        DH3=-G2*SL2
0033        DH=DH1+(G3*SL3-G2*SL2)
0034        H1=DH1/DH
0035        H2=DH2/DH
0036        H3=DH3/DH
0037        SUM=0.
0038        DO 20 I=1,N
0039        Z(I)=Z1(I)/E
0040        CX(I)=SX(I)/XIN
0041        CHX(I)=EXP(SL3/2)*(H1*EXP(-SL3/2)+H2*EXP(SL2*Z(I)-SL3/2)+H3*EXP
           2(SL3*Z(I)-SL3/2))
0042        CHX(I)=CHX(I)*XIN
0043        SUM=SUM+ABS((SX(I)-CHX(I))/SX(I))
0044     20 Z(I)=Z(I)*E
0045        AAPD(KK)=SUM*100./6.
0046    601 R=R+1.
0047        WRITE(3,502)RUN,X,R,AAPD(KK)
0048    502 FORMAT(4F18.8)
0049        CALL TSCALE(1.0,40.0,7.7)
0050        CALL YSCALE(0.0,45.0,5.0)
0051        CALL TPLT(AAPD,39,1,-1)
0052    600 X=X-0.02

0053        CALL TAXIS(1.0)
0054        CALL YAXIS(0.50)
0055        CALL SYM(-0.4,2.0,0.21,'AAPD',90.0,4)
```

```
0056        CALL SYM(3.0,-0.5,0.21,'R',0.0,1)
0057        CALL SYM(4.5,4.7,0.14,'RUN',0.0,3)
0058        CALL SYM(4.5,4.3,0.14,'L(LB/HR.SQFT)=',0.0,14)
0059        CALL NUM(5.5,4.7,0.14,RUN,0.0,-1)
0060        CALL NUM(6.6,4.3,0.14,FY,0.0,2)
0061        CALL SYM(4.5,4.0,0.14,'G(LB/HR.SQFT)=',0.0,14)
0062        CALL NUM(6.6,4.0,0.14,FX,0.0,3)
0063        R=1.
0064        DR=5.
0065        DO 801 MN=1,8
0066        CALL NUM(TSTOIN(R),-0.14,0.07,R,0.0,1)
0067        IF(ABS(R)-4.)31,31,32
0068     31 R=R+4.
0069        GO TO 801
0070     32 R=R+DR
0071    801 CONTINUE
0072        AAP=0
0073        DAAP=1.0
0074        DO 802 NM=1,21
0075        CALL NUM(-0.21,YSTOIN(AAP),0.07,AAP,0.0,1)
0076    802 AAP=AAP+DAAP
0077     10 FORMAT(3F18.8)
0078     48 FORMAT(F10.4)
0079     50 FORMAT(3F18.8)
0080        CALL ENDPLT
0081    700 CONTINUE
0082        CALL LSTPLT
0083        CALL EXIT
0084        END
```
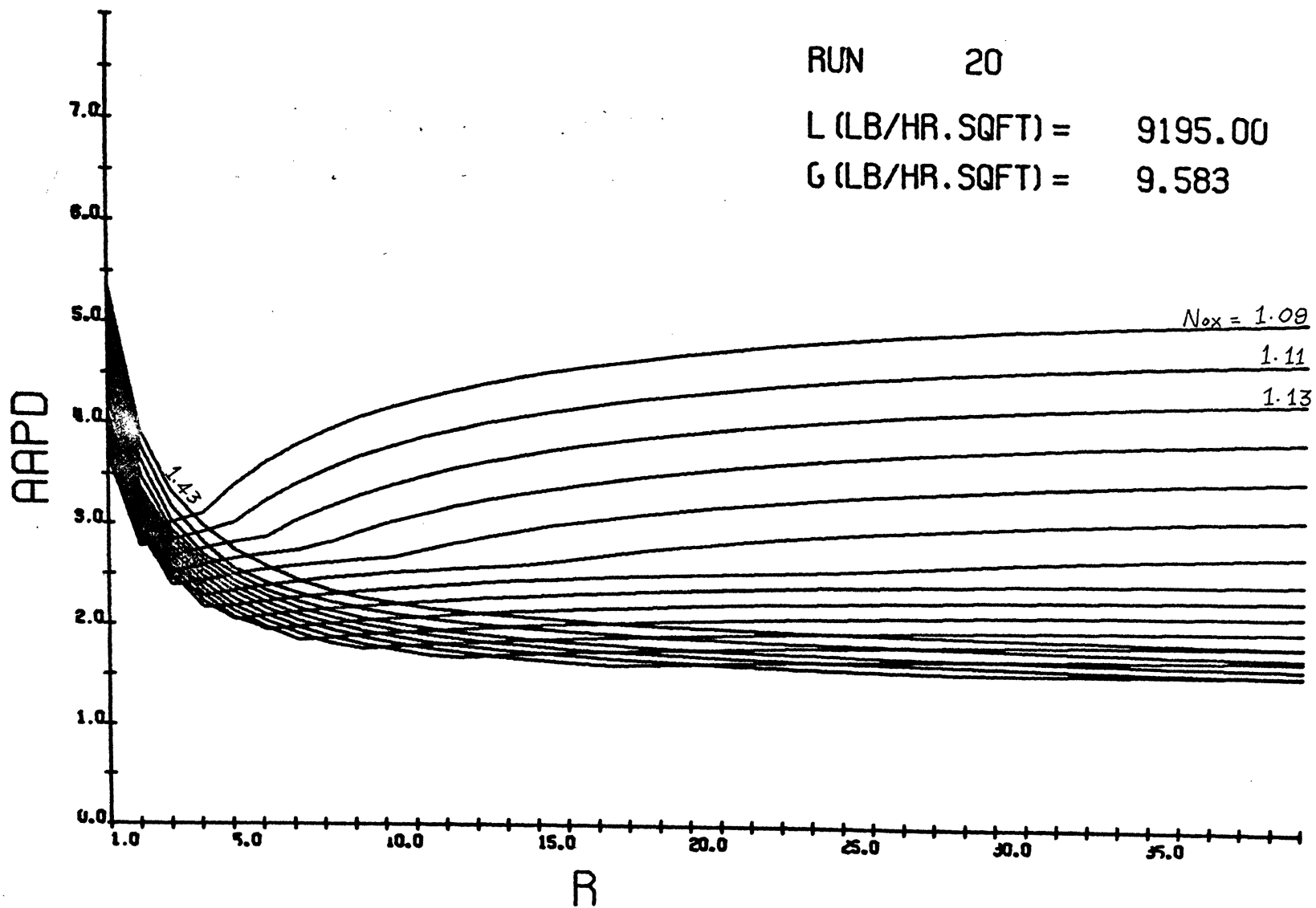
Fig. G-1. Effect of R on AAPD, N_{ox} as the parameter: Run 20. (L = 9195.00, G = 9.583, N_{ox} = 1.09 to 1.43)

RUN 25

L (LB/HR.SQFT) = 7356.00

G (LB/HR.SQFT) = 9.578
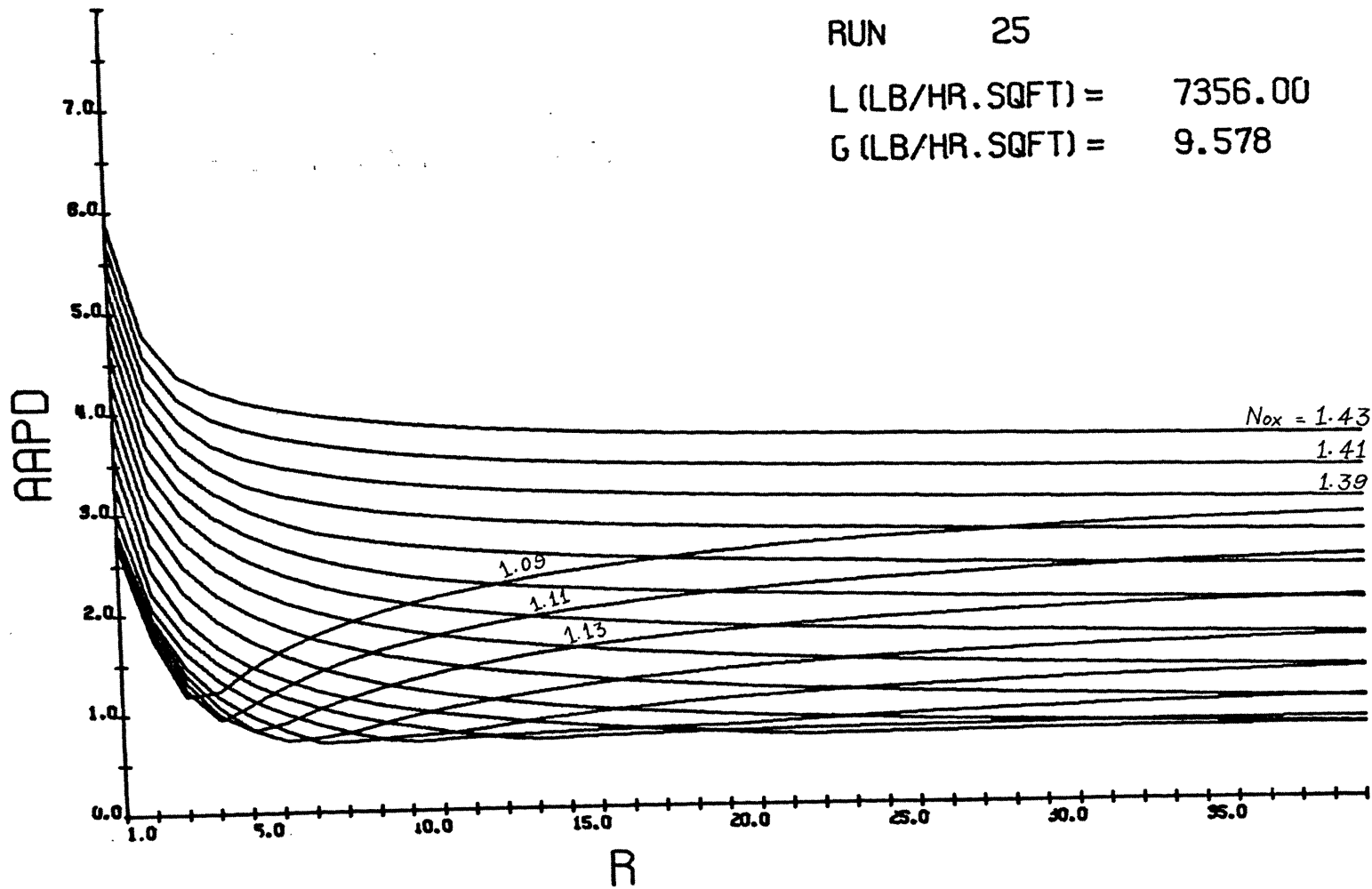
Fig. G-2. Effect of R on AAPD, N_{ox} as the parameter: Run 25. (L = 7356.00, G = 9.578, N_{ox} = 1.09 to 1.43)
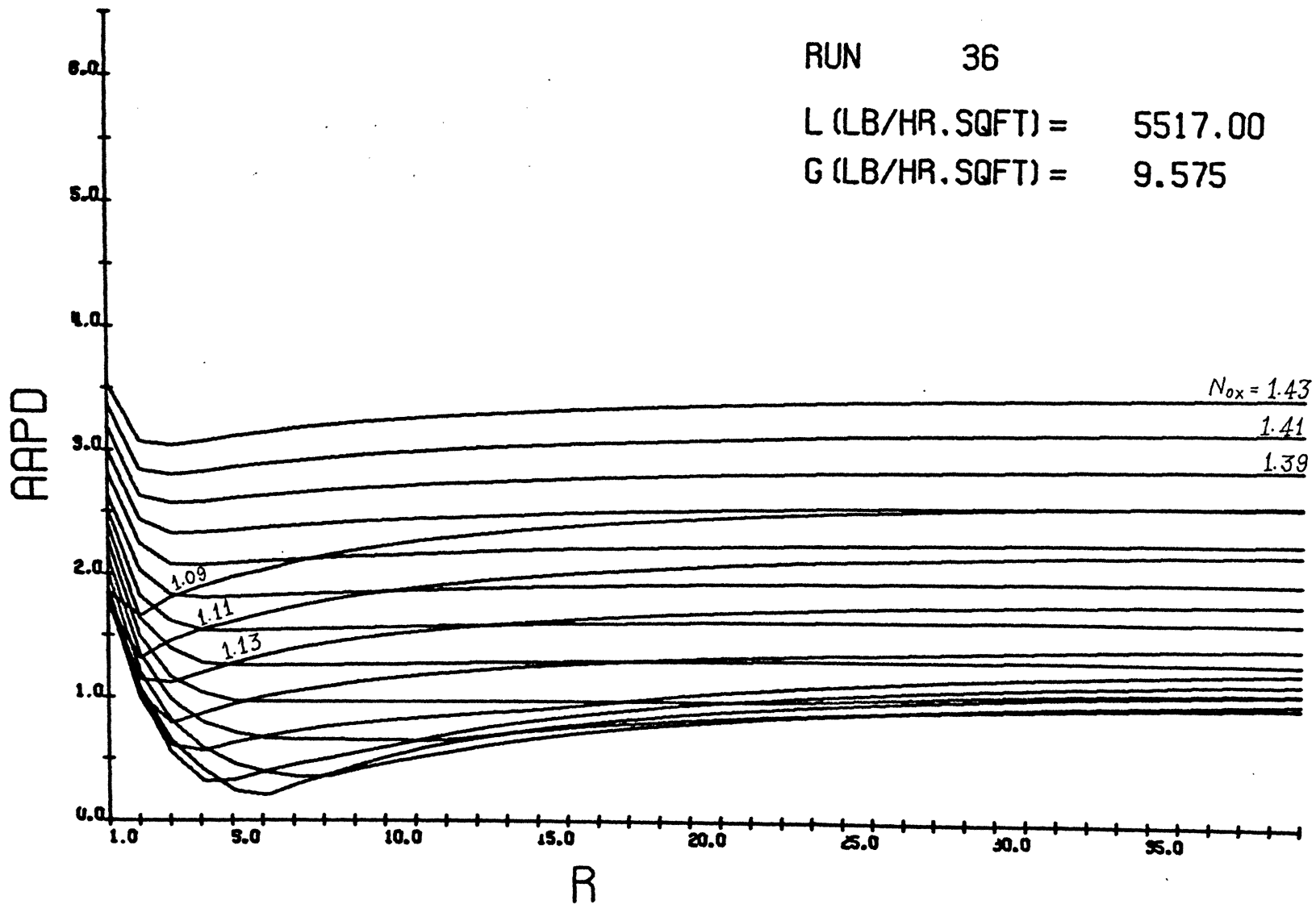
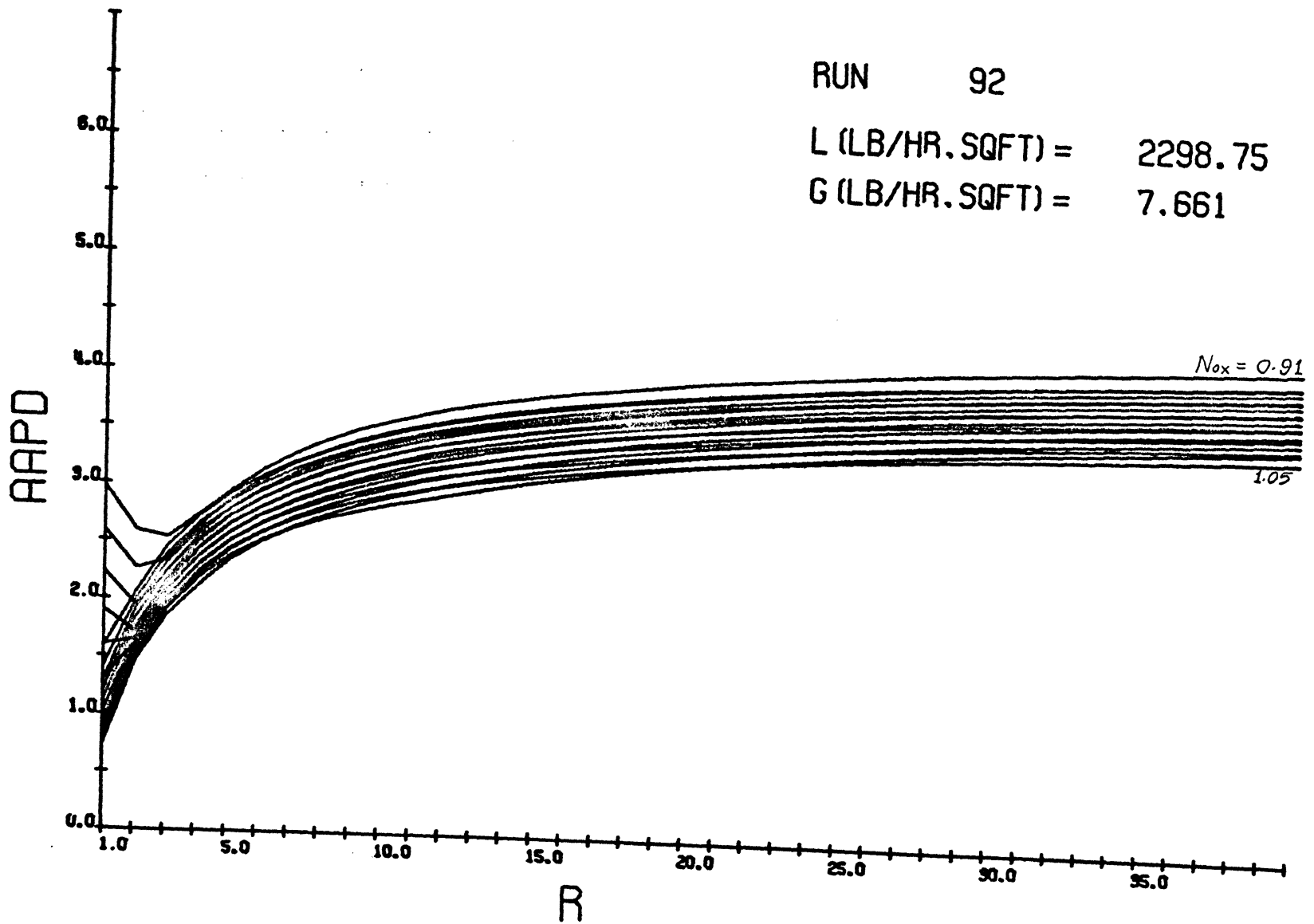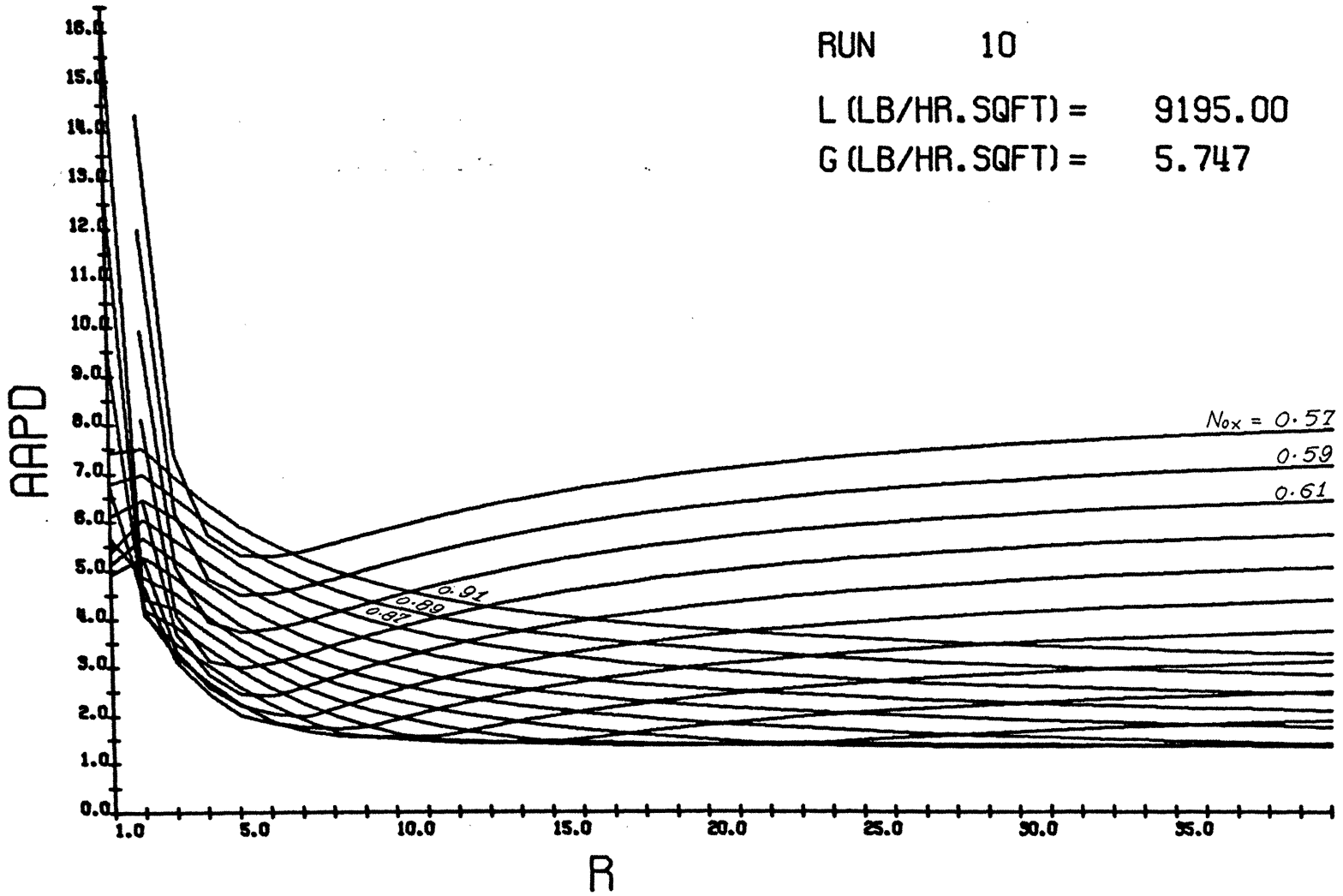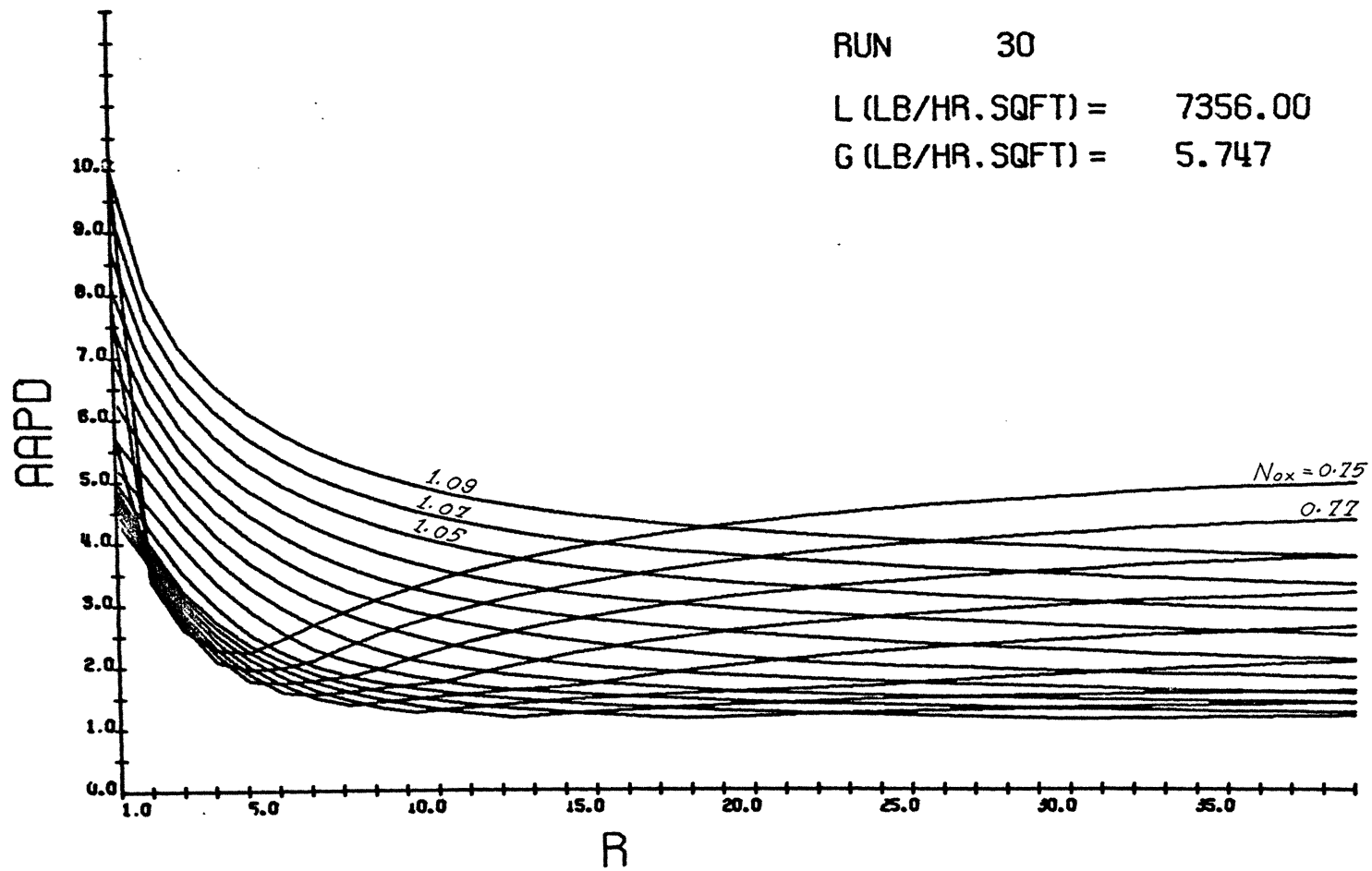Fig. G-3. Effect of R on AAPD, N_{ox} as the parameter: Run 36. (L = 5517.00, G = 9.575, N_{ox} = 1.09 to 1.43)
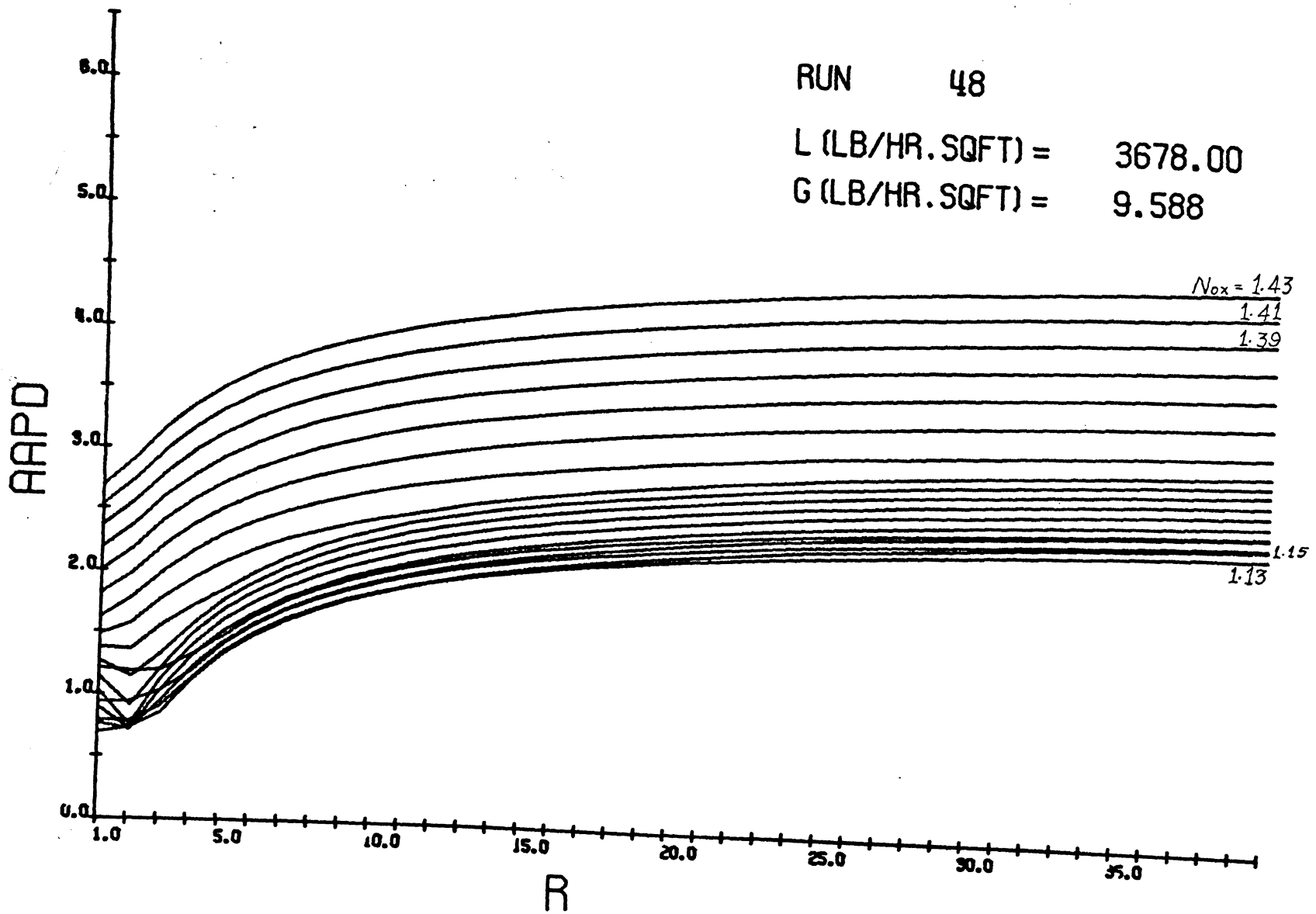
Fig. G-4. Effect of R on AAPD, N_{ox} as the parameter: Run 48. (L = 3678.00, G = 9.588, N_{ox} = 1.09 to 1.43)

RUN 14

L (LB/HR.SQFT) = 9195.00

G (LB/HR.SQFT) = 7.668

$N_{ox} = 1.43$
1.41
1.39

1.13
1.11
1.09
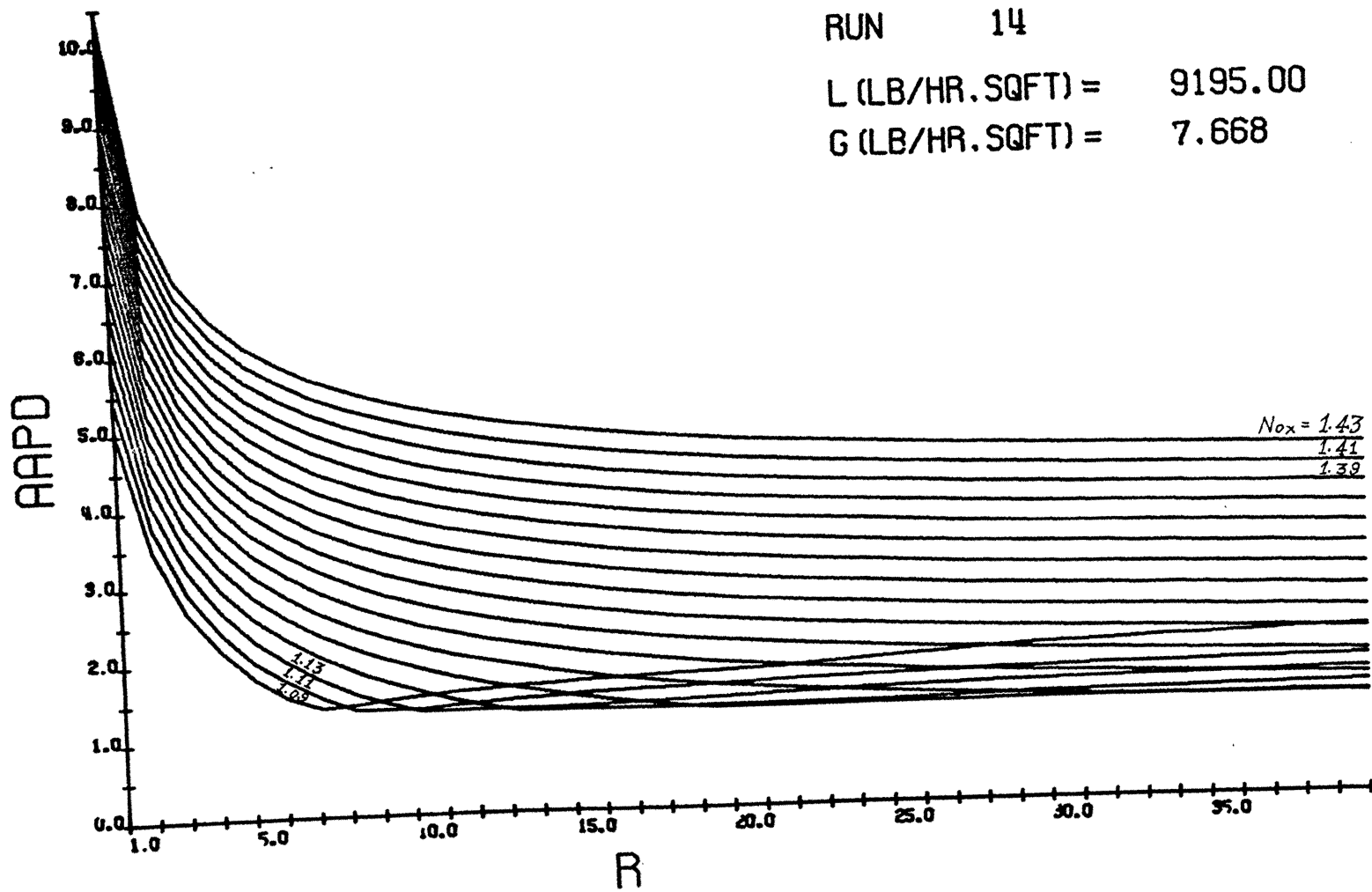
Fig. G-5. Effect of R on AAPD, N_{ox} as the parameter: Run 14. (L = 9195.00, G = 7.668, N_{ox} = 1.09 to 1.43)
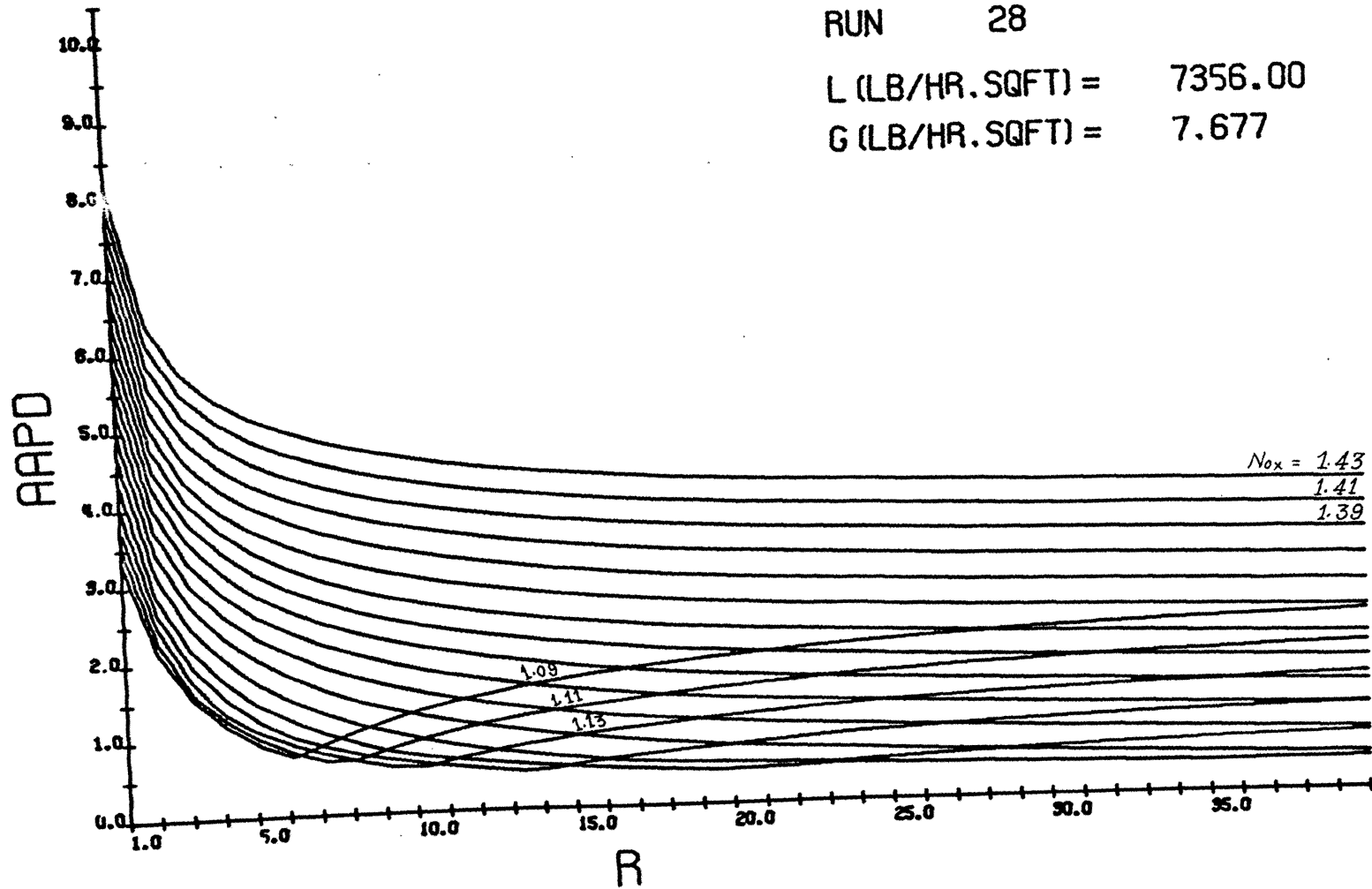
Fig. G-6. Effect of R on AAPD, N_{ox} as the parameter: Run 28. ($L = 7356.00$, $G = 7.677$, $N_{ox} = 1.09$ to 1.43)
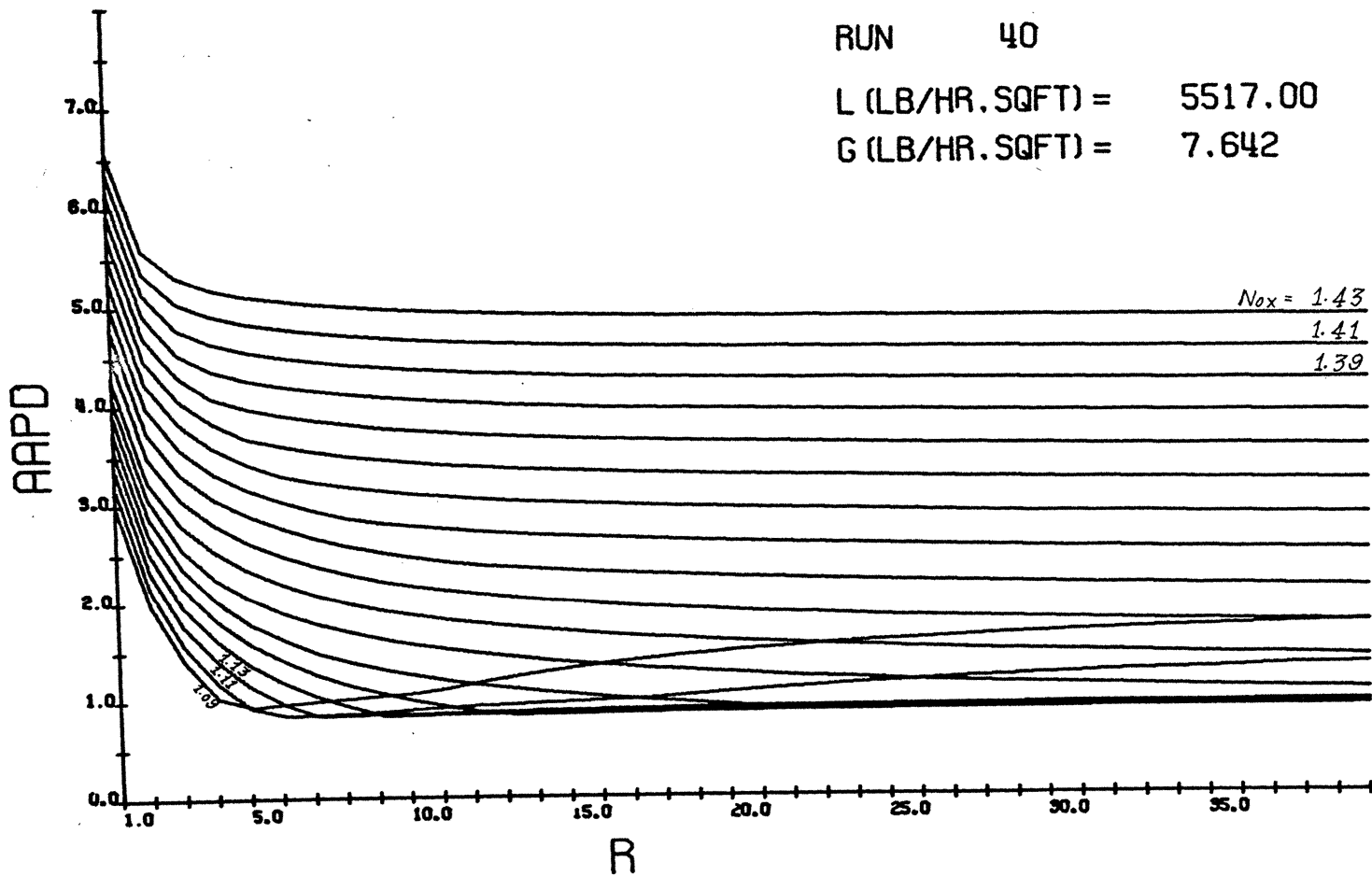
Fig. G-7. Effect of R on AAPD, N_{ox} as the parameter: Run 40. (L = 5517.00, G = 7.642, N_{ox} = 1.09 to 1.43)
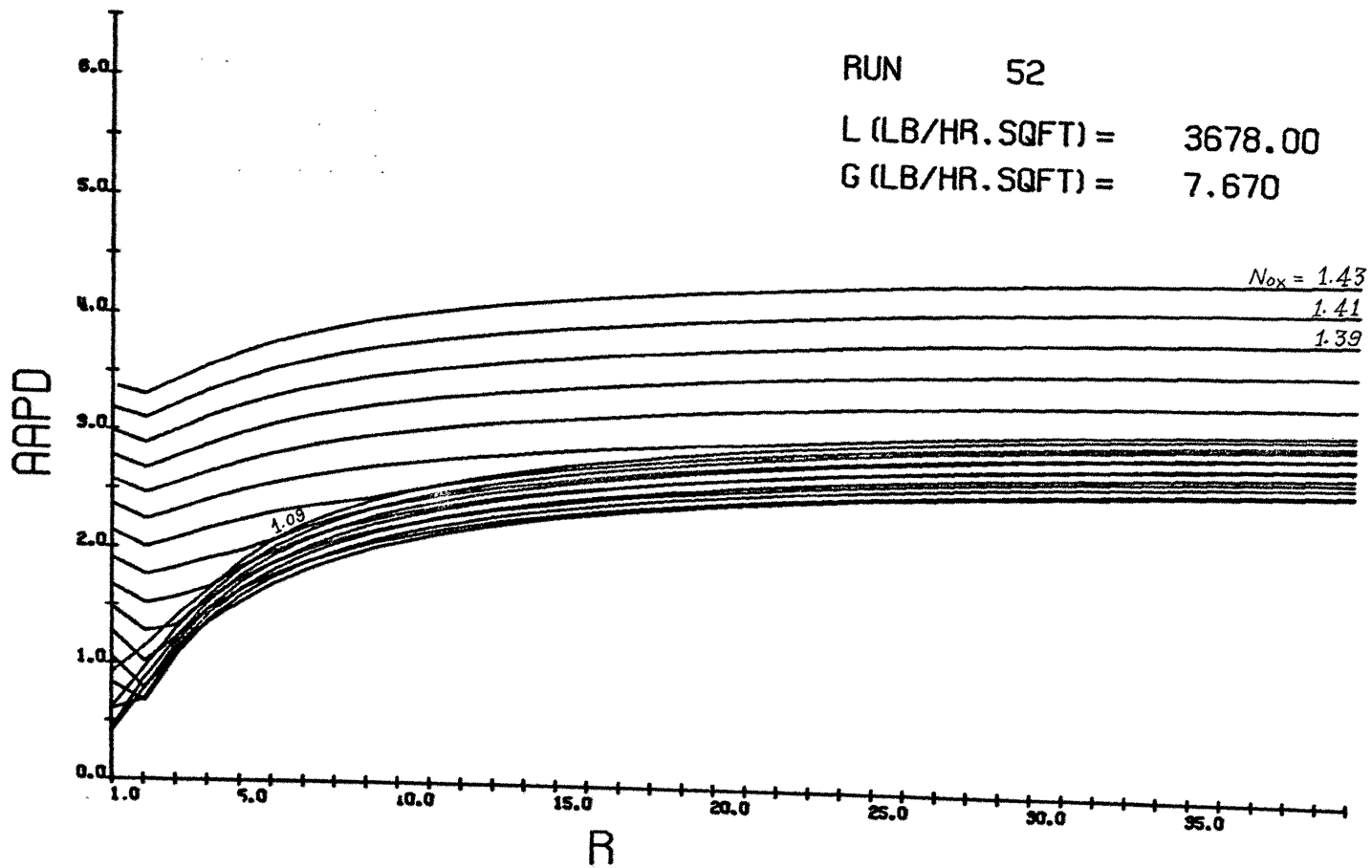
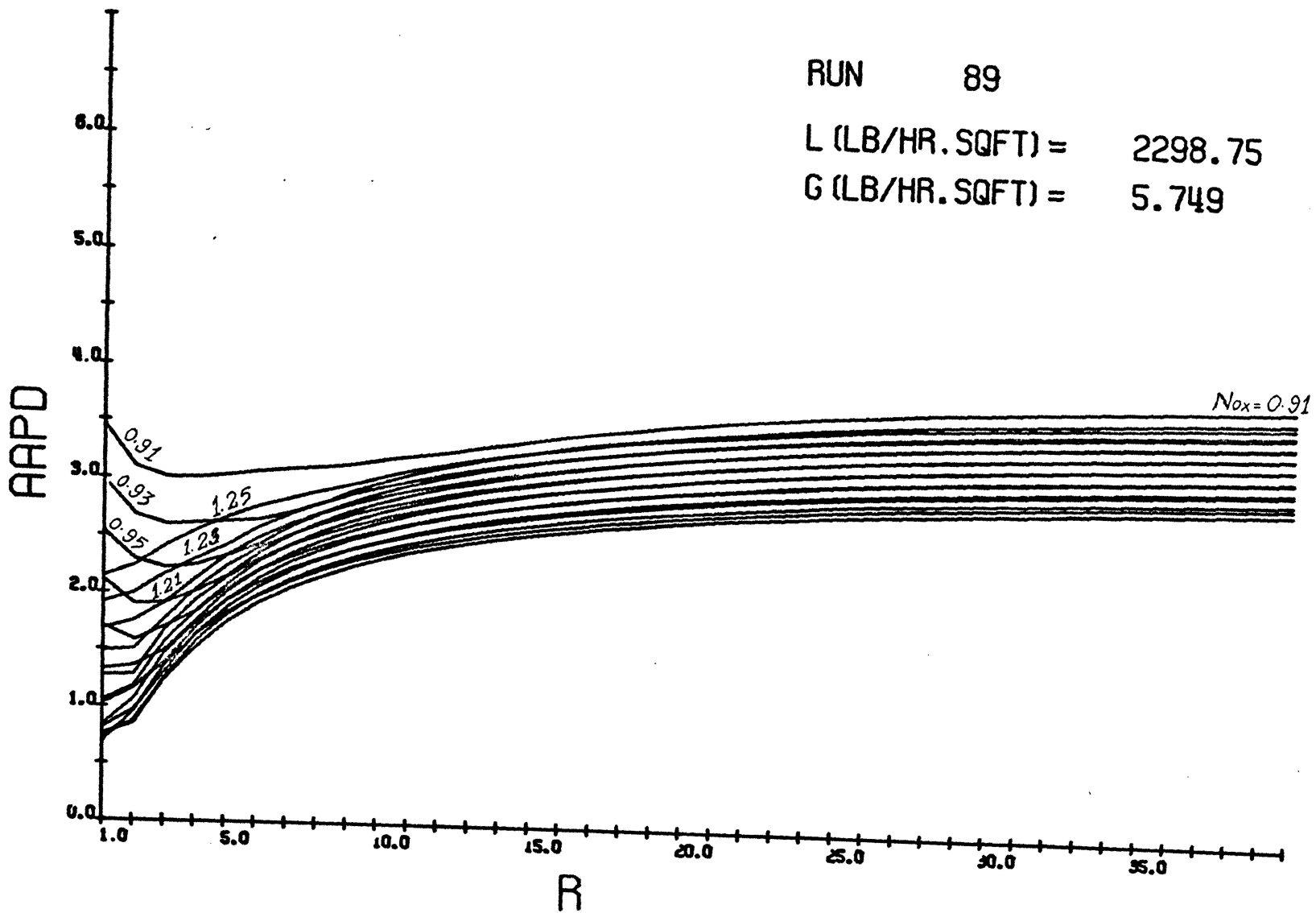Fig. G-8. Effect of R on AAPD, N_{ox} as the parameter: Run 52. (L = 3678.00, G = 7.670, N_{ox} = 1.09 to 1.43)

Fig. G-9. Effect of R on AAPD, N_{ox} as the parameter: Run 92. (L = 2298.75, G = 7.661, N_{ox} = 0.91 to 1.25)
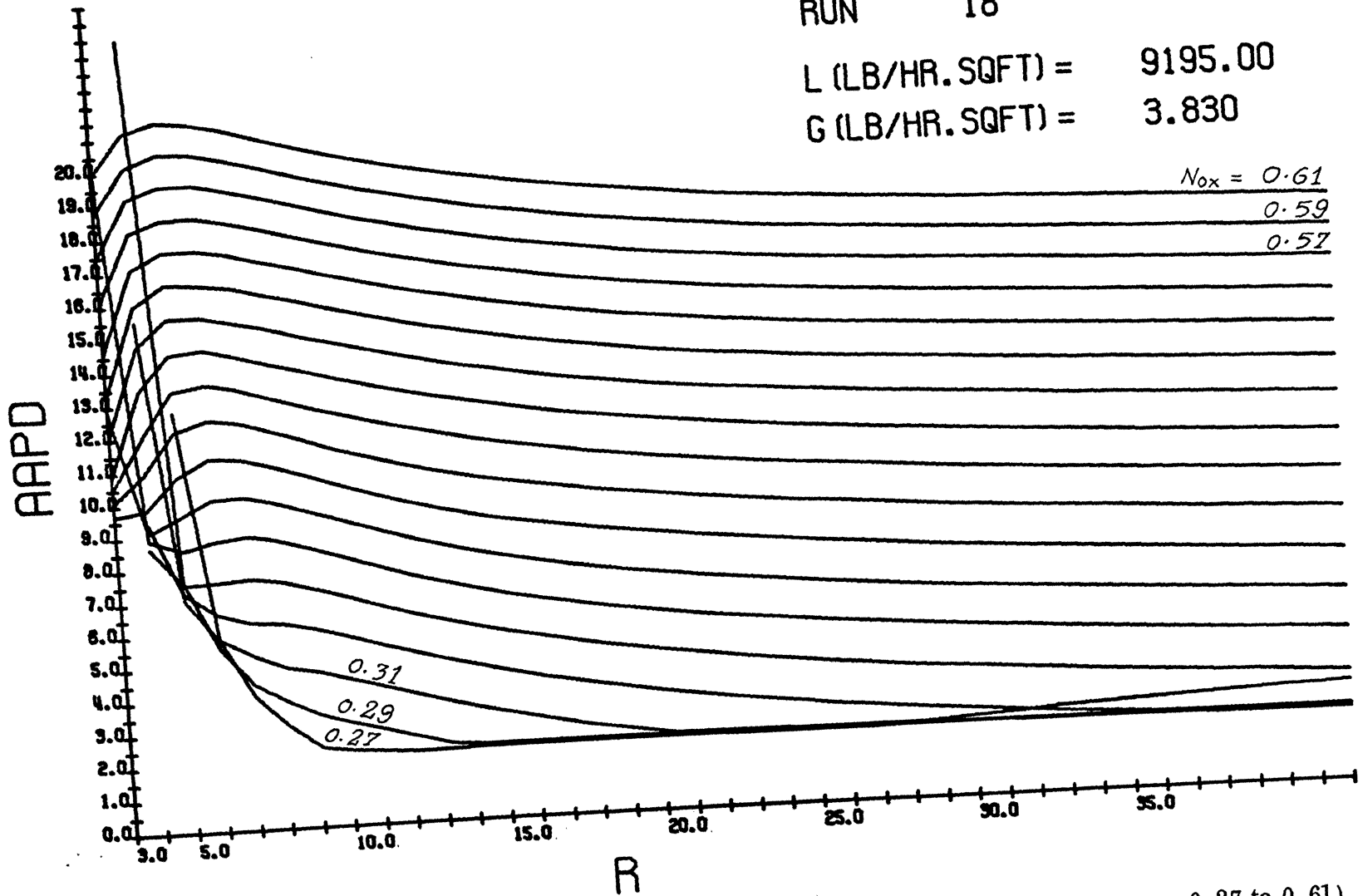
Fig. G-10. Effect of R on AAPD, N_{ox} as the parameter: Run 10. (L = 9195.00, G = 5.747, N_{ox} = 0.57 to 0.91)

RUN   30
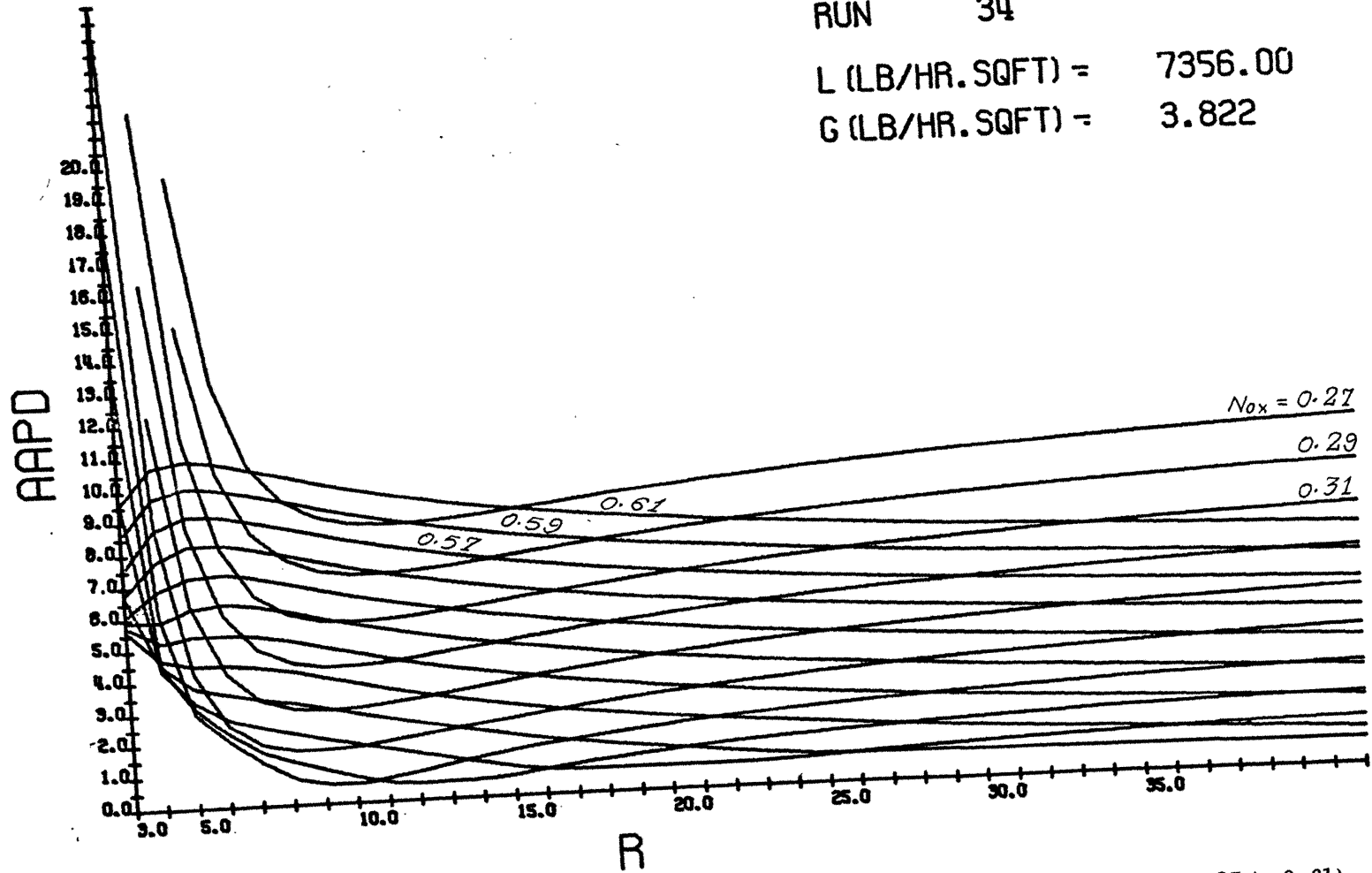
L (LB/HR.SQFT) =   7356.00
G (LB/HR.SQFT) =   5.747

$N_{ox} = 0.75$

0.77

1.09
1.07
1.05

AAPD

R

Fig. G-11. Effect of R on AAPD, N_{ox} as the parameter: Run 30. (L = 7356.00, G = 5.747, N_{ox} = 0.75 to 1.09)
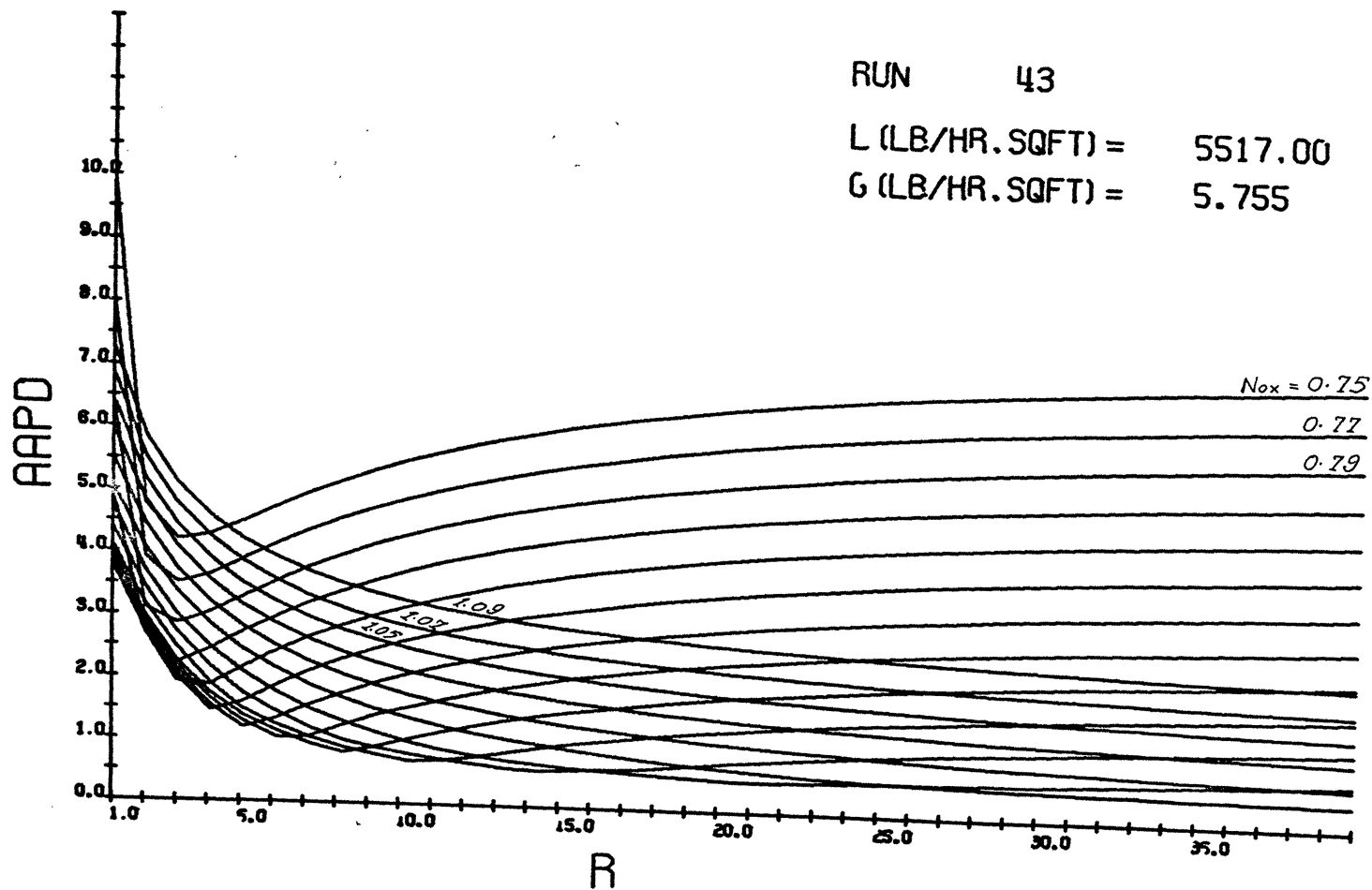
Fig. G -12. Effect of R on AAPD, N_{ox} as the parameter: Run 43. (L = 5517.00, G = 5.755, N_{ox} = 0.75 to 1.09)
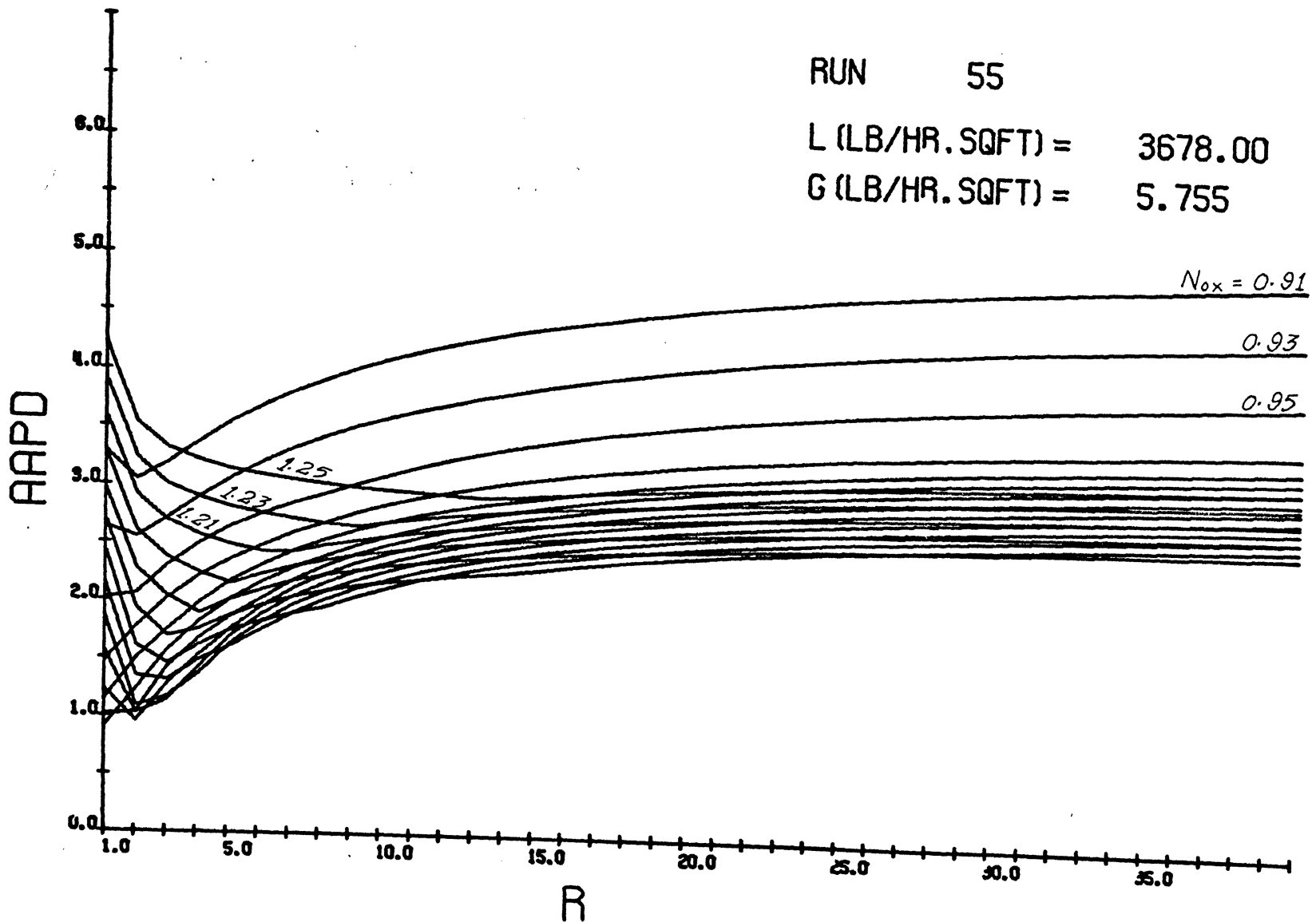
Fig. G-13. Effect of R on AAPD, N_{ox} as the parameter: Run 55. (L = 3678.00, G = 5.755, N_{ox} = 0.91 to 1.25)

Fig. G-14. Effect of R on AAPD, N_{ox} as the parameter: Run 89. (L = 2298.75, G = 5.749, N_{ox} = 0.91 to 1.25)

Fig. G-15. Effect of R on AAPD, N_{ox} as the parameter: Run 18. ($L = 9195.00$, $G = 3.830$, $N_{ox} = 0.27$ to 0.61)

Fig. G-16. Effect of R on AAPD, N_{ox} as the parameter: Run 34. (L = 7356.00, G = 3.822, N_{ox} = 0.27 to 0.61)
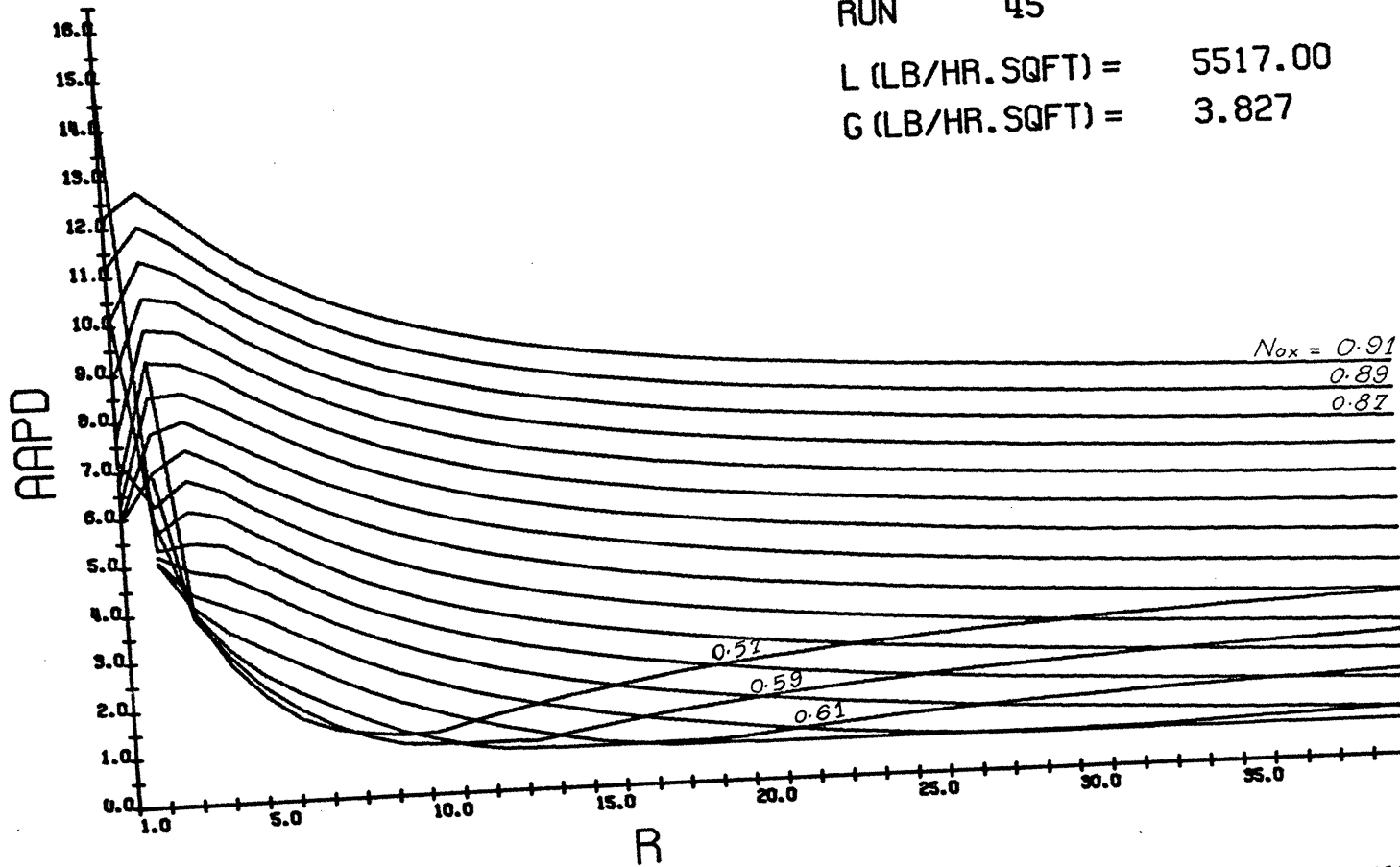
Fig. G-17. Effect of R on AAPD, N_{ox} as the parameter: Run 45. (L = 5517.00, G = 3.827, N_{ox} = 0.57 to 0.91)
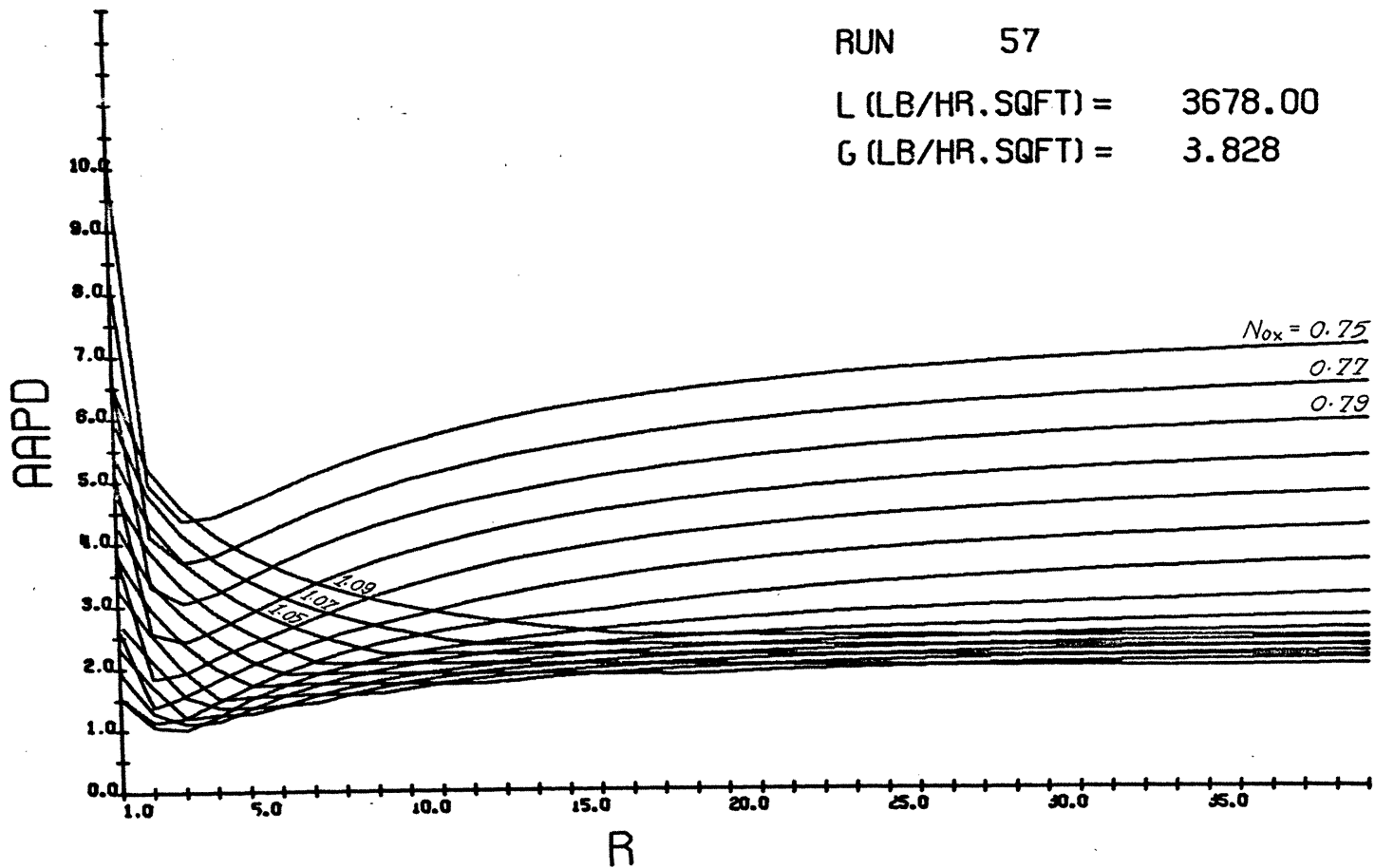
Fig. G-18. Effect of R on AAPD, N_{ox} as the parameter: Run 57. (L = 3678.00, G = 3.828, N_{ox} = 0.75 to 1.09)

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183304