Contrails

A STUDY OF THE THEORETICAL PERFORMANCE OF GASEOUS ADSORPTION SYSTEMS

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FOREWORD

This technical report has been reviewed and is approved.

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ABSTRACT

This study of the theoretical performance of gaseous adsorption systems is based on an equation for the time-dependent transmission of a gas through an adsorber bed of length, ℓ, and bulk density, ρ, and a gas-adsorber system characterized by an isothermal adsorption capacity, K, and a dispersivity, D. For a step-function gaseous input pulse injected into a stream of carrier gas which flows through the adsorber at a superficial flow velocity, u, the time-dependent expression for the transmission is a function only of the dimensionless dispersion number, $D/u\ell$, and the dimensionless time measured in units of the inflection time. A weighted least-squares analysis is developed and programmed on a digital computer to determine from an experimental transmission versus time curve the values of the two theoretical parameters (namely, the dispersivity and the adsorptivity) in the transmission equation. The errors in the values of the two theoretical parameters are evaluated also by propagating the errors in the experimental values of the transmission through the normal equations of the least-squares analysis. The Newton-Raphson method is used for obtaining the solution of the two simultaneous normal equations of the least-squares analysis. The theory is used to analyze experimental data on the transmission of carbon dioxide in air through molecular sieve adsorber beds. Values of the theoretical parameters have been deduced from the Christensen (1962) data for one mole percent carbon dioxide on 1/8-inch pellets, and from the Fox (1966) data for 0.64-mole percent carbon dioxide on both 1/16-inch and 1/8-inch pellets for various flow velocities, bed dimensions, and air temperatures. At each air temperature, the results are consistent with the dispersivity increasing with the square of the superficial flow velocity over the range studied. A log-log plot of the transmission at the inflection time versus the inflection time correlates all the data analyzed for the various experimental conditions of air temperature, adsorber bed dimensions, superficial flow velocity, and inlet concentration of carbon dioxide. For a given value of the transmission at the inflection time, a molecular sieve adsorber bed packed with 1/8-inch pellets has a longer inflection time then one packed with 1/16-inch pellets.

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LIST OF SYMBOLS

Symbol	Units	Identification
A	cm^2	Cross-sectional area of the adsorber bed
B	----	Effective adsorptivity
C	moles/cc	Concentration of adsorbate
D	cm^2/sec	Dispersion coefficient, or dispersivity
$\dfrac{D}{u\ell}$	----	Dispersion number for the fluid-adsorber bed system
E	----	Dynamic adsorption efficiency
K	cc/g	Isothermal adsorption coefficient, or adsorptivity
L	----	Adsorption load
ℓ	cm	Length of adsorber bed
p	----	Inflection time parameter
Q	gm/sec	Mass flow velocity
R	----	Sum of squares of weighted residuals
q	cc/sec	Volumetric flow velocity
$s_{\pm}$	----	Argument of complementary error functions
T	----	Transmission
t	sec	Time
t_i	sec	Inflection time
t_p	sec	Propagation time
u	cm/sec	Superficial flow velocity
W	----	Statistical weight
Y	----	Twice the difference between experimental and theoretical values of the transmission
ρ	g/cc	Adsorber bulk density
ρ_1	----	Convergence parameter

Symbol	Units	Identification
τ_i	----	Time in units of the inflection time
τ_p	----	Time in units of the propagation time
Θ	°K	Temperature

SECTION I

INTRODUCTION

Madey et al (1960) studied the adsorption process in an experiment conducted with the reactor facility at the Brookhaven National Laboratory. This experiment measured the time-dependent transmission of a radioactive gaseous isotope, namely metastable kryption-85m, which was carried by an helium stream through an activated carbon adsorber bed. The transmission of a gas through an adsorber bed is defined as the ratio of the concentration of the gas at the outlet of the adsorber bed to the concentration at the inlet to the bed. The transmission of a stable gaseous isotope flowing steadily through an adsorber bed reaches the value unity when the concentration of the isotope on the adsorber ceases to increase. When this steady-state value is reached, the adsorber is said to be "saturated." The saturation capacity of the adsorber depends upon the partial pressure or atom concentration of the isotope in the gas phase. The experiment with radioactive krypton-85m, which has a 4.4 hour half-life, was designed so that the time to saturate the adsorber bed was comparable with the lifetime for decay of the radioactive gas. The experimental results revealed that the transmission of radioactive krypton-85m reached a steady-state or equilibrium value less than unity.

The analysis and interpretation of the measurements obtained in this experiment led Madey (1961) to the development of a time-dependent physical theory of adsorption of a radioactive gas. He formulated a partial differential equation to represent the balance of gains and losses of radioactive atoms in any volume element of the adsorber resulting from the processes of flow, adsorption, difusion, and radioactive decay. The theory contains two parameters, namely, an isothermal adsorption capacity, K, and a diffusion or dispersion coefficient, D, for the gas-adsorber system. The adsorption capacity is a measure of the ability of a material to remove a particular gas; it is a static characteristic. The dispersivity is a measure of the dispersion of a particular gas through the porous medium; it is a dynamic characteristic. Values of these two parameters were deduced from the measurements at the Brookhaven reactor, and agreement was obtained between the theory and the experimental results.

Madey and Pflumm[1] (unpublished) subsequently obtained more general solutions to the differential equation that apply to stable as well as radioactive isotopes. The solution to the differential equation for the transmission of a

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[1]Madey, Richard and Pflumm, Eugene, Republic Aviation Corporation (unpublished) Report RAC 885 (1962), "A Physical Theory of Adsorption."

delta-function input pulse of a stable gaseous isotope through an adsorber bed was reported by Madey, Fiore, Pflumm, and Stephenson (1962). In this 1962 paper, these authors analyzed experimental data obtained previously by Browning et al (1959a; 1959b; 1962) at the Oak Ridge National Laboratory on the transmission of a pulse of krypton-85 gas through an activated carbon adsorber bed. In these experiments, the pulse of krypton gas was injected into a stream of oxygen carrier gas flowing through the adsorber bed. The asymmetric shape of the transmitted pulse is one of the principal features observed in a pulsed experiment of this type. Expressions for the adsorptivity and the dispersivity were derived from the transmission function in terms of experimentally measured times on the transmitted pulse. The analysis of the Oak Ridge experiments gave values for the two theoretical parameters, namely, the adsorptivity and the dispersivity. The theoretical transmission function faithfully reproduced the asymmetry in the observed transmitted pulse.

The solution to the differential equation obtained by Madey and Pflumm for the time-dependent transmission, T, of a step function input pulse of a stable gaseous isotope through an adsorber bed of length, ℓ, is

$$2T = e^{u\ell/D} \text{ erfc } s_+ + \text{ erfc } 2_- \tag{1}$$ [2]

with

$$2s_\pm = \left(\frac{u\ell}{D}\right)^{\frac{1}{2}} \left[\left(\frac{B\ell}{ut}\right)^{\frac{1}{2}} \pm \left(\frac{tu}{B\ell}\right)\right]^{\frac{1}{2}} \tag{2}$$

and

$$B \equiv K\rho + 1 \tag{3}$$

where ρ is the bulk density of the adsorber.

For convenience, the quantity B is called the effective adsorptivity. The superficial flow velocity, u, is the ratio of the volumetric flow velocity to the cross-sectional area of the bed.

Levenspiel and Bischoff (1963) review five dispersion models for the flow of fluid in empty tubes and packed beds:

1. General dispersion
2. General dispersion in cylindrical coordinates
3. Uniform dispersion
4. Dispersed plug flow
5. Axial dispersed plug flow (ADPF)

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[2] The complementary error function is defined:

$$\text{erfc } s \equiv 1 - \text{erf } s \equiv 1 - \frac{2}{\sqrt{\pi}} \int_0^s e^{-x^2} dx$$

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The first three of these models take into account the velocity profile of the fluid. The last two assume a flat velocity profile equal to the actual mean velocity. The first model has a very general vector dispersion coefficient; the next three models have both radial and longitudinal dispersion coefficients; and the last model has only an axial dispersion coefficient. The other parameters of these models depend on the assumptions made regarding the relationship between the adsorbed and fluid phases.

For laminar flow in empty cylindrical tubes, Taylor (1953) and Westhaver (1947a, 1947b) have shown that dispersion caused by molecular diffusion and radial velocity variations can be represented by an effective axial dispersion coefficient and a flat velocity profile equal to the actual mean velocity of the fluid. They show that the effective axial dispersion coefficient gives the same results as the more general dispersion models involving both radial and axial dispersion coefficients and the true velocity profile; accordingly, the ADPF model is equivalent to the more complicated models for laminar flow in empty tubes.

In the hierarchy of dispersion models listed above, the Madey-Pflumm equation represents a solution to the axial dispersed plug flow model for packed beds.

This study of the theoretical performance of gaseous adsorption systems is based on the Madey-Pflumm equation above. The objective of this study is to generate and to validate a computer program that will permit the determination of the two theoretical parameters (namely, the effective adsorptivity, B, and the dispersivity, D) of the Madey-Pflumm equation from an analysis of experimental data on adsorption. The purpose of this report is twofold:

(1) To describe the basic analytical techniques that have been developed to determine the values of the two theoretical parameters in the transmission function and their errors from an experimental transmission versus time curve, and

(2) To report the results of the analysis of experimental data on the transmission of carbon dioxide in air through molecular sieve adsorber beds.

SECTION II

THE TRANSMISSION AS A FUNCTION OF TIME IN UNITS OF THE INFLECTION TIME

1. THE PROPAGATION-TIME REPRESENTATION OF THE TRANSMISSION FUNCTION

According to the Eq 1 and 2, the transmission is a function of two dimensionless quantities

$$T = T_1 \ (D_{u\ell}, \ \tau_p) = D_{u\ell}^{-\frac{1}{2}} \ [\tau_p^{\frac{1}{2}} \pm \tau_p^{-\frac{1}{2}}] \tag{4}$$

where

$$D_{u\ell} \equiv D/u\ell \tag{5}$$

$$t_p \equiv B\ell/u \tag{6}$$

$$\tau_p \equiv t/tp \tag{7}$$

The dimensionless group denoted by the symbol, $D_{u\ell}$, is a dispersion number for the fluid-adsorber bed system. The quantity, t_p, is called the propagation time. For the case of a system with a zero dispersion number, the transmission versus time function is a step function with the step occurring at a time equal to the propagation time. The propagation time is not readily obtained from an experimental transmission versus time curve except for systems with zero or near zero dispersion numbers. Since the inflection time can be estimated from an experimental transmission versus time curve, it will prove useful to represent the theoretical transmission versus time curve in terms of the inflection time.

2. THE INFLECTION-TIME REPRESENTATION OF THE TRANSMISSION FUNCTION

The inflection time, t_i, which occurs when the second time derivative of the transmission equals zero, is:

$$t_i = t_p/p \qquad\qquad (p > 1) \tag{8}$$

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where the inflection time parameter, p, denotes the following function of the dispersion number

$$p \equiv 3 D_{u\ell} + (9D^2_{u\ell} + 1)^{\frac{1}{2}} \tag{9}$$

In terms of the inflection time parameter, the dispersion number is

$$D_{u\ell} = \frac{1}{6} \left(p - \frac{1}{p}\right) = \frac{p^2 - 1}{6p} \tag{10}$$

In terms of the inflection time and the inflection time parameter, the argument $s_{\pm}$ of the complementary error functions in the transmission equation become

$$s_{\pm} = \left(\frac{6p}{p^2 - 1}\right)^{\frac{1}{2}} \left(p \, \tau_i^{-\frac{1}{2}} \pm \tau_i^{\frac{1}{2}}\right) \tag{11}$$

where τ_i denotes the time measured in units of the inflection time; that is,

$$\tau_i \equiv t/t_i \tag{12}$$

The inflection time representation of the transmission equation is

$$2T = e^{(s_+^2 - s_-^2)} \, \text{erfc} \, s_+ + \text{erfc} \, s_- \tag{13}$$

with $s_{\pm}$ given by Eq 11. In this representation, the transmission is a function of p and τ_i;

$$T = T_2(p, \tau_i) \tag{14}$$

The inflection time representation of the transmission function has been programmed on a computer. The computer results for the transmission versus time in units of the inflection time are tabulated in table I for values of the inflection time parameter p equal to 1.001, 1.005, 1.01, 1.05, 1.1, 1.15, 2, 3, 5, 10, 20, 50, 100, and 1000. Transmission versus time curves for p = 1.001, 1.1, 2, 5 and 100 are plotted on a linear scale in fig. 1 and on a log-log scale in fig. 2.

3. THE TRANSMISSION AT THE INFLECTION TIME

Both the inflection time and the transmission at the inflection time can be estimated from the inflection point of an experimental transmission versus time curve. At the inflection time, $\tau_i = 1$ and

$$s_{\pm}(\tau_i = 1) = \left(\frac{3}{2}\right)^{\frac{1}{2}} \left(\frac{p \pm 1}{p \mp 1}\right)^{\frac{1}{2}} \tag{15}$$

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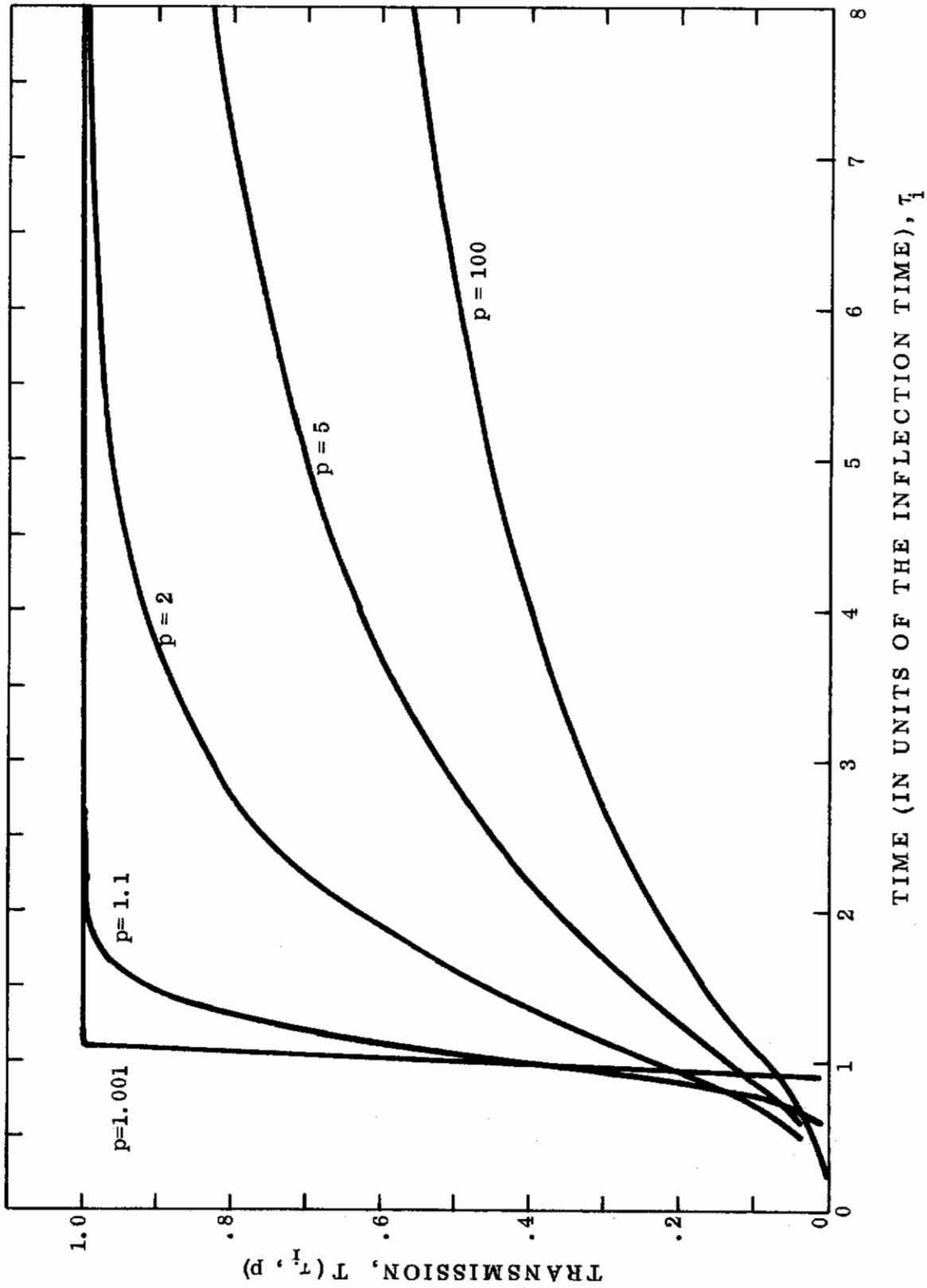
Figure 1. Transmission versus Time for Various Values of the Inflection Time Parameter
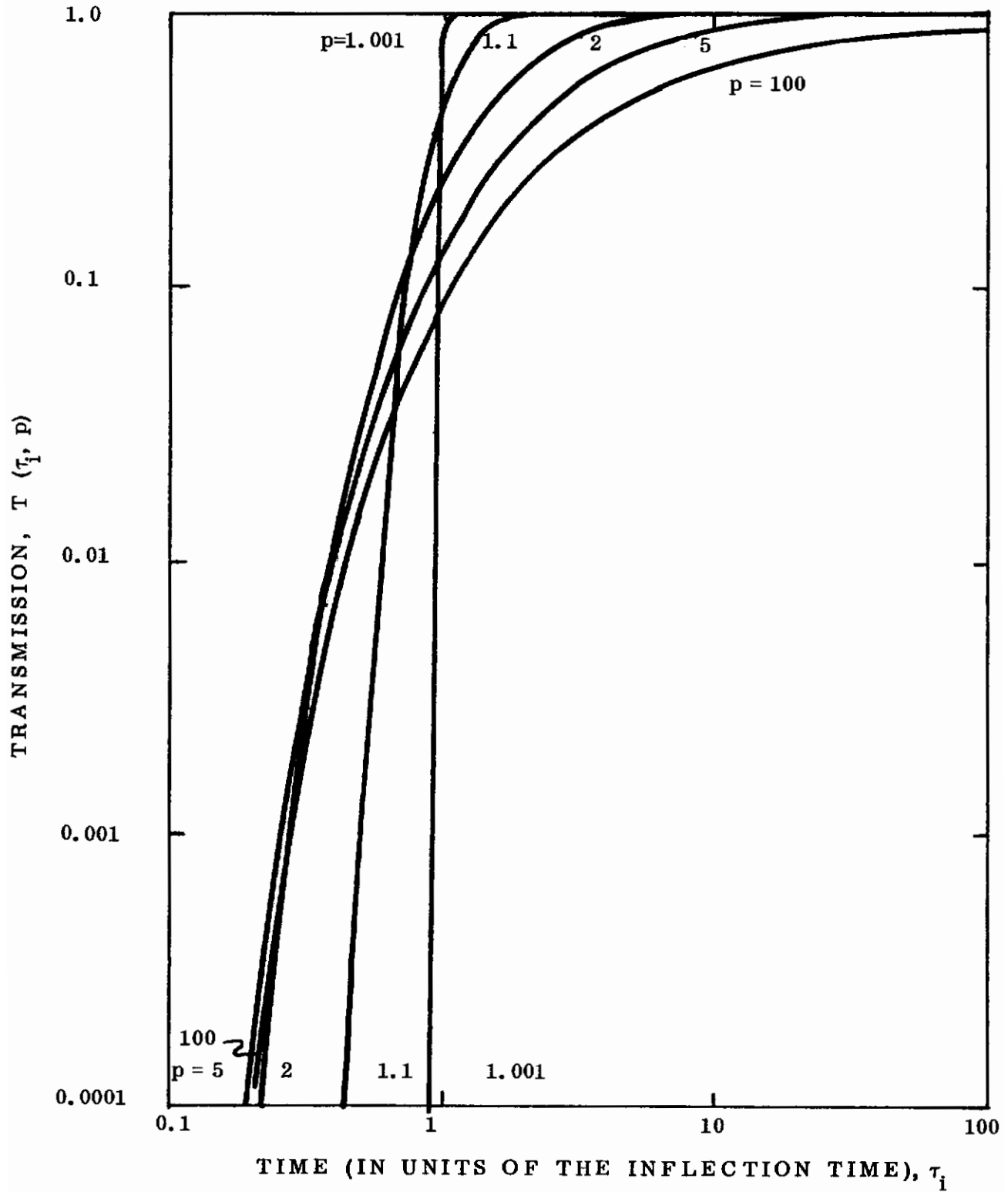
Figure 2. The Logarithm of the Transmission versus the Logarithm of the Time (in Units of the Inflection Time) for Various Values of the Inflection Time Parameter.

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This equation together with Eq 13 defines the transmission at the inflection time; obviously, the transmission at the inflection time is a function of the parameter p only. Values of the transmission at the inflection time for several values of the inflection time parameter are presented in table II and in fig. 3.

4. THE SLOPE OF THE TRANSMISSION AT THE INFLECTION TIME

The slope of the transmission versus time curve is

$$\frac{\partial T}{\partial \tau_i} = \frac{(s_+ + s_-)}{2 \sqrt{\pi \tau_i}} \; e^{-s_-^2} \tag{16}$$

with s_+ given by Eq 11. At the inflection time ($\tau_i = 1$), s_+ is given by Eq 15 and the slope is

$$\left(\frac{\partial T}{\partial \tau_i} \right)_{\tau_i = 1} = \left(\frac{3}{2\pi} \right)^{\frac{1}{2}} \frac{p}{(p^2 - 1)^{\frac{1}{2}}} \; e^{-\frac{3}{2} \frac{p-1}{p+1}} \tag{17}$$

This derivative is a function of p alone. As p approaches unity, the slope becomes infinite; as p approaches infinity, the slope is $(3/2\pi)^{\frac{1}{2}} e^{-3/2} = 0.1544$. Corresponding values of the slope of the transmission at the inflection time, the inflection time parameter, and the transmission at the inflection time are presented in table II.

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INFLECTION TIME PARAMETER, p
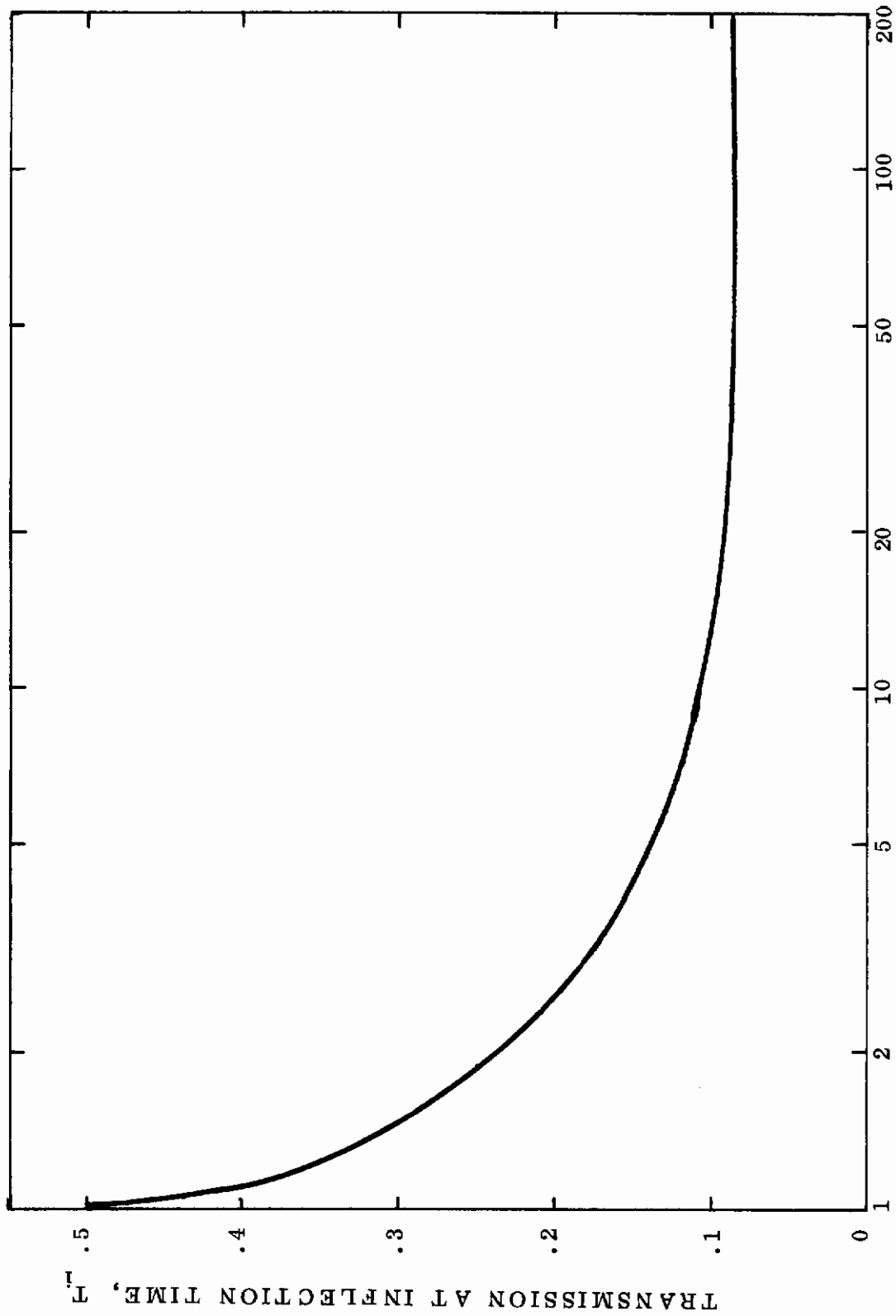
TRANSMISSION AT INFLECTION TIME, T_i

Figure 3.   Transmission at the Inflection Time ersus the Inflection Time Parameter

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SECTION III

THE LEAST-SQUARES ANALYSIS AND ERROR EVALUATION

1. **LEAST-SQUARES DETERMINATION OF THE EFFECTIVE ADSORPTIVITY AND THE DISPERSIVITY IN THE TRANSMISSION FUNCTION**

a. Statement of the Problem

We want to represent a set of observational points (t_k, T_k') by the theoretical equation

$$2\ T = e^{u\ell/D}\ \text{erfc}\ s_+ + \text{erfc}\ s_- \tag{1}$$

with

$$2\ s_{\pm} \equiv \left(\frac{u\ell}{D}\right)^{\frac{1}{2}} \quad \left(\frac{B\ell}{ut}\right)^{\frac{1}{2}} \pm \left(\frac{tu}{B\ell}\right)^{\frac{1}{2}} \tag{2}$$

We assume that the observed value of the transmission, T_k', is measured at an accurately known time, t_k, with an estimated standard deviation, $\delta\ T_k'$ It is assumed also that the adsorber bed length, ℓ, and the superficial flow velocity, u, of the gas through the adsorber bed are accurately known quantities. In order to represent these points by the smooth function, T, we shall use the least-squares method to evaluate the best values of the dispersivity, D, and the effective adsorptivity B.

The best values of D and B in the least-squares sense are such that the sum of the squares of the weighted residuals is a minimum; that is,

$$R \equiv \frac{1}{2} \sum_{k=1}^{n} W_k\ Y_k^2 = \text{a minimum} \tag{18}$$

with the residual

$$Y_k = T_k' - T_k\ (t_k,\ D,\ B) \tag{19}$$

and the weight W_k of a residual Y_k defined at t_k as

$$W_k = r^2 / (\delta \ T_k')^2 \tag{20}$$

The quantity, $\delta \ T_k'$, denotes the standard deviation in the experimental value of the transmission for the kth data point, and r is an arbitrary constant equal to a standard deviation in the transmission that is chosen to be of unit weight.

b.   The Normal Equations and Their Solution

In order to satisfy the least-squares criterion given in Eq 18, the first partial derivatives of R with respect to the theoretical parameters D and B should be zero:

$$\frac{\partial R}{\partial D} = \sum_{k=1}^{n} W_k Y_k \ \frac{\partial Y_k}{\partial D} = 0 \tag{21}$$

$$\frac{\partial R}{\partial B} = \sum_{k=1}^{n} W_k Y_k \ \frac{\partial Y_k}{\partial B} = 0 \tag{22}$$

Eq 21 and 22 are called the "normal" equations.

The normal equations may be solved numerically for the parameters D and B by the Newton-Raphson Method.[3]   Accordingly, we expand Eq 21 and 22 in a Taylor Series about the jth iterates D_j and B_j and obtain the $(j+1)^{st}$ values D_{j+1} and B_{j+1}.   The iteration is continued until a desired convergence criterion is satisfied.   The Taylor expansions of Eq 21 and 22 are

$$\frac{\partial R}{\partial D} = \left(\frac{\partial R}{\partial D}\right)_j + \left(\frac{\partial^2 R}{\partial D^2}\right)_j (D_{j+1} - D_j) + \left(\frac{\partial^2 R}{\partial D \partial B}\right)_j \left(B_{j+1} - B_j\right) = 0 \tag{23}$$

$$\frac{\partial R}{\partial B} = \left(\frac{\partial R}{\partial B}\right)_j + \left(\frac{\partial^2 R}{\partial D \partial B}\right)_j (D_{j+1} - D_j) + \left(\frac{\partial^2 R}{\partial B^2}\right)_j (B_{j+1} - B_j) = 0 \tag{24}$$

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[3] The Newton-Raphson Method for simultaneous equations is described in the book by Scarborough (1962)

is   Eq 23 and 24 are linear in D_{j+1} and B_{j+1}. The solution for D_{j+1} and B_{j+1}

$$D_{j+1} = D_j - \frac{1}{\Delta_j}\left[\left(\frac{\partial R}{\partial D}\right)_j \left(\frac{\partial^2 R}{\partial B^2}\right)_j - \left(\frac{\partial R}{\partial B}\right)_j \left(\frac{\partial^2 R}{\partial D\, \partial B}\right)_j\right] \quad (25)$$

$$B_{j+1} = B_j - \frac{1}{\Delta_j}\left[\left(\frac{\partial R}{\partial B}\right)_j \left(\frac{\partial^2 R}{\partial D^2}\right)_j - \left(\frac{\partial R}{\partial D}\right)_j \left(\frac{\partial^2 R}{\partial D\, \partial B}\right)_j\right] \quad (26)$$

where the determinant of the coefficients is

$$\Delta_j = \left[\left(\frac{\partial^2 R}{\partial D^2}\right)_j \left(\frac{\partial^2 R}{\partial B^2}\right)_j - \left(\frac{\partial^2 R}{\partial D\, \partial B}\right)_j^2\right] \quad (27)$$

After iterating until the convergence criterion is satisfied, Eq 25 and 26 give the "best" values in the least-squares sense of the theoretical parameters D and B.

It is possible to obtain an initial estimate of the solution of the normal equations from the inflection point of an experimental transmission versus time curve. From the value of the transmission at the inflection time, one can obtain a value of the inflection time parameter p from fig. 3. Then, Eq 10 can be used to obtain the initial guess for the dispersion number $D_{u\ell}$ and Eq 8 gives the propagation time as the product of the inflection time t_i and the inflection time parameter, p. The dispersivity, D, and the effective adsorptivity, B, can then be obtained from Eq 5 and 6 for known values of u and ℓ.

2. EVALUATION OF STANDARD DEVIATIONS IN THE EFFECTIVE ADSORP-
    TIVITY AND THE DISPERSIVITY

We now wish to propagate the errors in D and B through the normal equations with respect to the experimentally observed errors $\delta T_k'$ in the transmission. The errors in D and B are obtained from the law of propagation of small errors, viz:

$$(\Delta D)^2 = \sum_{k=1}^{n} (\delta T_k')^2 \left(\frac{\partial D}{\partial T_k}\right)^2 \quad (26)$$

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$$\left(\Delta B \right)^2 = \sum_{k=1}^{n} \left(\delta T'_k \right)^2 \left(\frac{\partial B}{\partial T_k} \right)^2 \tag{27}$$

In order to obtain the partial derivatives required in Eq 28 and 29, we shall differentiate the normal equations with respect to T'_j. Differentiating Eq 21 with respect to T'_j, we obtain

$$\sum_{k=1}^{n} W_k Y_k \left[\frac{\partial^2 Y_k}{\partial D^2} \frac{\partial D}{\partial T'_j} + Y_k \frac{\partial^2 Y_k}{\partial D \partial B} \frac{\partial B}{\partial T'_j} + \frac{\partial Y_k}{\partial D} \frac{\partial Y_k}{\partial D} \frac{\partial D}{\partial T'_j} \right.$$

$$\left. + \frac{\partial Y_k}{\partial D} \frac{\partial Y_k}{\partial B} \frac{\partial B}{\partial T'_j} + \frac{\partial Y_k}{\partial D} \frac{\partial Y_k}{\partial T'_j} \right] = 0 \tag{30}$$

Now, in the last term in Eq 30, we note that

$$\frac{\partial Y_k}{\partial T_j} = \delta_{jk} = \begin{array}{ll} 1 & \text{for } k=j \\ 0 & \text{for } K \neq j \end{array} \tag{31}$$

Accordingly, Eq 30 may be rewritten as follows:

$$\frac{\partial D}{\partial T'_j} \sum_{k=1}^{n} W_k \left[Y_k \frac{\partial^2 Y_k}{\partial D^2} + \left(\frac{\partial Y_k}{\partial D} \right)^2 \right] + \frac{\partial B}{\partial T'_j} \sum_{k=1}^{n} \left[Y_k \frac{\partial^2 Y_k}{\partial D \partial B} + \frac{\partial Y_k}{\partial D} \frac{\partial Y_k}{\partial B} \right]$$

$$\tag{32}$$

Here we note that Eq 32 can be simplified because the coefficients of the desired partial derivatives may be expressed in terms of the partial derivatives of Eq 21 and 23 with respect to D, viz:

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$$\frac{\partial^2 R}{\partial D^2} = \sum_{k=1}^{n} \left[W_k Y_k \frac{\partial^2 Y_k}{\partial D^2} + \left(\frac{\partial Y_k}{\partial D} \right)^2 \right] \tag{33}$$

and

$$\frac{\partial^2 R}{\partial D \partial B} = \sum_{k=1}^{n} W_k \left[Y_k \frac{\partial^2 Y_k}{\partial D \partial B} + \frac{\partial Y_k}{\partial D} \frac{\partial Y_k}{\partial B} \right] \tag{34}$$

Hence, Eq 30 simplifies:

$$\frac{\partial^2 R}{\partial D^2} \frac{\partial D}{\partial T'_j} + \frac{\partial^2 R}{\partial D \partial B} \frac{\partial B}{\partial T'_j} + W_j \frac{\partial T_j}{\partial D} = 0 \tag{35}$$

By interchanging the D's and B's of Eq 35, we obtain a similar result from the other normal equation, Eq 22:

$$\frac{\partial^2 R}{\partial D \partial B} \frac{\partial D}{\partial T_j} + \frac{\partial^2 R}{\partial B^2} \frac{\partial B}{\partial T'_j} + W_j \frac{\partial Y_j}{\partial B} = 0 \tag{36}$$

We now solve Eq 35 and 36 for $\partial D / \partial T'_j$ and $\partial B / \partial T'_j$:

$$\frac{\partial D}{\partial T'_j} = - \frac{W_j}{\Delta} \left(\frac{\partial Y_j}{\partial D} \frac{\partial^2 R}{\partial B^2} - \frac{\partial Y_j}{\partial B} \frac{\partial^2 R}{\partial B \partial D} \right) \tag{37}$$

$$\frac{\partial B}{\partial T'_j} = - \frac{W_j}{\Delta} \left(\frac{\partial Y_j}{\partial B} \frac{\partial^2 R}{\partial D^2} - \frac{\partial T_j}{\partial D} \frac{\partial^2 R}{\partial D \partial B} \right) \tag{38}$$

where the determinant of the coefficients is

$$\Delta = \left[\left(\frac{\partial^2 R}{\partial D^2} \frac{\partial^2 R}{\partial B^2} - \frac{\partial^2 R}{\partial D \partial B} \right)^2 \right] \tag{39}$$

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In calculating $\partial D/\partial T'_j$ and $\partial B/\partial T'_j$, the values of D and B to be used in evaluating the various partial derivatives are values determined by the least-squares procedure outlined in Section III-1.

Since there are n experimentally observed values of the transmission T'_j, Eq 37 and 38 give n pairs of partial derivatives. Then the standard derivations ΔD in D and ΔB in B are found from Eq 29 and 30.

SECTION IV

THE LEAST-SQUARES ADSORPTION COMPUTER PROGRAM

The Least-Squares Adsorption Program instructs a digital computer to solve the two simultaneous normal equations Eq 21 and 22 of the least-squares analysis presented in Section III for the values of the dispersivity, D, and the effective adsorptivity, B. The Newton-Raphson method[4] is used for the solution of two simultaneous equations in two unknowns. The computer iterates the parameters D and B until a convergence criterion is satisfied. The convergence criterion is that

$$\rho \equiv \sqrt{\left(\frac{D_{j+1} - D_j}{D_j}\right)^2 + \left(\frac{B_{j+1} - B_j}{B_j}\right)^2} \leq \rho_1 \tag{40}$$

where the convergence parameter, ρ_1, is an arbitrarily chosen number. For a sufficiently small value of ρ_1, this criterion insures that changes in the values of the parameters are insignificant upon further iteration. The value of the convergence parameter, ρ_1, used for the analyses reported in Section V is 10^{-5}. We observed that ρ_1 could be an order of magnitude larger without significantly changing the solution for the two parameters. After determining the least squares values of D and B, the computer calculates standard deviations $\triangle D$ in D and $\triangle B$ in B. When the standard deviations have been computed, a table of theoretical values of the transmission versus time is computed.

The Least-Squares Adsorption Program consists of a main program and several subprograms. The subprograms are either "subroutine" or "function" subprograms. The name (computer symbol), and function of each subprogram follows :

1. The Newton-Raphson (DNR) "subroutine" subprogram performs the Newton-Raphson iterative processes.

2. The Cycling (DCYCL) "function" subprogram shifts or "cycles" the initial estimates of the two theoretical parameters (viz, the dispersivity, D, and the effective adsorptivity, B, whenever iterated values of D and B are diverging.

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[4] Same as footnote 3 on page 8

3. The Least-Squares (LSTSQ) "subroutine" subprogram calculates the first and second derivatives of the weighted residuals, R, in the Eq 23 and 24 for the first-order Newton-Raphson solutions of the normal equations.

4. The Derivative (YDERV) "subroutine" subprogram calculates the residuals Y_k and their first and second partial derivatives.

5. The Transmission (DTRANS) Function "function" subprogram calculates the transmission for given values of the dimensionless dispersion number $D_{u\ell}$ (=$D/u\ell$) and the dimensionless time measured in units of the inflection time.

6. The Error Function (ERFCC) "function" subprogram calculates the complementary error functions for use in the transmission function. This subprogram uses the rational approximation to the error function from Hastings (1955) when the argument of the error function is less than 2.4. Since the relative error in the Hastings approximation becomes larger as the argument of the error function becomes large, the asymptotic series approximation to the error function is used when the argument of the error function is greater than 2.4.

7. The Parameter (PARAM) "function" subprogram determines the inflection time parameter p from a given value of the transmission at the inflection time.

The program has been executed on three different computing machines: first on an IBM-1620 at Clarkson College, later on an IBM-7044 at the University of Buffalo, and still later on an IBM System 360 Model 44 at Clarkson College[5]. The program is written in a Fortran IV language. The iteration time on the IBM-360/44 Computer is about 20 milliseconds per input data point; hence, for example, about 200 milliseconds is required per iteration for an experimental transmission versus time curve consisting of 10 data points. Figure 4 is a flow diagram of the Least-Squares Adsorption Computer Program.

The program points out information in the following categories:

1. Run Identification
2. Input Data
3. Initial Estimate of the Solution
4. Output
5. Comparison of Experimental and Theoretical Transmission

Under "run identification" will be brief identifying information such as

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[5] On 15 June 1967, Clarkson College replaced its IBM-1620 with an IBM System 360 Model 44.

WEIGHTED LEAST–SQUARES ADSORPTION PROGRAM (JUNE 1967)
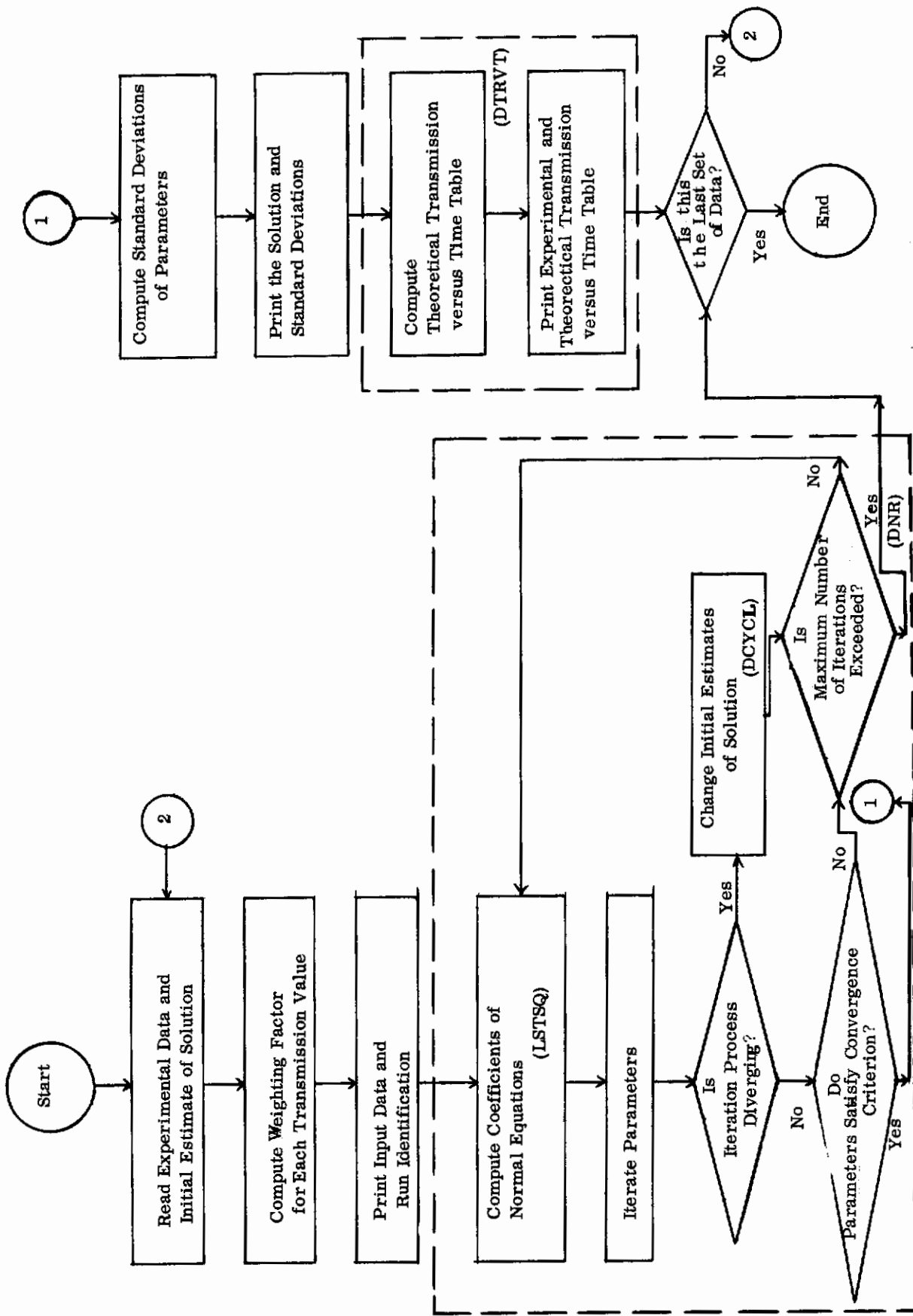
Figure 4.   A Flow Diagram of the Least–Squares Adsorption Computer Program

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CHRISTENSEN, .154 LB/MIN, 350 DEG R

CARBON DIOXIDE ON ONE EIGHTH INCH TYPE 5A MOLECULAR SIEVE PELLETS

Under "Input Data" are the name, symbol, value, error if known, and units of the following quantities: bed length, bed area, flow velocity, superficial flow velocity, adsorber bulk density, void fraction, inlet concentration, total pressure of gas, and temperature. Also listed are experimental values of the transmission and, if known, the uncertainty in the transmission versus time.

Under "intial estimate of solution" are printed the transmission at inflection time, the inflection time, and the inflection time parameter.

Under "output" are the name, symbol, value, error, and units for the various quantities of interest. First, the propagation time and the dispersivity are given in the same units as the units of the input data. Then, the following quantities are given in c. g. s units: propagation time, dimensionless dispersivity, dispersivity, effective adsorptivity, adsorptivity, inflection time parameter, inflection time, transmission at inflection time, and the slope of the transmission at the inflection time. Also listed are theoretical transmission versus time data and the reduced time in units of the inflection time.

Category 5 lists experimental and theoretical values of the transmission versus time.

SECTION V

COMPUTER ANALYSIS OF EXPERIMENTAL DATA ON THE TRANSMISSION
OF CARBON DIOXIDE IN AIR THROUGH MOLECULAR SIEVE ADSORBER BEDS

1. THE CHRISTENSEN DATA

The Christensen (1962) report contains data for one mole percent carbon
dioxide (CO_2) in air flowing through 3.55 inch diameter adsorber beds packed with
1/8 inch type 5A molecular sieve pellets.   These data are for air temperatures
of 350, 400, 450, 500 and 530° R and for mass flow velocities of 0.514, 0.308,
0.463, 0.616 and 0.720 pounds of air per minute.   Although the Christensen re-
port states on page 10 that the transmission versus time was measured directly,
these data are not included in the report; unfortunately, also these data are no
longer available.   The Christensen report presents curves of the adsorption load
L versus time with the air temperature and the mass flow velocity as parameters.
Also presented are curves of the adsorption load versus the air temperature (or
the mass flow velocity) with the mass flow velocity (or the air temperature) and
the dynamic adsorption efficiency E as parameters.   The adsorption load is the
amount of carbon dioxide adsorbed on the molecular sieve at any given time. It
is expressed as a fraction of the weight of the dry sieve.   The Christensen re-
port defines the dynamic adsorption efficiency E as

$$E = 1 - T \qquad (41)$$

where T is the transmission.

The procedure for obtaining values of the transmission versus time from
the Christensen report involves cross-referencing the adsorption load, the mass
flow velocity (or the air temperature), and the dynamic adsorption efficiency with
the corresponding time from the curves of adsorption load versus time.   The
transmission versus time data deduced by this procedure are presented in tables
III through VII.   Note that although the mass flow rate was held constant as the air
temperature was varied, the superficial flow velocity is different for each tem-
perature since the density of air is temperature dependent.   The superficial flow
velocities are listed in tables VIII through XI under data identification.

The transmission versus time data listed in the tables III through VII were
used as inputs to the computer program for obtaining the least-squares values and
the standard deviations of the dispersivity D, the effective adsorptivity B, the
adsorptivity K, the inflection time t_i and the inflection time parameter p.   The
computer results are given in tables VIII through XI.   The standard deviation in
the dispersivity and the effective adsorptivity were computed on the assumption
that the uncertainties in the experimental values of the transmissions are the same
for each value of the transmission.   As can be seen from Eq 18, this assumption

is equivalent to giving equal weight to each value of the transmission. The Christensen report does not give the uncertainties in the experimental values of the transmission. The standard deviations were computed for unit uncertainties in the transmissions. Actual values of the standard deviations may then be obtained by multiplying these computer values by the assigned uncertainty in the determination of the transmissions. The values of the standard deviations reported in tables VIII through XI are for assigned uncertainties of 0.1 in the experimental values of the transmissions.

In tables XII through XVI, the theoretical values of the transmission are compared with the experimental values. The theoretical transmission values are calculated for each case at the times corresponding to the experimental transmission values listed in the left-hand column of each table. The experimental transmission versus time data are listed in tables III through VII. Graphs of the time-dependent transmission are given in the Appendix. The solid lines represent the theoretical transmission functions whereas the points are experimental.

2. THE FOX DATA

Fox (1966) has obtained data for 0.64 mole percent carbon dioxide (CO_2) in air at a temperature of 75° F flowing through 0.85 inch diameter adsorber beds packed with 1/16 inch type 5A molecular sieve pellets. Fox also obtained similar data for 2.3 inch diameter adsorber beds packed with 1/8 inch type 5A molecular sieve pellets. Although the transmission versus time data do not appear in the Fox report, these data were furnished by Mr. W. B. Fox, Jr., and are listed in tables XVII through XXI. The conversion of the mass flow rate of the volumetric flow rate and the superficial flow velocity of dry air at a temperature of 75° F for the Fox data is given in table XXII.

The transmission versus time data listed in tables XVII through XXI were used as inputs to the computer program for obtaining the least-squares values and the standard deviations of the theoretical parameters. The computer results are given in tables XXIII through XXVI. Here as in the Christensen data, the standard deviations reported are for assumed uncertainties of 0.1 in the experimental values of the transmissions.

In tables XVII through XXI, the theoretical values of the transmission are compared with the experimental values. Graphs of the time-dependent transmission are given in the Appendix. The solid lines represent the theoretical transmission functions; whereas the points are experimental.

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SECTION VI

CORRELATION OF DATA ON THE ADSORPTION OF CARBON DIOXIDE IN AIR ON MOLECULAR SIEVES

1. VARIATION OF THE ADSORPTIVITY WITH THE AIR TEMPERATURE

The adsorptivities obtained from the analysis of the Christensen data (for the transmission of one mole percent carbon dioxide in air at various temperatures through 3.55 inch diameter adsorber beds packed with 1/8 inch type 5A molecular sieve pellets) are listed in tables VIII and IX. The lowest temperature of 194.4° K is the sublimation temperature of carbon dioxide. The data for a mass flow rate of 0.308 pounds of air per minute have been regrouped in table XXVII and plotted in fig. 5. As indicated in table XXVII, the data for the 6 inch and the 18 inch beds have been combined. The semi logarithmic plot in fig. 5 indicates that the adsorptivity does not vary with the air temperature for the lower air temperatures and that it decreases exponentially with air temperatures at the higher air temperatures. The adsorptivities at the higher air temperatures are given by equations of the form

$$K = K_o \exp(-\Theta/\Theta_o) \tag{42}$$

where Θ_o is a characteristic temperature. The temperature dependence of the adsorptivity is given by

$$K \ (cc/gm) = 8.14 \times 10^4 \exp(-\Theta/100) \quad (233 \le \Theta \ (°K) \le 300) \tag{43}$$

for a mass flow rate of 0.154 pounds of air per minute, and by

$$K \ (cc/gm) = 1.08 \times 10^5 \exp(-\Theta/90) \quad (255 \le \Theta \ (°K) \le 300) \tag{44}$$

for a mass flow rate of 0.308 pounds of air per minute. Note that a characteristic temperature Θ_o of 100 °K corresponds to a thermal energy $k \Theta_o = (1/120)$ eV.

2. VARIATION OF THE DISPERSIVITY WITH THE SUPERFICIAL FLOW VELOCITY

The dispersitivites obtained from the analyses of the experimental transmission-versus-time curves for carbon-dioxide on molecular sieve adsorbent are listed in tables VIII and IX for the Christensen data and in tables XXIII and XXVI for the Fox data. At each air temperature, these results are consistent with the dispersivity increasing as the square of the superficial flow velocity in the interval from about 15 to 70 cm/sec. More data are required in order to determine the superficial velocity dependence of the dispersivity at lower superficial flow velocities. It should be noted also that the dispersivity decreases as the temperature decreases.

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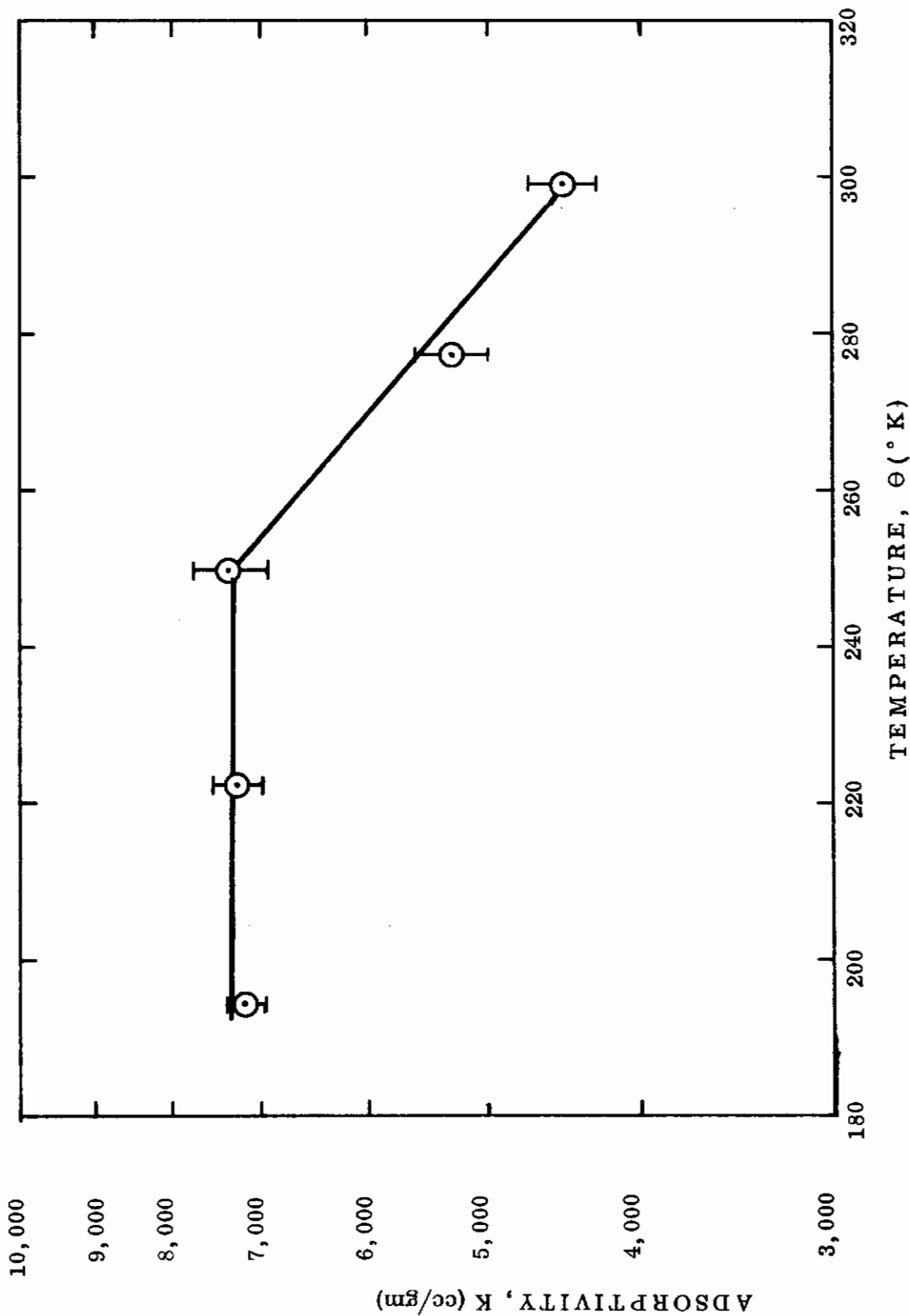
Figure 5. The Adsorptivity versus the Temperature of Air Containing One Mole Percent of Carbon
Dioxide Flowing at a Rate of 0.308 Pounds Per Minute through 3.55 Inch Diameter
Adsorber Beds Packed with 1/8 Inch Type 5A Molecular Sieve Pellets

Taylor (1953) and Aris (1956) have obtained relations for the velocity dependence of the dispersivity of a fluid in an empty tube of radius r when the concentration of the adsorbate is essentially uniform over the cross-section and disperses relative to the fluid which has a flat velocity profile and a mean velocity u along the axis of the tube. Aris's expression is

$$D = D_m + r^2 u^2 / 48 D_m \tag{48}$$

Aris showed that the numerical value of the coefficient of the molecular diffusivity D_m in Eq 48 is in general a function of the tube geometry and the velocity profile. Levenspiel and Bischoff (1963) state that use of Eq 48 for the effective dispersivity gives the same results as would be obtained from the more rigorous calculation involving radial and axial diffusion and a true velocity profile.

A survey of the literature does not reveal a suitable theoretical expression for the flow velocity dependence of the dispersivity in packed beds. Saffman (1959, 1960) provides theoretical expressions for the flow velocity dependence of the dispersivity for a bed composed of randomly distributed cylindrical pores of uniform length and cross-section. Saffman's expressions are expressed in terms of the length and cross-section of the pores. Application of Saffman's expressions to the analysis of packed beds would entail determining an "effective" pore length and cross-section for beds randomly packed with molecular sieve pellets. This work has not been attempted at this time.

3. INFLECTION POINT CORRELATIONS

The least-squares values and the standard deviations of the dispersivity, the adsorptivity, the inflection time and the inflection time parameter deduced from the Christensen and the Fox data are given in tables VIII through XI and tables XXIII through XXVI as shown in Section II, the transmission at the inflection time is a function only of the inflection time parameter p which in turn is a function only of the dimensionless dispersion number, $D_{u\ell}$ Arranged in table XXVIII in increasing order of the inflection time, t_i, for the Christensen and the Fox data are values of the transmission at the inflection time, T_i, and the inflection time parameter, p. The dimensionless dispersion number, $D_{u\ell}$, and the propagation time, t_p, are arranged in a similar manner in table XXIX.

Figure 6 is a log-log plot of the transmission at the inflection time versus the inflection time for the various experimental runs in both the Christensen and the Fox data. The values derived from the Fox data with the 1/16 inch pellets lie on one line which extends over about one order of magnitude in the inflection time. All of the values derived from the experimental data of both Christensen and Fox

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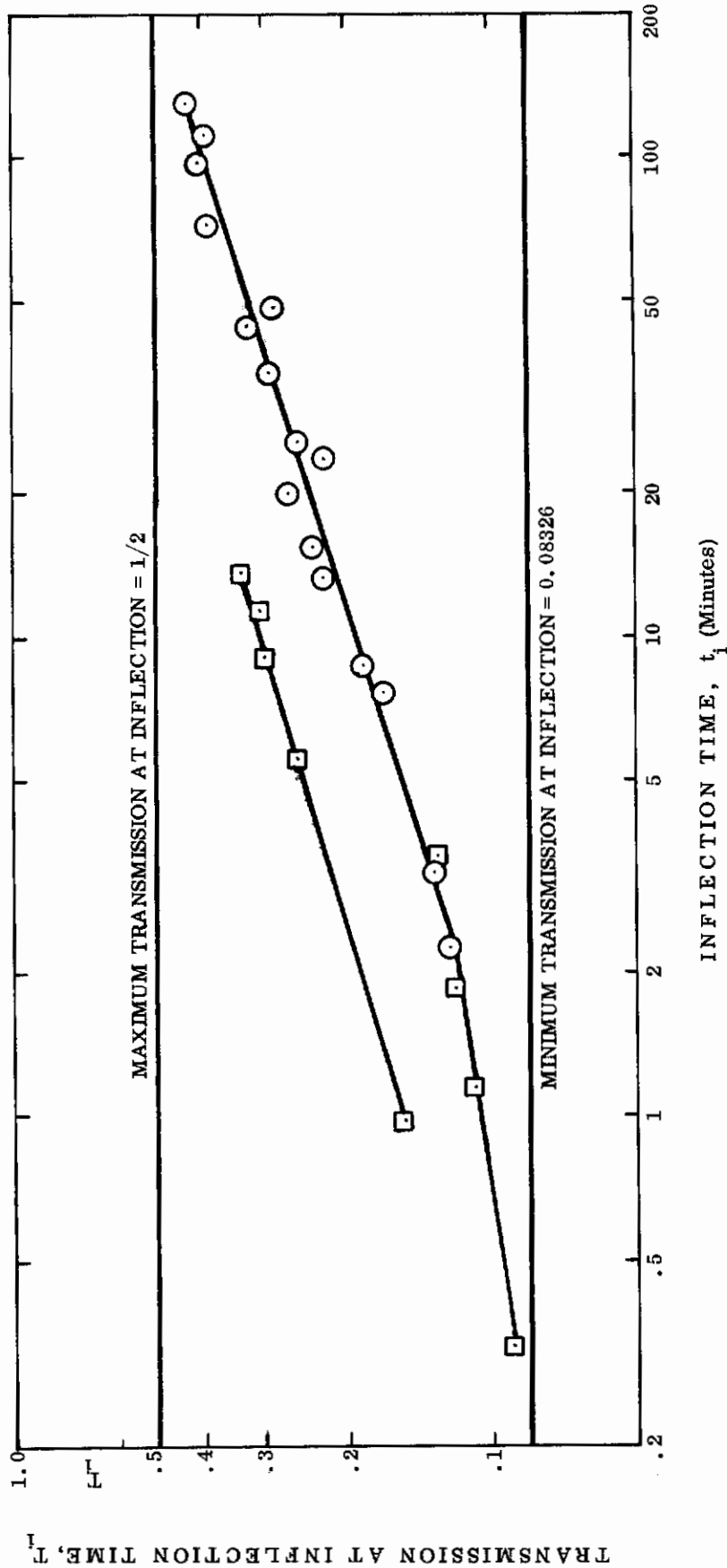
Figure 6. The Transmission at the Inflection Time versus the Inflection Time for Carbon Dioxide in Air on Type 5A Molecular Sieve Adsorbent. (The circled points have been deduced from the Christensen data and the points with squares from Fox data. Represented are different experimental conditions of air temperature, adsorber bed dimensions, molecular sieve pellet size, superficial flow velocity, and inlet concentration of carbon dioxide)

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for the 1/8 inch pellets correlates transmission versus time data obtained under various experimental conditions of air temperature, adsorber bed dimensions, superficial flow velocity, and inlet concentration of carbon dioxide. The Fox data for the 1/16 inch pellets were obtained at a temperature of 75° F for three different lengths of adsorber beds and for five different superficial flow velocities.

In the straight-line regions of the log-log plot, the transmission at the inflection time may be represented by a power-law of the form

$$T_i = kt_i^n \tag{49}$$

The coefficient k and the exponent n have the values indicated below: For 1/8 inch pellets,

$$T_i = 0.0930\, t_i^{0.32} \qquad (2 \leq t_i \text{ (min)} \leq 150) \tag{50}$$

For 1/16 inch pellets,

$$T_i = 0.155\, t_i^{0.26} \qquad (0.8 \leq \text{ (min)} \leq 20) \tag{51}$$

For a given value of the transmission at the inflection time, a molecular sieve adsorber bed packed with 1/8 inch pellets has a longer inflection time than one packed with 1/16 inch pellets.

SECTION VII

CONCLUSION

A weighted least-squares analysis has been developed to determine from an experimental transmission versus time curve the values of the two theoretical parameters of the Madey-Pflumm equation for the time-dependent transmission of a gas through an adsorber bed of length ℓ and bulk density ρ, and a gas-adsorber system characterized by an isothermal adsorption capacity and a dispersivity. The analysis has been extended to determining the errors in the two theoretical parameters by propagating the errors in the experimental values of the transmission through the normal equations of the least-square analysis. A digital computer program has been written in Fortran IV language with experimental transmission versus time data as input. The computer program prints out values for the two theoretical parameters and their errors. The output of the computer program also compares the experimental and theoretical values of transmission versus time.

The least-squares adsorption computer program has been used to analyze experimental data on the transmission of carbon dioxide (CO_2) in air through molecular sieve adsorber beds. Values of the theoretical parameters have been deduced from the Christensen (1962) data for one mole percent CO_2 on 1/8 inch pellets, and from the Fox (1966) data for 0.64 mole percent CO_2 on both 1/16 inch and 1/8 inch pellets for various flow velocities, bed dimensions, and air temperatures. At each air temperature, the results are consistent with the dispersivity increasing with the square of the superficial flow velocity over the range studied. A log-log plot of the transmission at the inflection time versus the inflection time correlates all the data analyzed for the various experimental conditions of air temperature, adsorbed bed dimensions, superficial flow velocity, and inlet concentration of carbon dioxide. For a given value of the transmission at the inflection time, a molecular sieve adsorber bed packed with 1/8 inch pellets has a longer inflection time than one packed with 1/16 inch pellets.

TABLE I

TRANSMISSION VERSUS TIME IN UNITS OF THE INFLECTION TIME
FOR SEVERAL VALUES OF THE INFLECTION TIME PARAMETER P

REDUCED TIME		TRANSMISSION		
T/TI	P= 1.001	1.005	1.010	
.10	0.000E-99	0.000E-99	0.000E-99	
.20	0.000E-99	0.000E-99	0.000E-99	
.30	0.000E-99	0.000E-99	1.343E-56	
.40	0.000E-99	1.186E-61	3.419E-32	
.50	0.000E-99	3.080E-35	8.285E-19	
.60	1.396E-89	9.411E-20	6.318E-11	
.70	2.448E-44	1.691E-10	3.563E-06	
.80	1.824E-18	4.113E-05	2.326E-03	
.90	1.980E-05	2.960E-02	8.424E-02	
1.00	4.897E-01	4.769E-01	4.674E-01	
1.10	9.998E-01	9.447E-01	8.621E-01	
1.20	1.000E-00	9.990E-01	9.846E-01	
1.30	1.000E-00	9.999E-01	9.991E-01	
1.40	1.000E-00	9.999E-01	9.999E-01	
1.50	1.000E-00	1.000E-00	9.999E-01	
1.60	1.000E-00	1.000E-00	9.999E-01	
1.70	1.000E-00	1.000E-00	1.000E-00	

TABLE I

TRANSMISSION VERSUS TIME IN UNITS OF THE INFLECTION TIME
FOR SEVERAL VALUES OF THE INFLECTION TIME PARAMETER P

REDUCED TIME   TRANSMISSION

T/TI	P= 1.050	1.100	1.150
.10	1.956E-59	5.795E-33	3.858E-24
.20	7.105E-25	2.393E-14	7.904E-11
.30	1.001E-13	2.675E-08	1.769E-06
.40	1.966E-08	2.133E-05	2.246E-04
.50	1.765E-05	9.391E-04	3.606E-03
.60	1.082E-03	9.766E-03	2.060E-02
.70	1.451E-02	4.482E-02	6.554E-02
.80	7.652E-02	1.243E-01	1.451E-01
.90	2.208E-01	2.486E-01	2.536E-01
1.00	4.277E-01	3.988E-01	3.772E-01
1.10	6.362E-01	5.495E-01	5.012E-01
1.20	7.976E-01	6.816E-01	6.144E-01
1.30	8.997E-01	7.859E-01	7.108E-01
1.40	9.550E-01	8.621E-01	7.885E-01
1.50	9.814E-01	9.143E-01	8.487E-01
1.60	9.928E-01	9.483E-01	8.937E-01
1.70	9.974E-01	9.696E-01	9.264E-01
1.80	9.991E-01	9.825E-01	9.497E-01
1.90	9.997E-01	9.901E-01	9.661E-01
2.00	9.999E-01	9.945E-01	9.773E-01
3.00	9.999E-01	9.999E-01	9.997E-01
4.00	1.000E-00	9.999E-01	9.999E-01
5.00	1.000E-00	1.000E-00	9.999E-01
6.00	1.000E-00	1.000E-00	1.000E-00

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TABLE I

TRANSMISSION VERSUS TIME IN UNITS OF THE INFLECTION TIME
FOR SEVERAL VALUES OF THE INFLECTION TIME PARAMETER P

RECUCED TIME		TRANSMISSION	
T/TI	P= 1.500	2.000	3.000
.10	6.534E-12	1.789E-09	1.896E-08
.20	5.947E-06	5.220E-05	1.188E-04
.30	5.826E-04	1.686E-03	2.334E-03
.40	5.705E-03	9.738E-03	1.062E-02
.50	2.211E-02	2.807E-02	2.675E-02
.60	5.380E-02	5.689E-02	4.988E-02
.70	1.002E-01	9.425E-02	7.824E-02
.80	1.581E-01	1.374E-01	1.100E-01
.90	2.231E-01	1.841E-01	1.436E-01
1.00	2.913E-01	2.323E-01	1.782E-01
1.10	3.595E-01	2.805E-01	2.127E-01
1.20	4.256E-01	3.277E-01	2.467E-01
1.30	4.880E-01	3.733E-01	2.798E-01
1.40	5.459E-01	4.168E-01	3.118E-01
1.50	5.989E-01	4.580E-01	3.426E-01
1.60	6.468E-01	4.967E-01	3.720E-01
1.70	6.899E-01	5.330E-01	4.001E-01
1.80	7.283E-01	5.668E-01	4.269E-01
1.90	7.623E-01	5.984E-01	4.524E-01
2.00	7.924E-01	6.276E-01	4.766E-01
3.00	9.483E-01	8.244E-01	6.607E-01
4.00	9.872E-01	9.150E-01	7.724E-01
5.00	9.968E-01	9.577E-01	8.430E-01
6.00	9.991E-01	9.785E-01	8.893E-01
7.00	9.997E-01	9.889E-01	9.206E-01
8.00	9.999E-01	9.941E-01	9.422E-01
9.00	9.999E-01	9.968E-01	9.575E-01
10.00	9.999E-01	9.983E-01	9.684E-01
12.00	9.999E-01	9.995E-01	9.821E-01
14.00	9.999E-01	9.998E-01	9.896E-01
16.00	9.999E-01	9.999E-01	9.939E-01
18.00	1.000E-00	9.999E-01	9.963E-01
20.00	1.000E-00	9.999E-01	9.978E-01
30.00	1.000E-00	9.999E-01	9.997E-01
40.00	1.000E-00	1.000E-00	9.999E-01

TABLE I

REDUCED TIME	TRANSMISSION		
T/TI P=	5.000	10.00	20.00
.10	4.213E-08	4.996E-08	4.828E-08
.20	1.426E-04	1.339E-04	1.224E-04
.30	2.297E-03	1.998E-03	1.793E-03
.40	9.493E-03	7.969E-03	7.087E-03
.50	2.262E-02	1.860E-02	1.646E-02
.60	4.078E-02	3.309E-02	2.919E-02
.70	6.254E-02	5.032E-02	4.430E-02
.80	8.660E-02	6.927E-02	6.089E-02
.90	1.119E-01	8.917E-02	7.831E-02
1.00	1.378E-01	1.094E-01	9.607E-02
1.10	1.636E-01	1.297E-01	1.138E-01
1.20	1.892E-01	1.498E-01	1.313E-01
1.30	2.142E-01	1.694E-01	1.485E-01
1.40	2.384E-01	1.885E-01	1.653E-01
1.50	2.619E-01	2.071E-01	1.815E-01
1.60	2.845E-01	2.250E-01	1.972E-01
1.70	3.062E-01	2.423E-01	2.124E-01
1.80	3.271E-01	2.589E-01	2.270E-01
1.90	3.472E-01	2.749E-01	2.411E-01
2.00	3.664E-01	2.903E-01	2.546E-01
3.00	5.203E-01	4.162E-01	3.659E-01
4.00	6.246E-01	5.051E-01	4.452E-01
5.00	6.986E-01	5.711E-01	5.048E-01
6.00	7.534E-01	6.223E-01	5.514E-01
7.00	7.952E-01	6.631E-01	5.891E-01
8.00	8.279E-01	6.966E-01	6.203E-01
9.00	8.540E-01	7.245E-01	6.467E-01
10.00	8.751E-01	7.483E-01	6.693E-01
12.00	9.069E-01	7.865E-01	7.064E-01
14.00	9.291E-01	8.159E-01	7.356E-01
16.00	9.452E-01	8.393E-01	7.593E-01
18.00	9.571E-01	8.583E-01	7.791E-01
20.00	9.661E-01	8.741E-01	7.958E-01
40.00	9.955E-01	9.502E-01	8.854E-01
60.00	9.992E-01	9.754E-01	9.230E-01
80.00	9.998E-01	9.866E-01	9.440E-01
100.00	9.999E-01	9.922E-01	9.574E-01

TABLE I

TRANSMISSION VERSUS TIME IN UNITS OF THE INFLECTION TIME
FOR SEVERAL VALUES OF THE INFLECTION TIME PARAMETER P

REDUCED TIME		TRANSMISSION	
T/TI	P= 50.00	100.0	1000.
.10	4.559E-08	4.445E-08	4.333E-08
.20	1.137E-04	1.106E-04	1.078E-04
.30	1.658E-03	1.612E-03	1.570E-03
.40	6.539E-03	6.354E-03	6.188E-03
.50	1.516E-02	1.473E-02	1.434E-02
.60	2.687E-02	2.611E-02	2.542E-02
.70	4.075E-02	3.959E-02	3.854E-02
.80	5.600E-02	5.439E-02	5.296E-02
.90	7.200E-02	6.993E-02	6.809E-02
1.00	8.831E-02	8.577E-02	8.351E-02
1.10	1.046E-01	1.016E-01	9.894E-02
1.20	1.207E-01	1.172E-01	1.141E-01
1.30	1.365E-01	1.326E-01	1.291E-01
1.40	1.519E-01	1.475E-01	1.436E-01
1.50	1.668E-01	1.620E-01	1.577E-01
1.60	1.812E-01	1.760E-01	1.714E-01
1.70	1.952E-01	1.895E-01	1.845E-01
1.80	2.086E-01	2.026E-01	1.972E-01
1.90	2.215E-01	2.152E-01	2.095E-01
2.00	2.340E-01	2.273E-01	2.213E-01
3.00	3.365E-01	3.268E-01	3.182E-01
4.00	4.098E-01	3.981E-01	3.876E-01
5.00	4.649E-01	4.517E-01	4.398E-01
6.00	5.083E-01	4.938E-01	4.809E-01
7.00	5.434E-01	5.280E-01	5.142E-01
8.00	5.725E-01	5.564E-01	5.419E-01
9.00	5.973E-01	5.805E-01	5.653E-01
10.00	6.186E-01	6.013E-01	5.856E-01
12.00	6.536E-01	6.354E-01	6.189E-01
14.00	6.814E-01	6.625E-01	6.453E-01
16.00	7.041E-01	6.847E-01	6.669E-01
18.00	7.231E-01	7.033E-01	6.851E-01
20.00	7.393E-01	7.192E-01	7.006E-01
40.00	8.288E-01	8.071E-01	7.865E-01
60.00	8.688E-01	8.468E-01	8.255E-01
80.00	8.927E-01	8.707E-01	8.489E-01
100.00	9.088E-01	8.870E-01	8.650E-01

TABLE II

CORRESPONDING VALUES OF THE INFLECTION TIME PARAMETER, THE
TRANSMISSION AT THE INFLECTION TIME, AND THE SLOPE OF THE
TRANSMISSION AT THE INFLECTION TIME.

Inflection–Time Parameter p	Transmission at Inflection Time T_i	Slope of Transmission at the Inflection Time $(\partial T/\partial T_i)_i$
1.0000	0.5000	∞
1.0001		48.86
1.0005		21.85
1.001	0.4897	15.45
1.005	0.4769	6.910
1.01	0.4674	4.886
1.05	0.4277	2.185
1.1	0.3988	1.544
1.15	0.3772	1.260
1.5	0.2913	0.6868
2	0.2323	0.4939
3	0.1782	0.3462
5	0.1378	0.2594
10	0.1094	0.2035
20	0.09607	0.1781
50	0.08831	0.1636
100	0.08577	0.1588
1000	0.08351	0.1546
∞	0.08326	0.1544

TABLE III

TRANSMISSION OF ONE MOLE PERCENT OF CARBON DIOXIDE IN AIR AT A TEMPERATURE OF 530°R THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 650 GRAMS OF 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS VERSUS TIME WITH THE MASS FLOW RATE AS A PARAMETER

Transmission, T	Time, t (minutes)				
	Mass Flow Rate, Q (pounds air/minute)				
	0.154	0.308	0.463	0.616	0.720
0.0	10	3.0	1.4	---	1.1
0.1	15.7	5.6	2.4	2.2	1.5
0.2	21.7	7.5	3.9	2.8	2.2
0.3	27.1	11.1	6.1	4.2	3.3
0.4	32.9	14.2	7.8	5.6	4.6
0.5	38.3	17.5	10.0	8.0	6.4
0.6	44.0	21.9	13.3	11.1	8.9
0.7	52.3	27.8	18.3	15.6	12.3
0.8	60.0	35.1	25.6	21.1	17.0
0.9	70.0	45.5	38.6	33.3	26.8

TABLE IV

TRANSMISSION OF ONE MOLE PERCENT OF CARBON DIOXIDE IN AIR AT A TEMPERATURE OF 400°R THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 650 GRAMS OF 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS VERSUS TIME WITH THE MASS FLOW RATE AS A PARAMETER

Transmission, T	Time, t (minutes)				
	Mass Flow Rate, Q (pounds air/minute)				
	0.154	0.308	0.463	0.616	0.720
0.1	72.5	24.6	15.0	10.0	5.8
0.2	85.0	30.8	18.3	12.5	8.8
0.3	92.5	35.2	21.7	15.0	11.8
0.4	99.2	42.1	25.0	18.8	14.2
0.5	103.9	47.5	27.5	21.4	17.5
0.6	112.3	53.5	33.3	25.8	22.1
0.7	115.8	60.0	39.5	32.2	28.8
0.8	122.1	71.7	50.0	41.0	35.8
0.9	136.2	87.9	64.2	53.4	41.2

TABLE V

TRANSMISSION OF ONE MOLE PERCENT OF CARBON DIOXIDE IN AIR AT A MASS FLOW RATE OF 0.154 POUNDS PER MINUTE THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 650 GRAMS OF 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS VERSUS TIME WITH THE AIR TEMPERATURE AS A PARAMETER

Transmission, T	Time, t (minutes)				
	Air Temperature, θ (°R)				
	350	400	450	500	530
0.1	86	72.5	56.0	34.2	15.7
0.2	95	85.0	63.5	41.2	21.8
0.3	104	92.5	68.0	46.0	27.1
0.4	114	99.2	73.5	51.0	32.9
0.5	121	103.9	77.6	58.0	38.3
0.6	131	112.3	86.0	66.0	44.0
0.7	140	115.8	91.8	74.0	52.3
0.8	150	122.1	100.0	82.5	60.0
0.9	162	136.2	112.0	96.0	70.0

TABLE VI

TRANSMISSION OF ONE MOLE PERCENT OF CARBON DIOXIDE IN AIR AT A MASS FLOW RATE OF 0.308 POUNDS PER MINUTE THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 650 GRAMS OF 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS VERSUS TIME WITH THE AIR TEMPERATURE AS A PARAMETER

Transmission, T	Time, t (minutes)				
	Air Temperature, θ (°R)				
	350	400	450	500	530
0.0	25.8	17.5	9.2	4.2	3.0
0.1	33.4	24.6	15.4	7.9	5.6
0.2	38.4	30.8	21.8	13.8	7.5
0.3	43.3	35.2	28.5	17.9	11.1
0.4	48.6	42.1	34.2	21.8	14.2
0.5	54.7	47.5	40.0	26.2	17.5
0.6	61.8	53.5	46.8	30.0	21.9
0.7	69.0	60.0	55.9	37.0	27.8
0.8	80.0	71.7	70.0	42.0	35.1
0.9	91.7	87.9	100.0	48.5	45.5

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TABLE VII

TRANSMISSION OF ONE MOLE PERCENT OF CARBON DIOXIDE IN AIR AT A MASS
FLOW RATE OF 0.308 POUNDS PER MINUTE THROUGH 3.55 INCH DIAMETER
ADSORBER BEDS, 18 INCHES LONG, PACKED WITH 1850 GRAMS OF 1/8 INCH
TYPE 5A MOLECULAR SIEVE PELLETS VERSUS TIME WITH THE AIR
TEMPERATURE AS A PARAMETER

Transmission, T	Time, t (minutes)	
	Air Temperature, θ (°R)	
	450	530
0.1	113.2	33.3
0.2	117.2	40.7
0.3	124.0	50.0
0.4	128.0	57.3
0.5	134.0	64.3
0.6	138.8	72.7
0.7	144.8	82.7
0.8	157.2	97.7
0.9	166.7	126.7

TABLE VIII

LEAST-SQUARES VALUES AND STANDARD DEVIATIONS OF THE DISPERSIVITY, THE EFFECTIVE ADSORPTIVITY, AND THE ADSORPTIVITY DEDUCED FROM THE CHRISTENSEN (1962) DATA FOR THE TRANSMISSION OF ONE MOLE PERCENT CARBON DIOXIDE IN AIR AT VARIOUS TEMPERATURES THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS.

Run	Data Identification				Theoretical Parameters Obtained by Least-Squares Analysis[i]		
	Mass Flow Rate Q (lbs. air/min)	Temperature Θ (°R)	(°K)	Superficial Flow Velocity u (cm/sec)	Dispersivity D (cm²/sec)	Effective Adsorptivity B	Adsorptivity[ii] K (cc/gm)
1	0.154	350	194.4	10.1	5.57 ± .99	4976 ± 73	7463 ± 110
2	0.308	350	194.4	20.3	29.7 ± 5.4	4781 ± 131	7170 ± 200
3	0.154	400	222.2	12.0	4.74 ± .98	5043 ± 61	7563 ± 92
4	0.308	400	222.2	23.0	47.9 ± 9.4	4823 ± 164	7233 ± 247
5	0.463	400	222.2	34.5	99.3 ± 20.2	4681 ± 217	7020 ± 325
6	0.616	400	222.2	46.0	196 ± 40	5065 ± 291	7596 ± 436
7	0.720	400	222.2	54.5	342 ± 76	5242 ± 367	7862 ± 550
8	0.154	450	250.0	13.0	7.77 ± 1.41	4189 ± 68	6282 ± 101
9	0.308	450	250.0	25.9	111 ± 25	5138 ± 298	7706 ± 447
10	0.308	500	277.8	28.8	107.5 ± 25.8	3514 ± 169	5270 ± 253
11	0.154	530	294.4	15.25	46.2 ± 9.6	2660 ± 109	3988 ± 164
12	0.308	530	294.4	30.5	229 ± 53	3000 ± 239	4500 ± 358
13	0.463	530	294.4	45.75	644 ± 183	3349 ± 449	5022 ± 673
14	0.616	530	294.4	61.0	1092 ± 304	3891 ± 595	5836 ± 892

(i) Standard deviations are based on assumed uncertainties of 0.1 in the transmission

(ii) Based on an adsorber bulk density $\rho = 0.666$ gm/cc

TABLE IX

LEAST-SQUARES VALUES AND STANDARD DEVIATIONS OF THE DISPERSIVITY, THE EFFECTIVE ADSORPTIVITY AND THE ADSORPTIVITY DEDUCED FROM THE CHRISTENSEN (1962) DATA FOR THE TRANSMISSION OF ONE MOLE PERCENT CARBON DIOXIDE IN AIR AT VARIOUS TEMPERATURES THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 18 INCHES LONG, PACKED WITH 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS.

Data Identification					Theoretical Parameters Obtained by Least-Squares Analysis[i]		
Run	Mass Flow Rate Q (lbs. air/min)	Temperature Θ (°R)	(°K)	Superficial Flow Velocity u (cm/sec)	Dispersivity D (cm²/sec)	Effective Adsorptivity B	Adsorptivity[ii] K (cc/gm)
15	0.308	450	250.0	25.9	15.1 ± 2.8	4624 ± 420	6935 ± 630
16	0.308	530	294.4	30.5	197 ± 41	2920 ± 105	4379 ± 157

(i) Standard deviations are based on assumed uncertainties of 0.1 in the transmission

(ii) Based on an adsorber bulk density $\rho = 0.666$ gm/cc

TABLE X

LEAST-SQUARES VALUES AND STANDARD DEVIATIONS OF THE INFLECTION TIME PARAMETER AND THE INFLECTION TIME DEDUCED FROM THE CHRISTENSEN (1962) DATA FOR THE TRANSMISSION OF ONE MOLE PERCENT CARBON DIOXIDE IN AIR AT VARIOUS TEMPERATURES THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS.

Run	Data Identification				Theoretical Parameters Obtained by Least-Squares Analysis[i]	
	Mass Flow Rate Q (lbs. air/min)	Temperature Θ (°R)	(°K)	Superficial Flow Velocity u (cm/sec)	Inflection Time Parameter p	Inflection Time t_i (min)
1	0.154	350	194.4	10.1	$1.114 \pm .004$	112.2 ± 1.7
2	0.308	350	194.4	20.3	$1.33 \pm .01$	45.2 ± 1.3
3	0.154	400	222.2	12.0	$1.081 \pm .003$	98.4 ± 1.2
4	0.308	400	222.2	23.0	$1.49 \pm .02$	35.7 ± 1.3
5	0.463	400	222.2	34.5	$1.72 \pm .03$	20.1 ± 1.0
6	0.616	400	222.2	46.0	$2.14 \pm .05$	$13.0 \pm .8$
7	0.720	400	222.2	54.5	$2.82 \pm .08$	$8.64 \pm .65$
8	0.154	450	250.0	13.0	$1.125 \pm .004$	73.0 ± 1.2
9	0.308	450	250.0	25.9	$2.15 \pm .05$	23.4 ± 1.5
10	0.308	500	277.8	28.8	$1.97 \pm .05$	$15.7 \pm .8$
11	0.154	530	294.4	15.25	$1.76 \pm .03$	25.2 ± 1.1
12	0.308	530	294.4	30.5	$3.27 \pm .11$	$7.65 \pm .66$
13	0.463	530	294.4	45.75	$5.72 \pm .25$	$3.25 \pm .46$
14	0.616	530	294.4	61.0	$7.19 \pm .32$	$2.26 \pm .36$

(i) Standard deviations are based on assumed uncertainties of 0.1 in the transmission

(ii) Based on an adsorber bulk density $\rho = 0.666$ gm/cc

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TABLE XI

LEAST-SQUARES VALUES AND STANDARD DEVIATIONS OF THE INFLECTION TIME PARAMETER AND THE INFLECTION TIME DEDUCED FROM THE CHRISTENSEN (1962) DATA FOR THE TRANSMISSION OF ONE MOLE PER CENT CARBON DIOXIDE IN AIR AT VARIOUS TEMPERATURES THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 18 INCHES LONG, PACKED WITH 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS.

Data Identification					Theoretical Parameters Obtained by Least-Squares Analysis [i]	
Run	Mass Flow Rate Q_e (lbs. air/min)	Temperature Θ (°R)	(°K)	Superficial Flow Velocity u (cm/sec)	Inflection Time Parameter p	Inflection [ii] Time t_i (min)
15	0.308	450	250.0	25.9	1.039 ± .001	130.9 ± 1.2
16	0.308	530	294.4	30.5	1.51 ± .02	48.3 ± 1.8

(i)   Standard deviations are based on assumed uncertainties of 0.1 in the transmission

(ii) Based on an adsorber bulk density $\rho = 0.666$ gm/cc

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TABLE XII

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUES OF THE TRANSMISSION OF ONE MOLE PERCENT OF CARBON DIOXIDE IN AIR AT A PRESSURE OF ONE ATMOSPHERE AND A TEMPERATURE OF 530° R THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 650 GRAMS OF 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS WITH MASS FLOW RATE AS A PARAMETER

Experimental Transmission	Theoretical Transmission			
	Mass Flow Rate , Q (pounds air/minute)			
	0.154	0.308	0.463	0.616
0.1	.066	.083	.065	.117
0.2	.181	.163	.179	.172
0.3	.297	.311	.324	.293
0.4	.419	.418	.412	.395
0.5	.521	.514	.505	.515
0.6	.611	.613	.603	.618
0.7	.715	.709	.704	.714
0.8	.787	.790	.794	.789
0.9	.854	.864	.880	.897

TABLE XIII

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUES OF THE TRANSMISSION OF ONE MOLE PERCENT OF CARBON DIOXIDE IN AIR AT A PRESSURE OF ONE ATMOSPHERE AND A TEMPERATURE OF 400° R THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 650 GRAMS OF 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS WITH MASS FLOW RATE AS A PARAMETER

Experimental Transmission	Theoretical Transmission				
	Mass Flow Rate , Q (pounds air/minute)				
	0.154	0.308	0.463	0.616	0.720
0.1	.055	.095	.122	.118	.073
0.2	.189	.200	.212	.203	.190
0.3	.306	.284	.307	.289	.315
0.4	.421	.416	.398	.410	.399
0.5	.503	.511	.463	.484	.501
0.6	.638	.604	.592	.591	.611
0.7	.688	.688	.699	.706	.725
0.8	.765	.800	.822	.813	.806
0.9	.887	.895	.913	.898	.849

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TABLE XIV

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUE OF THE TRANSMISSION OF ONE MOLE PERCENT OF CARBON DIOXIDE IN AIR AT A MASS FLOW RATE OF 0.154 POUNDS PER MINUTE THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 650 GRAMS OF 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS WITH THE AIR TEMPERATURE AS A PARAMETER

Experimental Transmission	Theoretical Transmission			
	Air Temperature, Θ ($^\circ$R)			
	350	400	450	530
.1	.102	.055	.106	.066
.2	.186	.189	.215	.181
.3	.282	.306	.294	.297
.4	.415	.421	.397	.419
.5	.504	.503	.474	.521
.6	.621	.638	.619	.611
.7	.711	.688	.705	.715
.8	.793	.765	.802	.787
.9	.866	.887	.896	.854

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TABLE XV

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUE OF THE TRANSMISSION OF ONE MOLE PERCENT OF CARBON DIOXIDE IN AIR AT A MASS FLOW RATE OF 0.308 POUNDS PER MINUTE THROUGH 3.55 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 650 GRAMS OF 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS WITH THE AIR TEMPERATURE AS A PARAMETER

Experimental Transmission	Theoretical Transmission				
	Air Temperature, θ (°R)				
	350	400	450	500	530
.1	.118	.095	.075	.029	.083
.2	.199	.200	.189	.176	.163
.3	.290	.284	.317	.304	.311
.4	.388	.416	.417	.418	.418
.5	.497	.511	.506	.530	.514
.6	.610	.604	.594	.609	.613
.7	.704	.688	.688	.723	.709
.8	.811	.800	.791	.783	.790
.9	.886	.895	.907	.842	.864

TABLE XVI

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUE OF THE TRANSMISSION OF ONE MOLE
PERCENT OF CARBON DIOXIDE IN AIR AT A MASS FLOW RATE OF 0.308 POUNDS PER MINUTE
THROUGH 3.55 INCH DIAMETER ADSORBED BEDS, 18 INCHES LONG, PACKED WITH 1850 GRAMS OF
1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS WITH THE AIR TEMPERATURE AS A PARAMETER

Experimental Transmission	Theoretical Transmission	
	Air Temperature, Θ (°R)	
	450	530
.1	.141	.094
.2	.196	.184
.3	.308	.313
.4	.381	.413
.5	.495	.502
.6	.582	.597
.7	.682	.690
.8	.839	.794
.9	.913	.909

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TABLE XVII

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUES OF THE TRANSMISSION OF 0.64 MOLE PERCENT OF CARBON DIOXIDE IN DRY AIR AT A PRESSURE OF ONE ATMOSPHERE AND A TEMPERATURE OF 75° F THROUGH 0.85 INCH DIAMETER ADSORBER BEDS, 6 INCHES LONG, PACKED WITH 1/16 INCH TYPE 5A MOLECULAR SIEVE PELLETS WITH THE SUPERFICIAL FLOW VELOCITY AS A PARAMETER

Time (Min)	Run 19F $u = 51.8$ cm/sec Transmission		Run 23F $u = 38.9$ cm/sec Transmission	
	Experimental	Theoretical	Experimental	Theoretical
2	.03	.004	.03	.010
4	.15	.109	.10	.077
6	.31	.304	.22	.205
8	.48	.491	.36	.355
10	.60	.638	.47	.496
12	.73	.745	.60	.615
14	.82	.821	.70	.711
16	.87	.874	.79	.785
18	.94	.911	.84	.841
20	.97	.938	.88	.883
22	1.00	.956	.92	.914
24			.95	.937
26			.98	.954
28			1.00	.966
30				

TABLE XVIII

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUES OF THE TRANSMISSION OF 0.64 MOLE PERCENT OF CARBON DIOXIDE IN DRY AIR AT A PRESSURE OF ONE ATMOSPHERE AND A TEMPERATURE OF 75°F THROUGH 0.85 INCH DIAMETER ADSORBED BEDS, 8 INCHES LONG, PACKED WITH 1/16 INCH TYPE 5A MOLECULAR SIEVE PELLETS WITH THE SUPERFICIAL FLOW VELOCITY AS A PARAMETER

Time (Min)	Run 1F $u = 45.6$ cm/sec Transmission Experimental	Theoretical	Run 9F $u = 38.9$ cm/sec Transmission Experimental	Theoretical
2				
4	.02	.002	.02	.004
6	.06	.028	.04	.032
8	.13	.103	.11	.102
10	.24	.218	.22	.210
12	.34	.349	.33	.336
14	.45	.473	.45	.462
16	.56	.583	.58	.577
18	.66	.675	.68	.675
20	.75	.750	.75	.754
22	.81	.809	.81	.816
24	.86	.855	.85	.864
26	.90	.890	.89	.901
28	.93	.917	.93	.928
30	.96	.937	.97	.948
32				
33	1.0	.959		
34			.98	.962
35			1.0	.968

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TABLE XIX

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUES OF THE TRANSMISSION OF 0.64 MOLE PERCENT OF CARBON DIOXIDE IN DRY AIR AT A PRESSURE OF ONE ATMOSPHERE AND A TEMPERATURE OF 75° F THROUGH 0.85 INCH DIAMETER ADSORBED BEDS, 3 INCHES LONG, PACKED WITH 1/16 INCH TYPE 5A MOLECULAR SIEVE PELLETS WITH THE SUPERFICIAL FLOW VELOCITY AS A PARAMETER

Time (Min)	Run 29F $u = 68.5$ cm/sec Transmission		Run 39F $u = 31.9$ cm/sec Transmission	
	Experimental	Theoretical	Experimental	Theoretical
2	.44	.410	.03	
4	.64	.683	.27	
6	.78	.809	.42	
8	.88	.878	.56	
10	.94	.918	.68	
12	1.0	.944	.76	
14			.84	
16			.89	
18			.92	
20			.95	
22			.985	
23			1.0	

TABLE XX

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUES OF THE TRANSMISSION OF 0.64 MOLE PERCENT OF CARBION DIOXIDE IN DRY AIR AT A PRESSURE OF ONE ATMOSPHERE AND A TEMPERATURE OF 75° F THROUGH 2.3 INCH DIAMETER ADSORBED BEDS, 6 INCHES LONG, PACKED WITH 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS WITH THE SUPERFICIAL FLOW VELOCITY AS A PARAMETER

Time (Min)	Run 5A u = 31.3 cm/sec Transmission Experimental	Run 5A u = 31.3 cm/sec Transmission Theoretical	Run 6A u = 45.6 cm/sec Transmission Experimental	Run 6A u = 45.6 cm/sec Transmission Theoretical
2	.13	.036	.22	.134
4	.23	.173	.38	.338
6	.33	.302	.48	.474
8	.42	.405	.53	.568
10	.47	.487	.60	.636
12	.53	.552	.64	.688
14	.57	.605	.69	.729
16	.60	.649	.72	.762
18	.64	.686	.75	.789
20	.67	.717	.78	.812
22	.70	.744	.81	.831
24	.74	.767	.83	.847
26	.77	.788	.86	.861
28	.80	.806	.88	.874
30	.83	.821	.90	.885
32	.85	.836	.92	.894
34	.87	.848	.94	.903
36	.88	.860	.96	.910
38	.90	.870	.98	.917
40	.92	.879	.99	.923
42	.93	.887	1.00	.929
44	.95	.895		
.				
.				
.				
54	1.00	.925		

TABLE XXI

COMPARISON OF THEORETICAL AND EXPERIMENTAL VALUES OF THE
TRANSMISSION OF 0.64 MOLE PERCENT OF CARBON DIOXIDE IN DRY
AIR AT A PRESSURE OF ONE ATMOSPHERE AND A TEMPERATURE OF
75° F THROUGH 2.3 INCH DIAMETER ADSORBED BEDS, 3 INCHES LONG,
PACKED WITH 1/8 INCH TYPE 5 A MOLECULAR SIEVE PELLETS WITH
THE SUPERFICIAL FLOW VELOCITY AS A PARAMETER

Time (Min)	Run 10AA u = 51.2 cm/sec Transmission Experimental	Theoretical	Run 11AA u = 31.3 cm/sec Transmission Experimental	Theoretical
2	.55	.526	.28	.245
4	.67	.675	.47	.457
6	.74	.746	.56	.578
8	.78	.790	.64	.656
10	.81	.819	.69	.711
12	.83	.841	.73	.753
14	.84	.858	.77	.785
16	.85	.872	.80	.810
18	.87	.883	.82	.831
20	.88	.893	.85	.849
22	.90	.901	.87	.864
24	.91	.908	.88	.876
26	.92	.914	.89	.887
28	.93	.919	.90	.897
30	.94	.924	.91	.905
32			.92	.913
34			.93	.919
35	1.00	.934		
36			.94	.925
38				
40				
42			1.00	.934

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TABLE XXII

CONVERSION OF THE MASS FLOW RATE TO THE VOLUMETRIC FLOW RATE
AND TO THE SUPERFICIAL VELOCITY OF DRY AIR AT A TEMPERATURE OF
75°F FOR THE FOX (1966) DATA

Run	Mass Flow Rate Q (lbs/hr)	Volumetric Flow Rate q		Superficial Flow Velocity u	
		(cc/sec)	(cu. ft/min)	(cm/sec)	(ft/min)
5A	7.92	838.7	1.777	31.3	61.7
6A	11.52	1220	2.585	45.6	89.8
10AA	12.95	1371	2.906	51.2	101
11AA	7.92	838.7	1.777	31.3	61.7
19F	1.77	187.4	.3972	51.8	102
23F	1.33	140.8	.2985	38.9	76.5
29F	2.34	247.8	.5251	68.5	135
39F	1.09	115.4	.2446	31.9	62.7
1F	1.56	165.2	.3501	45.6	89.8
9F	1.33	140.8	.2985	38.9	76.5

(i) The density of dry air ($A = 28.966$) at 75°F (= 296.7°K) is $\rho\,(\theta = 75°F) = 1.190$ 1.190×10^{-3} gm/cc; therefore, q (cc/sec) = 105.9 Q (lbs/hr) and q (cu. ft/min) = 0.2244 Q (lb/hr)

(ii) The cross-sectional area of the adsorber bed $A = 0.0288$ ft^2 (= 26.76 cm^2) for runs 5A, 6A, 10AA and 11AA; and $A = 0.0039$ ft^2 (= 3.62 cm^2) for runs 19F, 23F, 29F, 39F, 1F and 9F

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TABLE XXIII

LEAST-SQUARES VALUES AND STANDARD DEVIATIONS OF THE DISPERSIVITY, THE EFFECTIVE ADSORPTIVITY AND THE ADSORPTIVITY DEDUCED FROM THE FOX (1966) DATA FOR THE TRANSMISSION OF 0.64 MOLE PERCENT CARBON DIOXIDE IN AIR AT A TEMPERATURE OF 75° F THROUGH 0.85 INCH DIAMETER ADSORBER BEDS PACKED WITH 1/16 INCH TYPE 5A MOLECULAR SIEVE PELLETS.

Data Identification				Theoretical Parameters Obtained by Least-Squares Analysis[i]		
Run	Superficial Flow Velocity u (cm/sec)	Length of Bed ℓ (in)	(cm)	Dispersivity D (cm²/sec)	Effective Adsorptivity B	Adsorptivity[ii] K (cc/g)
19F	51.8	6	15.25	153 29	1965 ± 70	2949 ± 106
23F	38.9	6	15.25	79.0 13.0	2035 ± 55	3055 ± 84
29F	68.5	3	7.62	327 95	2109 ± 186	3165 ± 280
1F	45.6	8	20.3	111 17	2121 ± 51	3182 ± 78
9F	38.9	8	20.3	66.6 10.0	2011 ± 42	3017 ± 63

(i)   Standard deviations are based on assumed uncertainties of 0.1 in the transmission.

(ii)   Based on an adsorber bulk density ρ = 0.666 gm/cc.

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TABLE XXIV

LEAST-SQUARES VALUES AND STANDARD DEVIATIONS OF THE INFLECTION TIME PARAMETER AND THE INFLECTION TIME DEDUCED FROM THE FOX (1966) FOR THE TRANSMISSION OF 0.64 MOLE PER CENT CARBON DIOXIDE IN AIR AT A TEMPERATURE OF 75° F THROUGH 3.55 INCH DIAMETER ABSORBER BEDS PACKED WITH 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS.

Data Identification				Theoretical Parameters Obtained by Least-Squares Analysis (i)	
Run	Superficial Flow Velocity u (cm/sec)	Length of Bed ℓ (in)	(cm)	Inflection Time Parameter p	Inflection (ii) Time t_i (sec)
19F	51.8	6	15.25	$1.74 \pm .03$	333 ± 13
23F	38.9	6	15.25	$1.49 \pm .02$	550 ± 16
29F	68.5	3	7.62	$4.11 \pm .17$	58.7 ± 5.8
1F	45.6	8	20.3	$1.43 \pm .01$	679 ± 18
9F	38.9	8	20.3	$1.293 \pm .008$	838 ± 18

(i) Standard deviations are based on assumed uncertainties of 0.1 in the transmission

(ii) Based on an adsorber bulk density $\rho = 0.666$ gm/cc.

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TABLE XXV

LEAST-SQUARES VALUES AND STANDARD DEVIATIONS OF THE DISPERSIVITY, THE EFFECTIVE ADSORPTIVITY AND THE ADSORPTIVITY DEDUCED FROM THE FOX (1966) DATA FOR THE TRANSMISSION OF 0.64 MOLE PERCENT CARBON DIOXIDE IN AIR AT A TEMPERATURE OF 75°F THROUGH 2.3 INCH DIAMETER ADSORBER BEDS PACKED WITH 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS

Data Identification			Theoretical Parameters Obtained by Least-Squares Analysis[i]		
Run	Superficial Flow Velocity u (cm/sec)	Length of Bed ℓ (in) (cm)	Dispersivity D (cm²/sec)	Effective Adsorptivity B	Adsorptivity[ii] K (cc/g)
5A	31.3	6 15.25	440 ± 80	2395 ± 145	3591 ± 218
6A	45.6	6 15.25	845 ± 163	2497 ± 177	3745 ± 266
10AA	51.2	3 7.62	2048 ± 991	4222 ± 1220	6333 ± 1829
11AA	31.3	3 7.62	401.2 ± 91.0	2919 ± 293	4377 ± 440

(i)   Standard deviations are based on assumed uncertainties of 0.1 in the transmission

(ii)   Based on an adsorber bulk density $\rho = 0.666$ gm/cc

TABLE XXVI

LEAST-SQUARES VALUES AND STANDARD DEVIATIONS OF THE INFLECTION TIME PARAMETER AND THE INFLECTION TIME DEDUCED FROM THE FOX (1966) DATA FOR THE TRANSMISSION OF 0.64 MOLE PERCENT CARBON DIOXIDE IN AIR AT A TEMPERATURE OF 75°F THROUGH 2.3 INCH DIAMETER ADSORBER BEDS PACKED WITH 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS

Data Identification				Theoretical Parameters Obtained by Least-Squares Analysis[i]	
Run	Superficial Flow Velocity u (cm/sec)	Length of Bed ℓ (in) (cm)		Inflection Time Parameter p	Inflection[ii] Time t_i (sec)
5A	31.3	6	15.25	5.69 ± 0.16	204.5 ± 13.7
6A	45.6	6	15.25	7.43 ± 0.23	112.3 ± 8.7
10AA	51.2	3	7.62	31.46 ± 2.53	19.9 ± 6.0
11AA	31.3	3	7.62	10.19 ± 0.38	69.7 ± 7.5

(i) Standard deviations are based on assumed uncertainties of 0.1 in the transmission

(ii) Based on an adsorber bulk density $\rho = 0.666$ gm/cc

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TABLE XXVII

THE ADSORPTIVITY VS THE TEMPERATURE OF AIR CONTAINING ONE MOLE PER CENT CARBON
DIOXIDE FLOWING AT A RATE OF 0.308 POUNDS/MINUTE THROUGH 3.55 INCH DIAMETER
ADSORBER BEDS PACKED WITH 1/8 INCH TYPE 5A MOLECULAR SIEVE PELLETS

Temperature Θ (°K)	Adsorptivity K (cc/gm)	Christensen Run No.
194.4	7170 $\pm$ 200	2
222.2	7233 $\pm$ 247	4
250.0	7320 $\pm$ 387	9, 15
277.8	5270 $\pm$ 253	10
294.4	4440 $\pm$ 196	12, 16

TABLE XXVIII

CORRESPONDING VALUES OF THE INFLECTION TIME, THE TRANSMISSION AT THE INFLECTION TIME, AND THE INFLECTION TIME PARAMETER DEDUCED FROM THE CHRISTENSEN AND THE FOX DATA FOR THE TRANSMISSION OF CARBON DIOXIDE THROUGH MOLECULAR SIEVE ADSORBER BEDS.

Run Identification	Inflection Time t_i (min.)	Transmission at Inflection Time T_i	Inflection Time Parameter p
C14	2.25 $\pm$ .37	.1203 $\pm$ .0396	7.19 $\pm$ .32
C13	3.25 $\pm$ .47	.1305 $\pm$ .0410	5.72 $\pm$ .25
C12	7.65 $\pm$ .65	.1697 $\pm$ .0343	3.27 $\pm$ .11
C 7	8.63 $\pm$ .65	.1848 $\pm$ .0326	2.82 $\pm$ .08
C 6	13.03 $\pm$ .80	.2213 $\pm$ .0293	2.14 $\pm$ .05
C10	15.67 $\pm$ .83	.2346 $\pm$ .0337	1.97 $\pm$ .05
C 5	20.07 $\pm$ .98	.2610 $\pm$ .0272	1.72 $\pm$ .03
C 9	23.45 $\pm$ 1.48	.2208 $\pm$ .0326	2.15 $\pm$ .05
C11	25.17 $\pm$ 1.13	.2557 $\pm$ .0282	1.76 $\pm$ .03
C 4	35.67 $\pm$ 1.30	.2932 $\pm$ .0243	1.49 $\pm$ .02
C 2	45.17 $\pm$ 1.30	.3245 $\pm$ .0203	1.33 $\pm$ .01
C16	48.35 $\pm$ 1.85	.2896 $\pm$ .0258	1.51 $\pm$ .02
C 8	73.00 $\pm$ 1.20	.3874 $\pm$ .0142	1.125 $\pm$ .004
C 3	98.45 $\pm$ 1.22	.4089 $\pm$ .0134	1.081 $\pm$ .003
C 1	112.2 $\pm$ 1.68	.3921 $\pm$ .0134	1.114 $\pm$ .004
C15	130.9 $\pm$ 17.0	.4362 $\pm$ .0088	1.039 $\pm$ .001
Fox 29F	.978 $\pm$ .096	.1507 $\pm$ .0425	4.11 $\pm$ .18
19F	5.55 $\pm$ .32	.2583 $\pm$ .0259	1.74 $\pm$ .03
23F	9.17 $\pm$ .27	.2925 $\pm$ .0204	1.49 $\pm$ .02
1F	11.3 $\pm$ .3	.3032 $\pm$ .0193	1.43 $\pm$ .01
9F	14.0 $\pm$ .3	.3333 $\pm$ .0161	1.293 $\pm$ .008
Fox 10AA	.333 $\pm$ .100	.0913 $\pm$ .0642	31.5 $\pm$ 2.5
11AA	1.16 $\pm$ .12	.1090 $\pm$ .0316	10.2 $\pm$ 0.4
6A	1.87 $\pm$ .14	.1191 $\pm$ .0273	7.43 $\pm$ 0.23
5A	3.41 $\pm$ .23	.1307 $\pm$ .0263	5.69 $\pm$ 0.16

TABLE XXIX

CORRESPONDING VALUES OF THE INFLECTION TIME, THE DIMENSIONLESS DISPERSION NUMBER, AND THE PROPAGATION TIME DEDUCED FROM THE CHRISTENSEN AND THE FOX DATA FOR THE TRANSMISSION OF CARBON DIOXIDE THROUGH MOLECULAR SIEVE ADSORBED BEDS

| Run Identification	Inflection Time t_i (sec)			Dispersion Number $D_{u\ell}$			Propagation Time t_p (sec)		
C14	135	$\pm$	22	1.175	$\pm$	.327	973	$\pm$	149
C13	195	$\pm$	28	.9248	$\pm$	.2626	1116	$\pm$	150
C12	459	$\pm$	39	..4935	$\pm$	.1148	1500	$\pm$	119
C 7	518	$\pm$	39	.4115	$\pm$	.0911	1463	$\pm$	102
C 6	783	$\pm$	48	.2790	$\pm$	.0573	1675	$\pm$	96
C10	940	$\pm$	50	.2445	$\pm$	.0587	1856	$\pm$	89
C 5	1204	$\pm$	59	.1887	$\pm$	.0384	2065	$\pm$	96
C 9	1407	$\pm$	89	.2804	$\pm$	.0640	3022	$\pm$	175
C11	1510	$\pm$	68	.1989	$\pm$	.0415	2660	$\pm$	109
C 4	2140	$\pm$	78	.1362	$\pm$	.0269	3187	$\pm$	109
C 2	2710	$\pm$	78	.0963	$\pm$	.0176	3604	$\pm$	99
C 8	4380	$\pm$	72	.394	$\pm$	.0071	4928	$\pm$	80
C 3	5907	$\pm$	73	.0259	$\pm$	.0053	6303	$\pm$	77
C 1	6732	$\pm$	101	.0361	$\pm$	.0064	7502	$\pm$	110
C15	7854	$\pm$	719	.0127	$\pm$	.0024	8160	$\pm$	74
Fox									
29F	587	$\pm$	58	.644	$\pm$	.186	241	$\pm$	21
19F	333	$\pm$	13	.1938	$\pm$	.0372	578	$\pm$	21
23F	550	$\pm$	16	.1372	$\pm$	.0226	822	$\pm$	22
1F	679	$\pm$	18	.1224	$\pm$	.0197	972	$\pm$	24
9F	838	$\pm$	18	.3333	$\pm$	.0161	1083	$\pm$	23
Fox									
10AA	19.9	$\pm$	6.0	5.237	$\pm$	2.536	627	$\pm$	181
11AA	69.7	$\pm$	7.5	1.682	$\pm$	.381	710	$\pm$	71
6A	112.3	$\pm$	8.7	1.215	$\pm$	.233	834	$\pm$	59
5A	204.5	$\pm$	13.7	.9195	$\pm$	.1671	1164	$\pm$	71

APPENDIX

GRAPHS OF THE TIME-DEPENDENT TRANSMISSION OF CARBON DIOXIDE IN AIR THROUGH MOLECULAR SIEVE ADSORBER BEDS

Figure	Christensen Run Number
7	1
8	2
9	3
10	4
11	5
12	6
13	7
14	8
15	9
16	10
17	11
18	12
19	13
20	14
21	15
22	16

Figure	Fox Run Number
23	19F
24	23F
25	29F
26	1F
27	9F
28	5A
29	6A
30	10AA
31	11AA

TRANSMISSION

TIME (MINUTES)
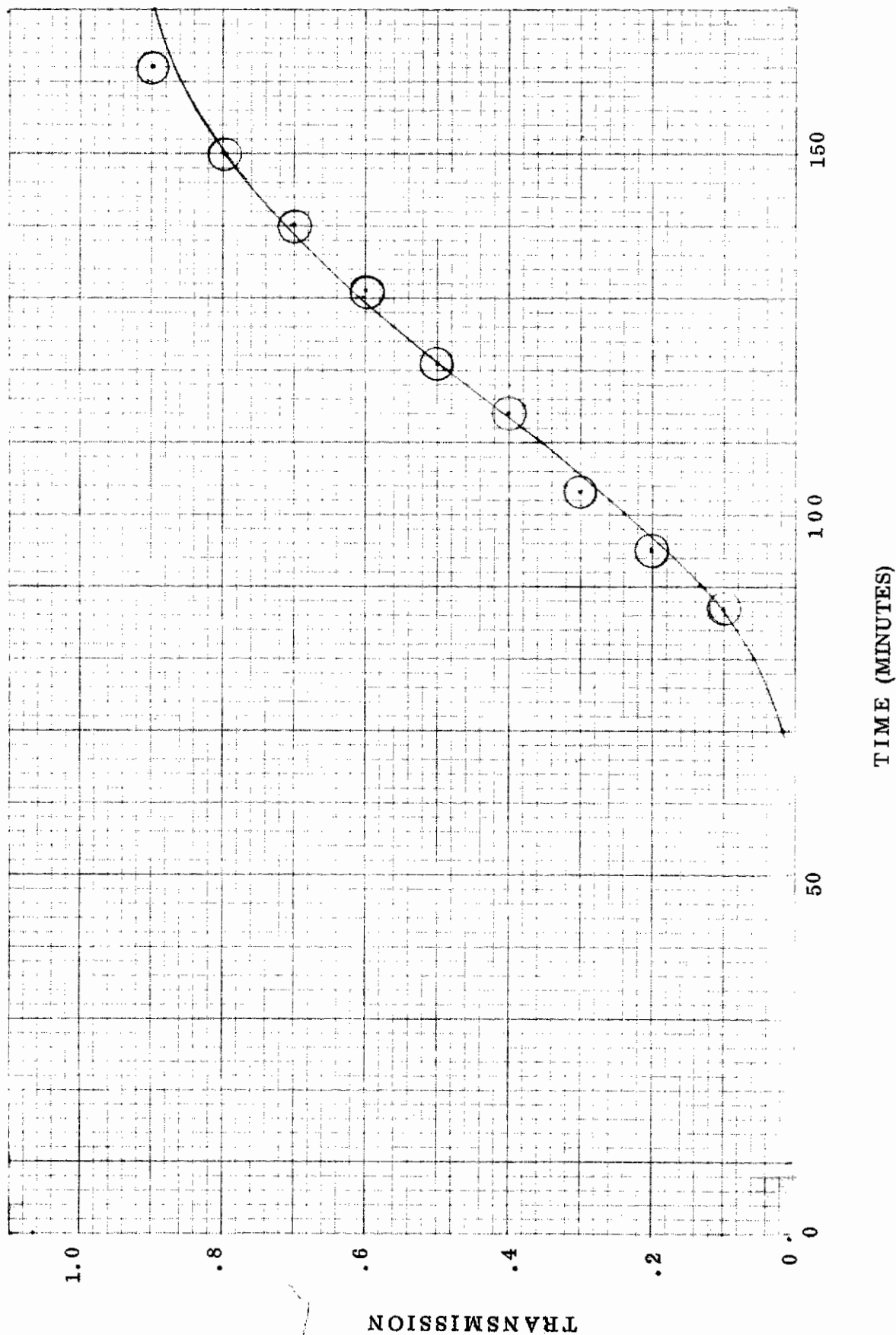
Christensen Run 1

Figure 7.

62

Christensen Run 2

TIME (MINUTES)
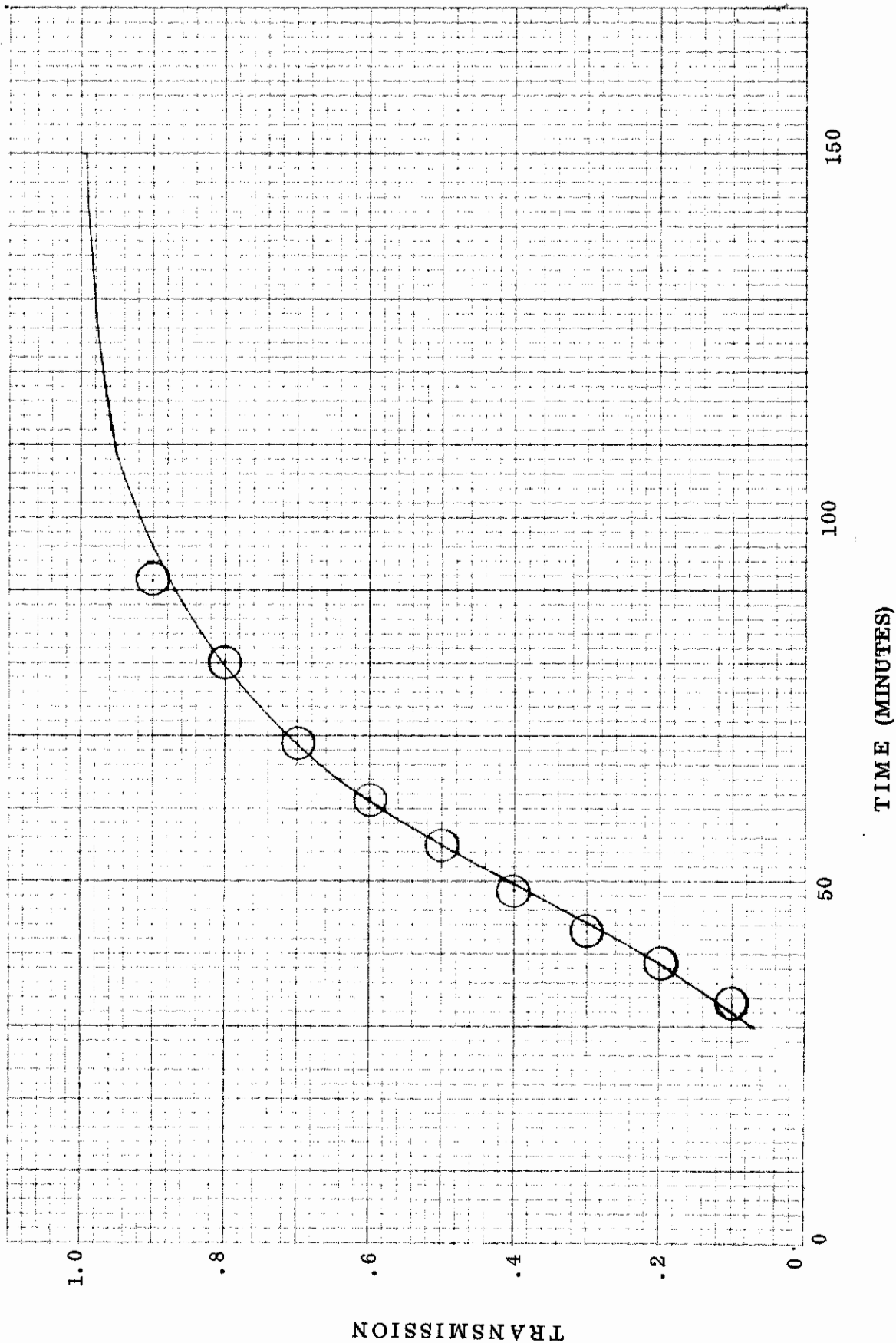
TRANSMISSION

Figure 8.

63
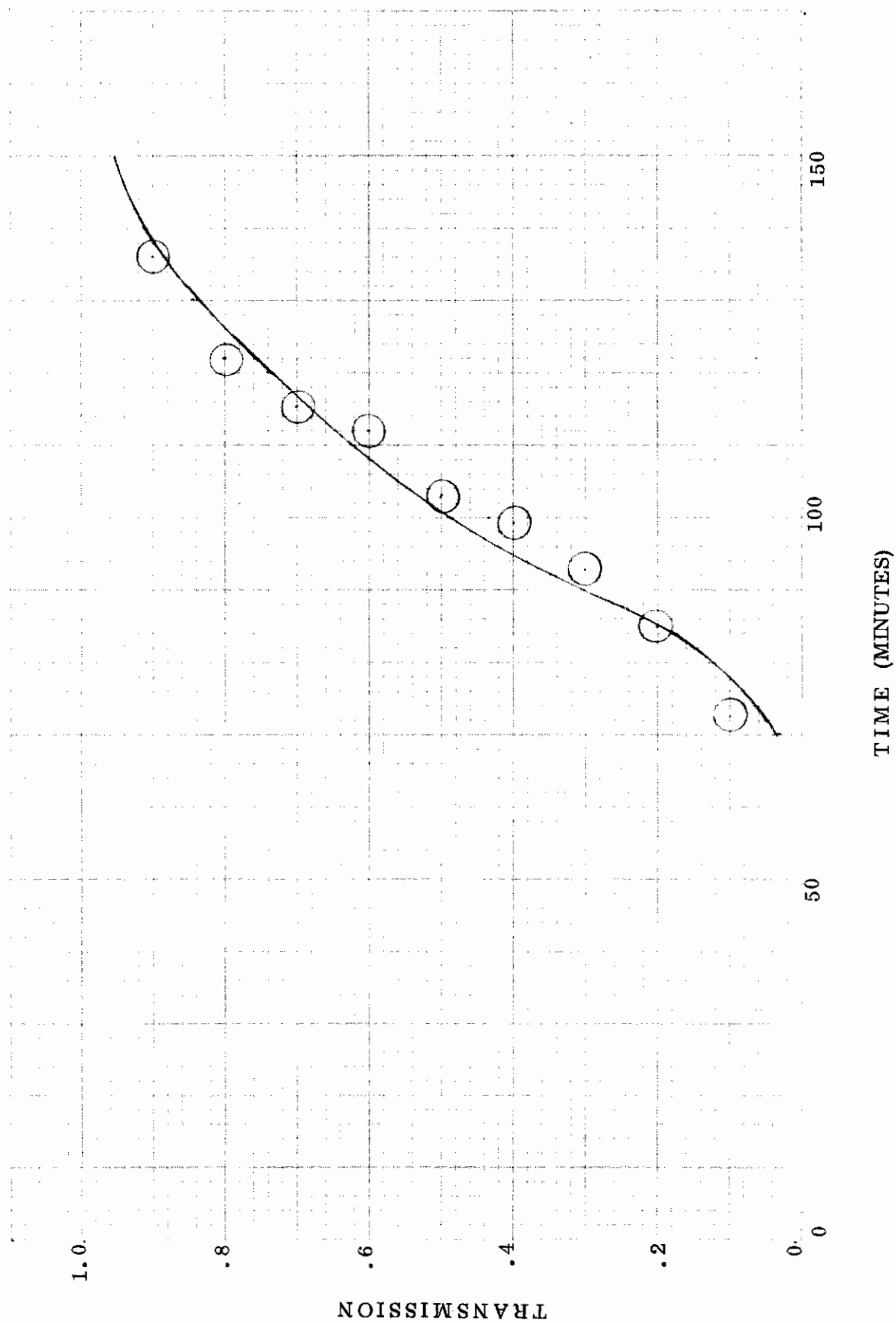
Christensen Run 3

Figure 9.

TIME (MINUTES)

TRANSMISSION

64

TRANSMISSION

TIME (MINUTES)
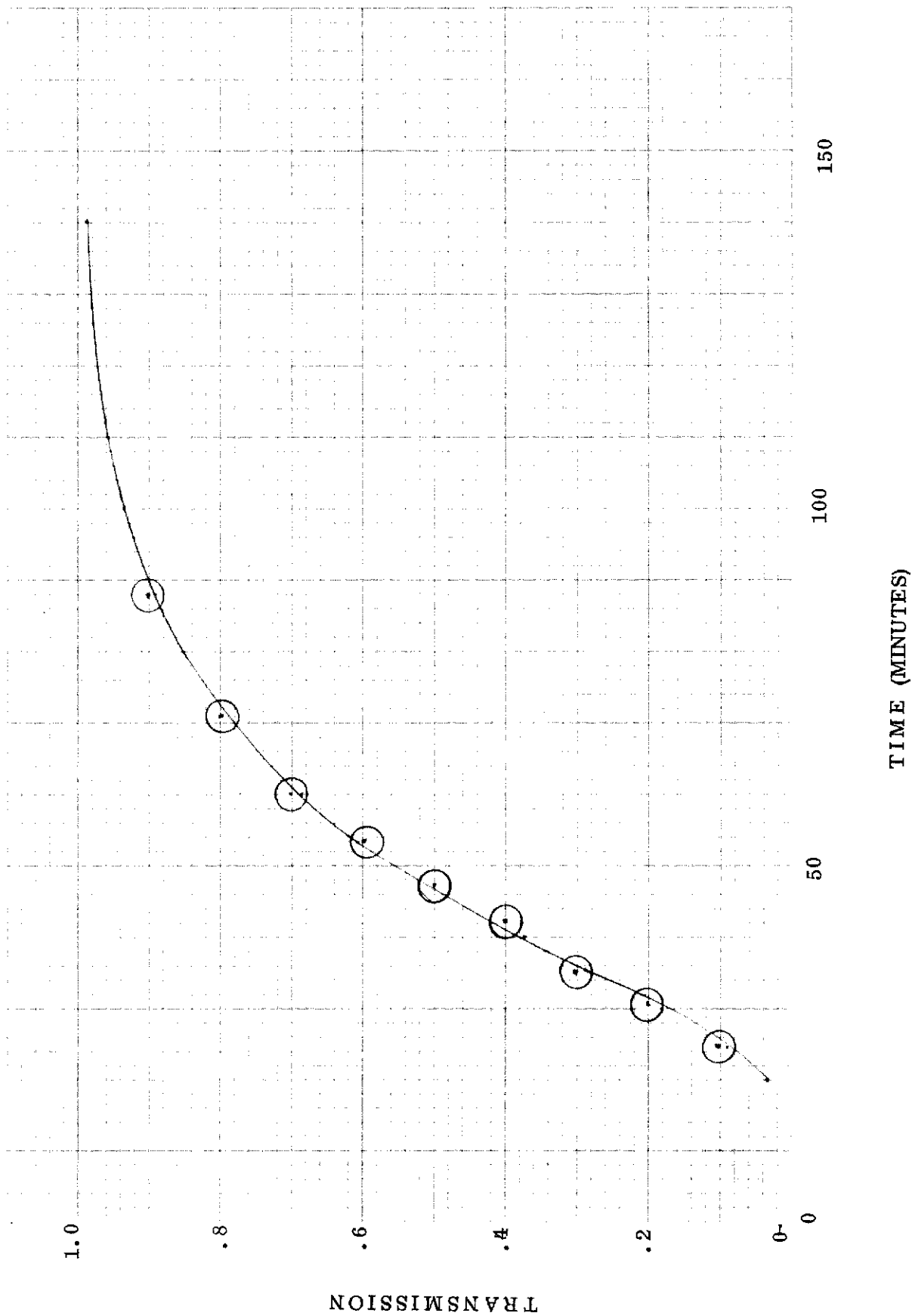
Christensen Run 4

Figure 10.

65

TIME (MINUTES)
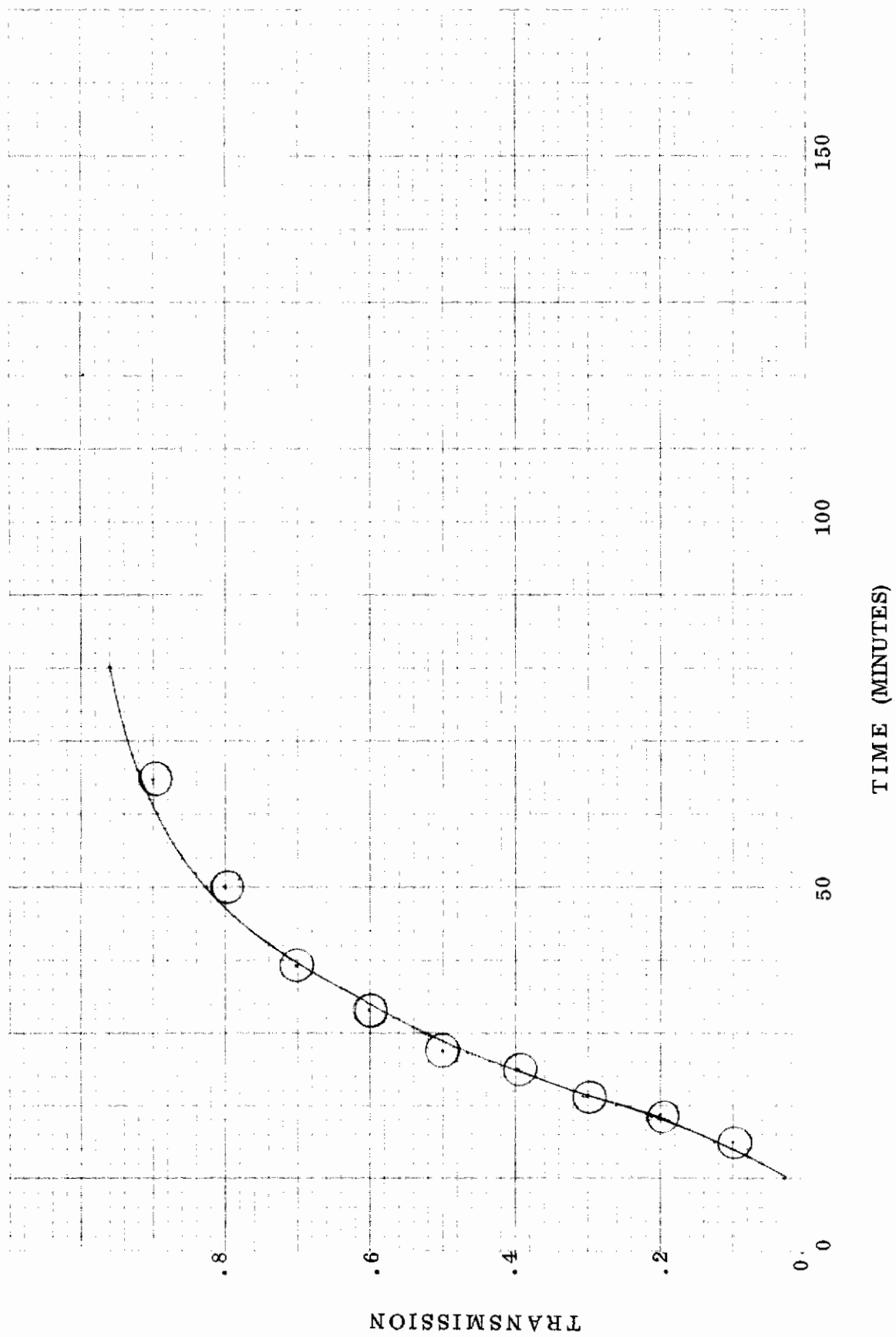
TRANSMISSION

Christensen Run 5

Figure 11.

66

TIME (MINUTES)
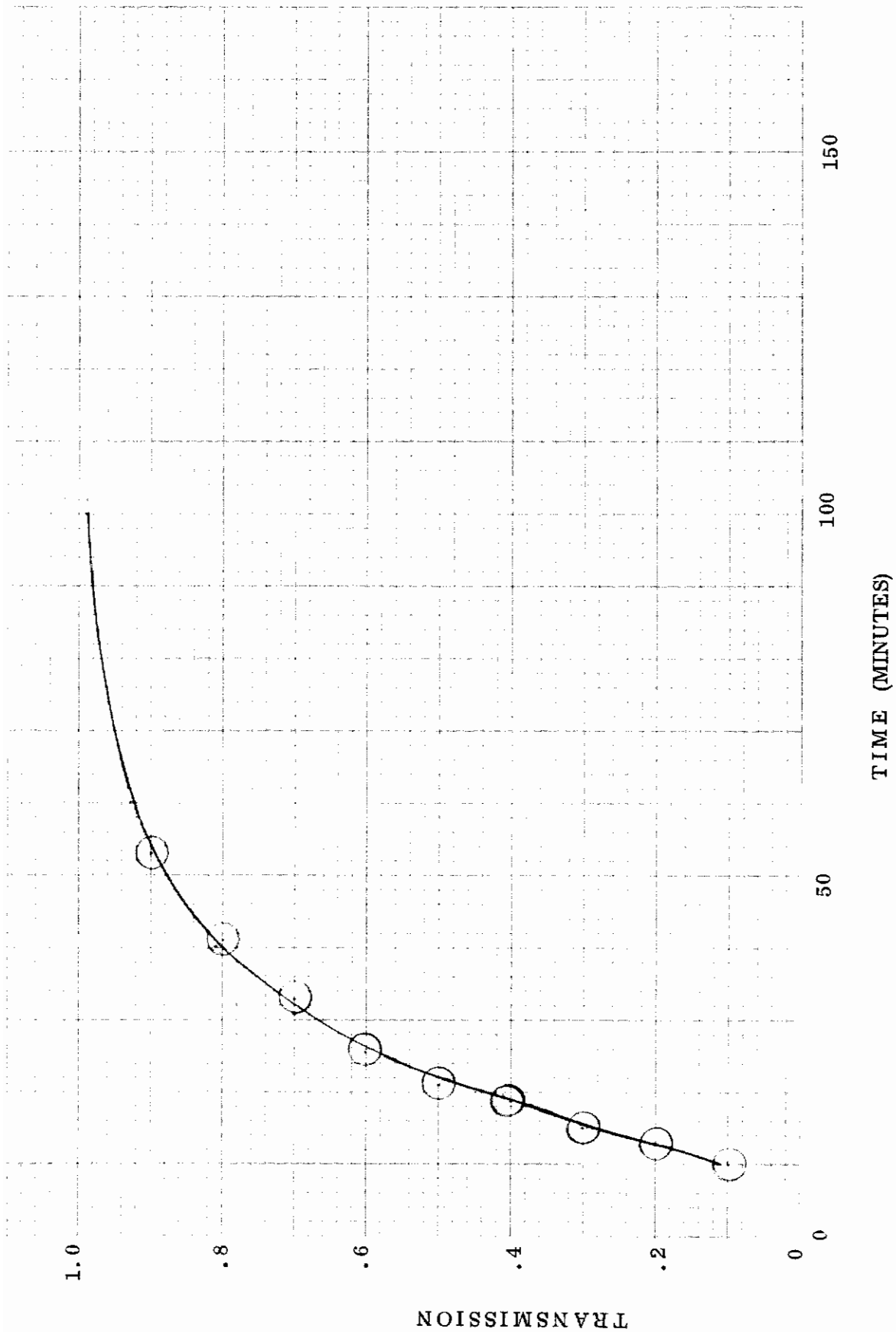
TRANSMISSION

Christensen Run 6

Figure 12.
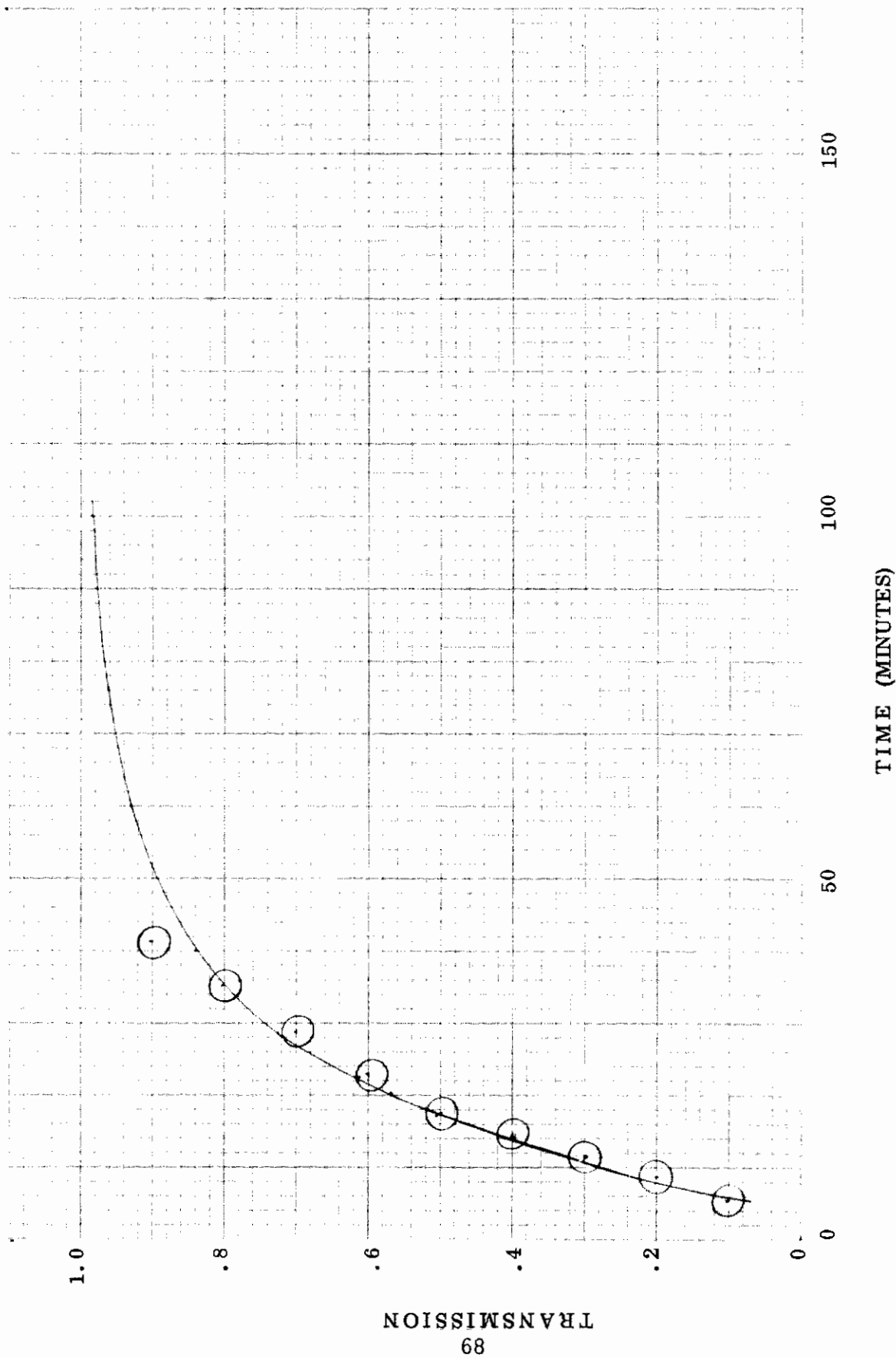
67

Figure 13.

Christensen Run 7

TIME (MINUTES)

TRANSMISSION

68
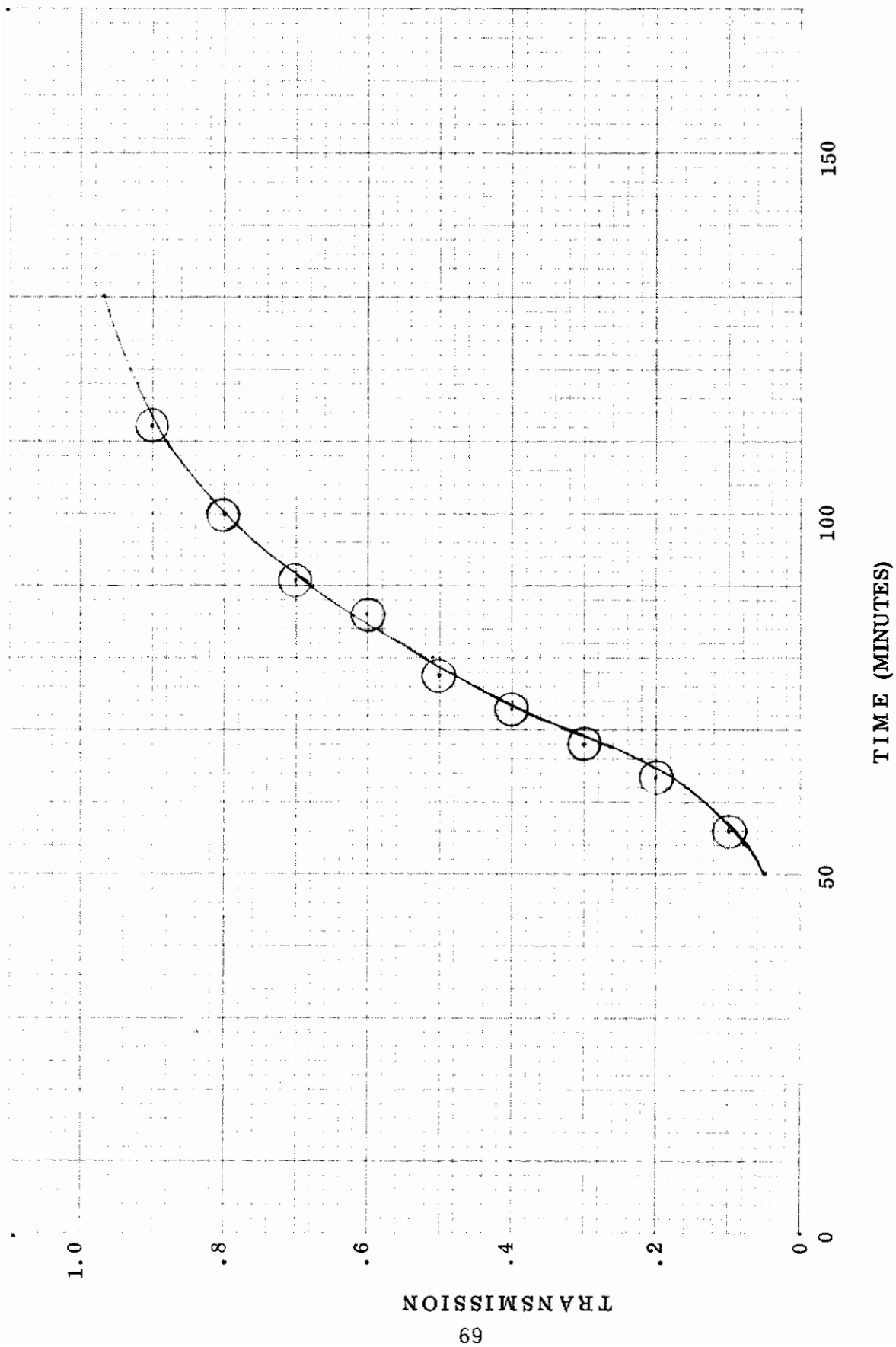
TIME (MINUTES)

Christensen Run 8

Figure 14.

TRANSMISSION

TIME (MINUTES)
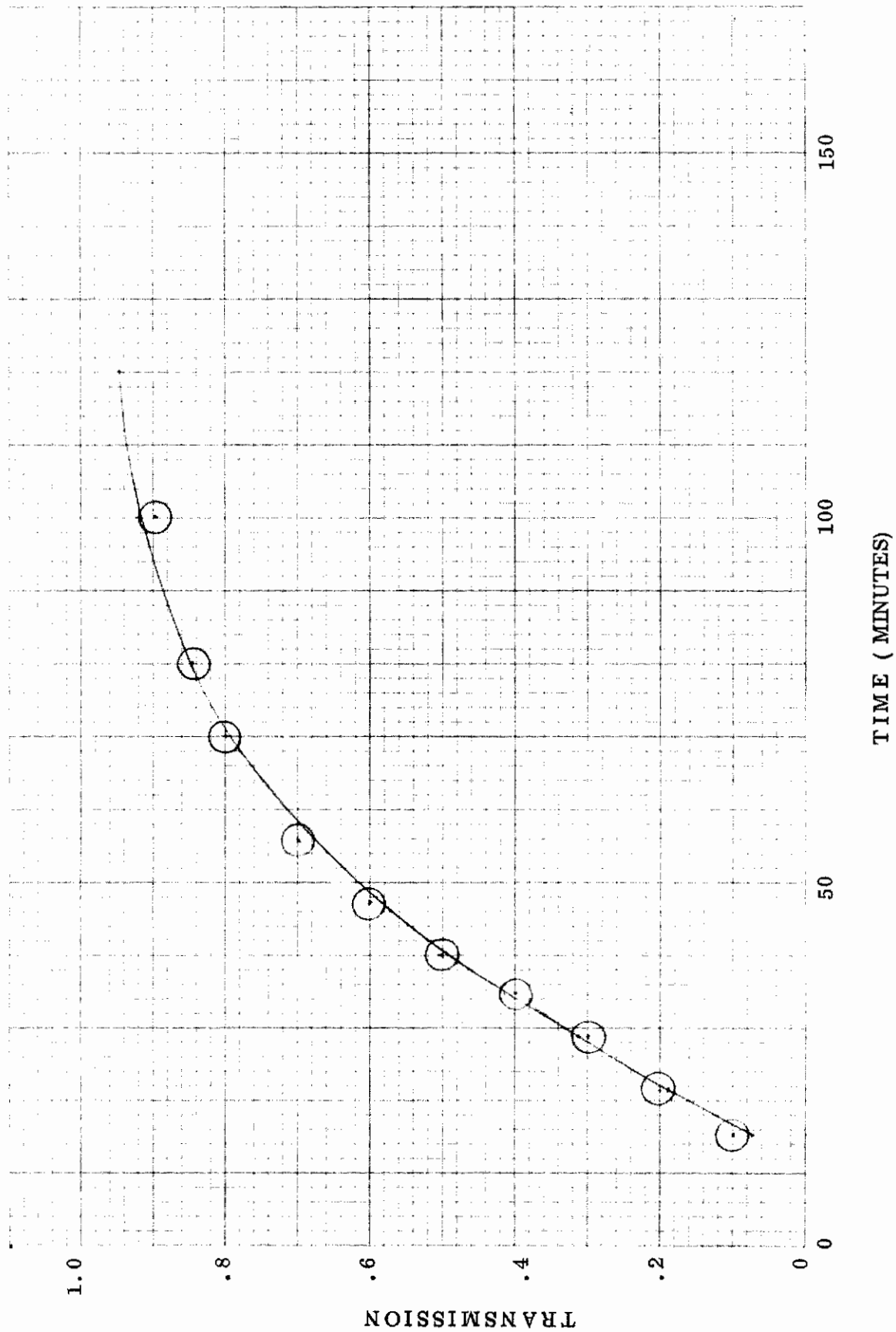
TRANSMISSION

Christensen Run 9

Figure 15.

70

Christensen Run 10

TIME (MINUTES)

TRANSMISSION

Figure 16.

71
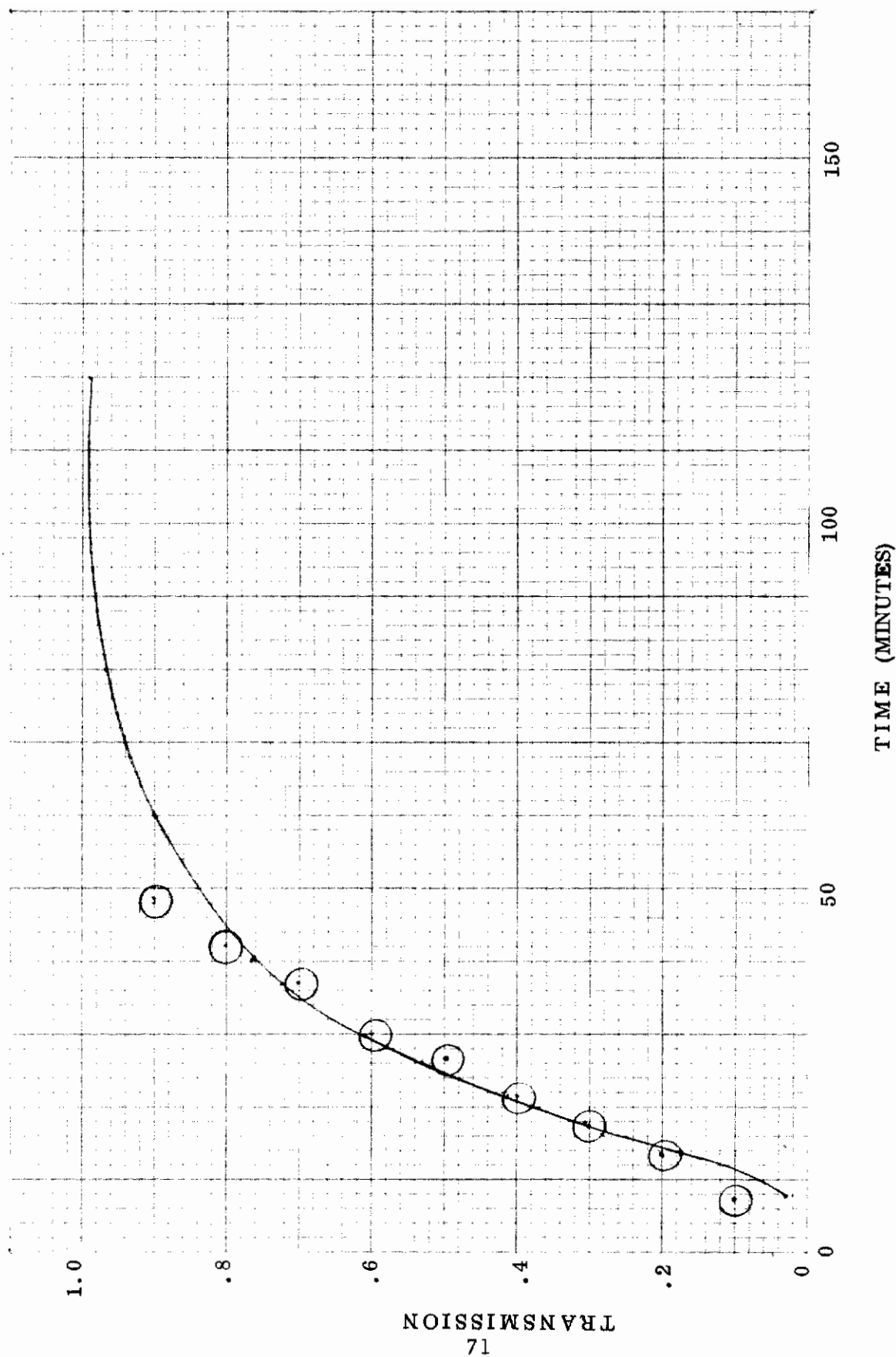
TIME (MINUTES)
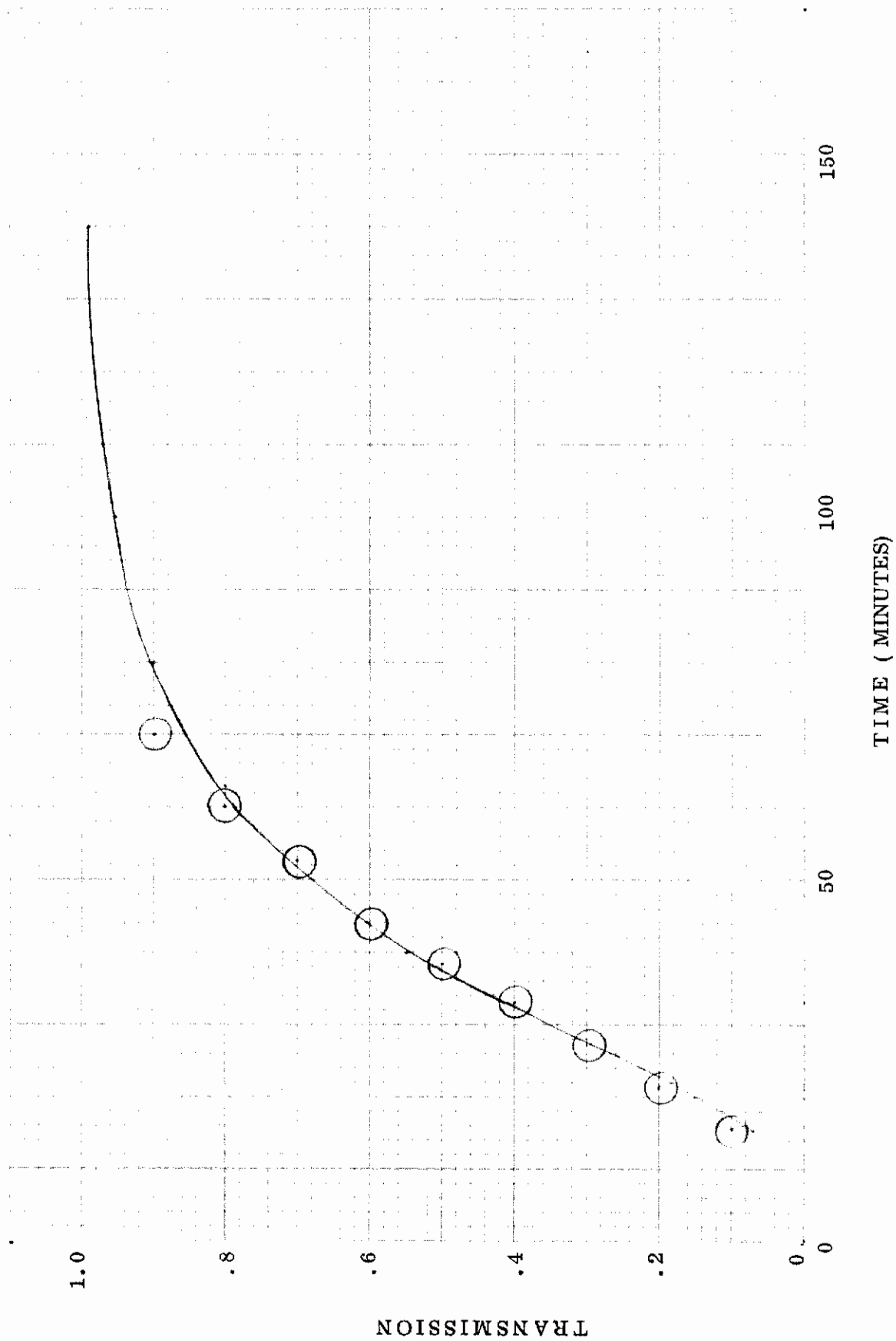
TRANSMISSION

Christensen Run 11

Figure 17.

72
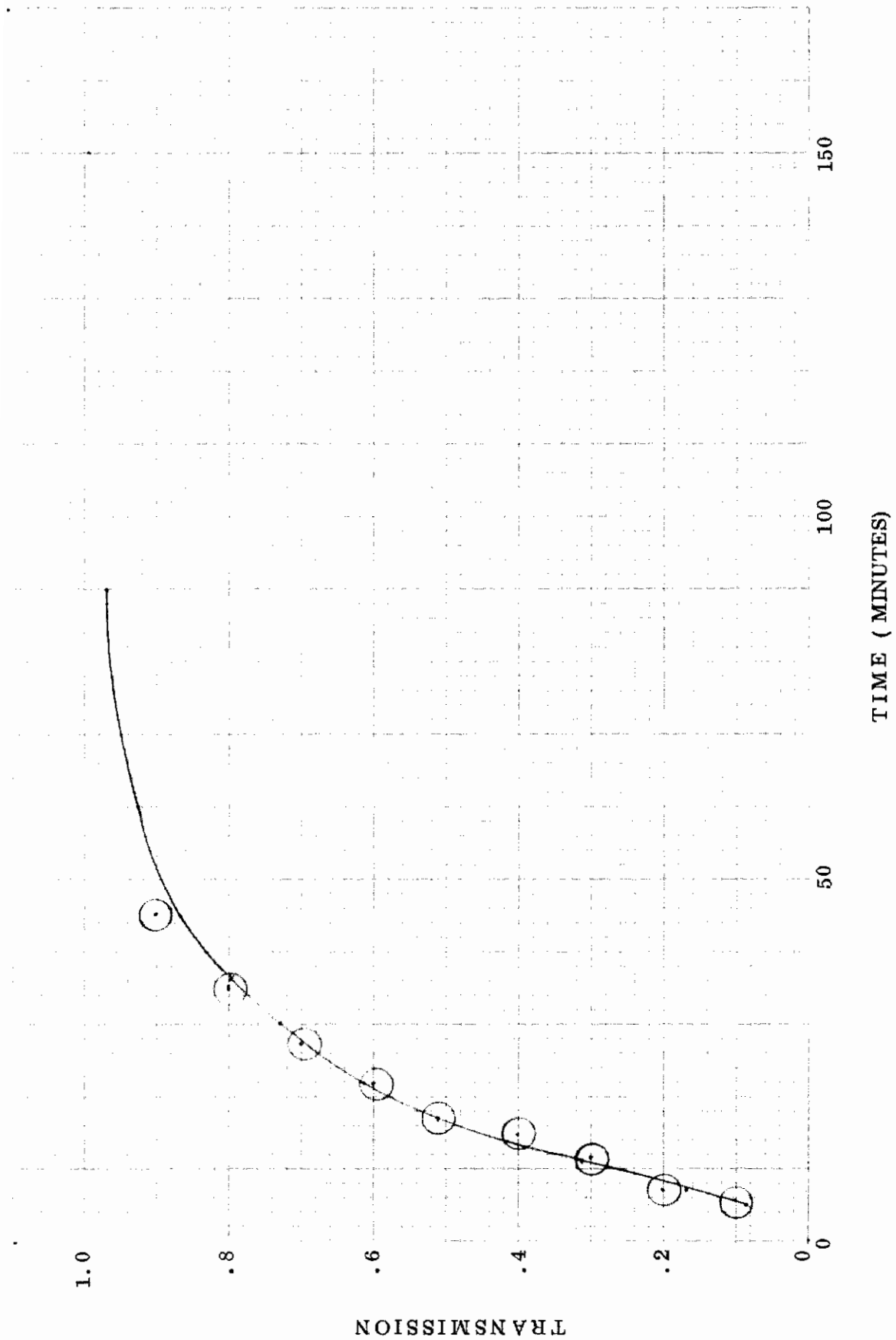
Christensen Run 12

TIME (MINUTES)

TRANSMISSION

Figure 18.

73

TIME (MINUTES)
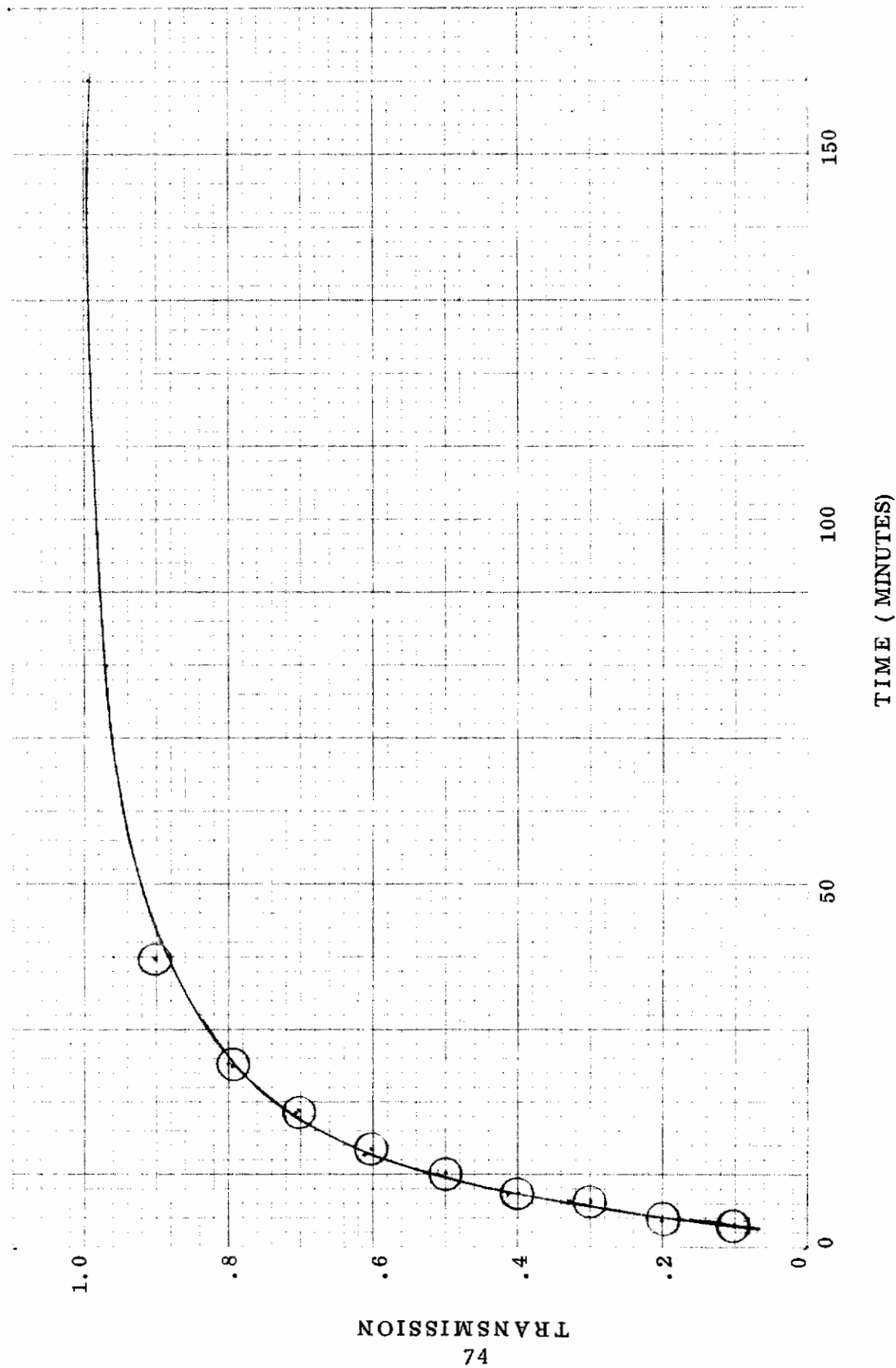
TRANSMISSION

Christensen Run 13

Figure 19.

74

Christensen Run 14

TIME (MINUTES)

TRANSMISSION

Figure 20.

75

TIME (MINUTES)
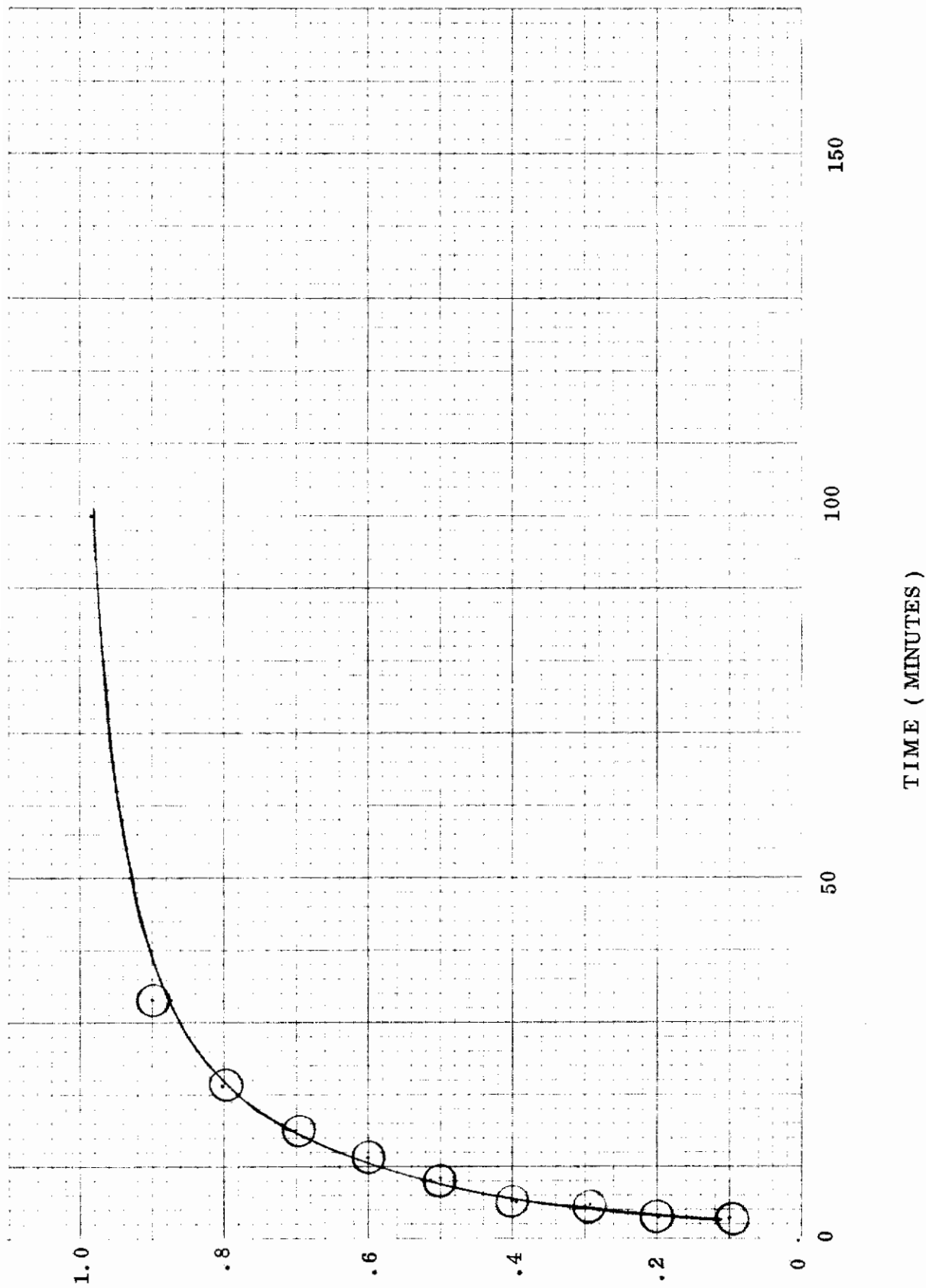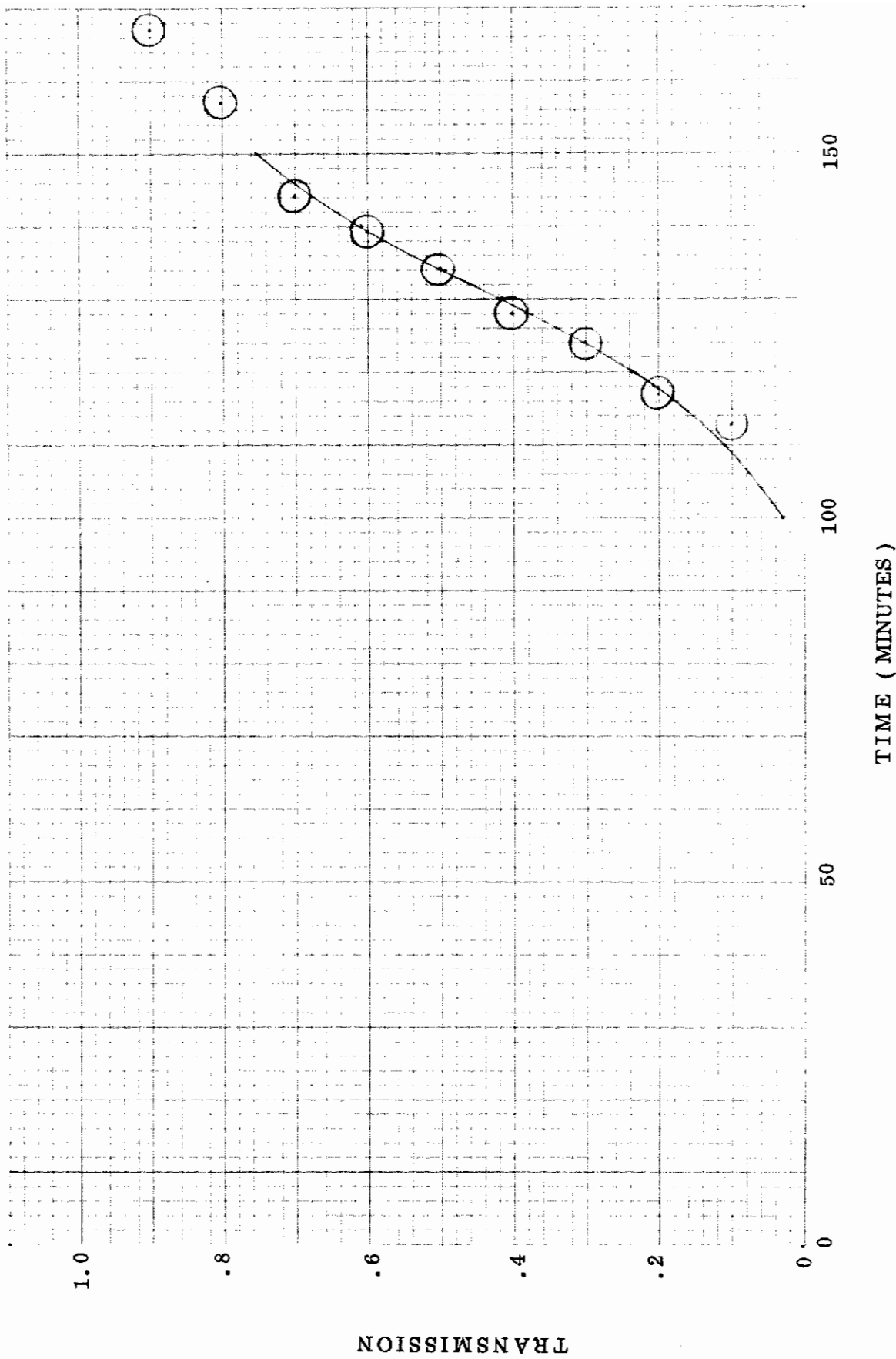
TRANSMISSION

Christensen Run 15

Figure 21.
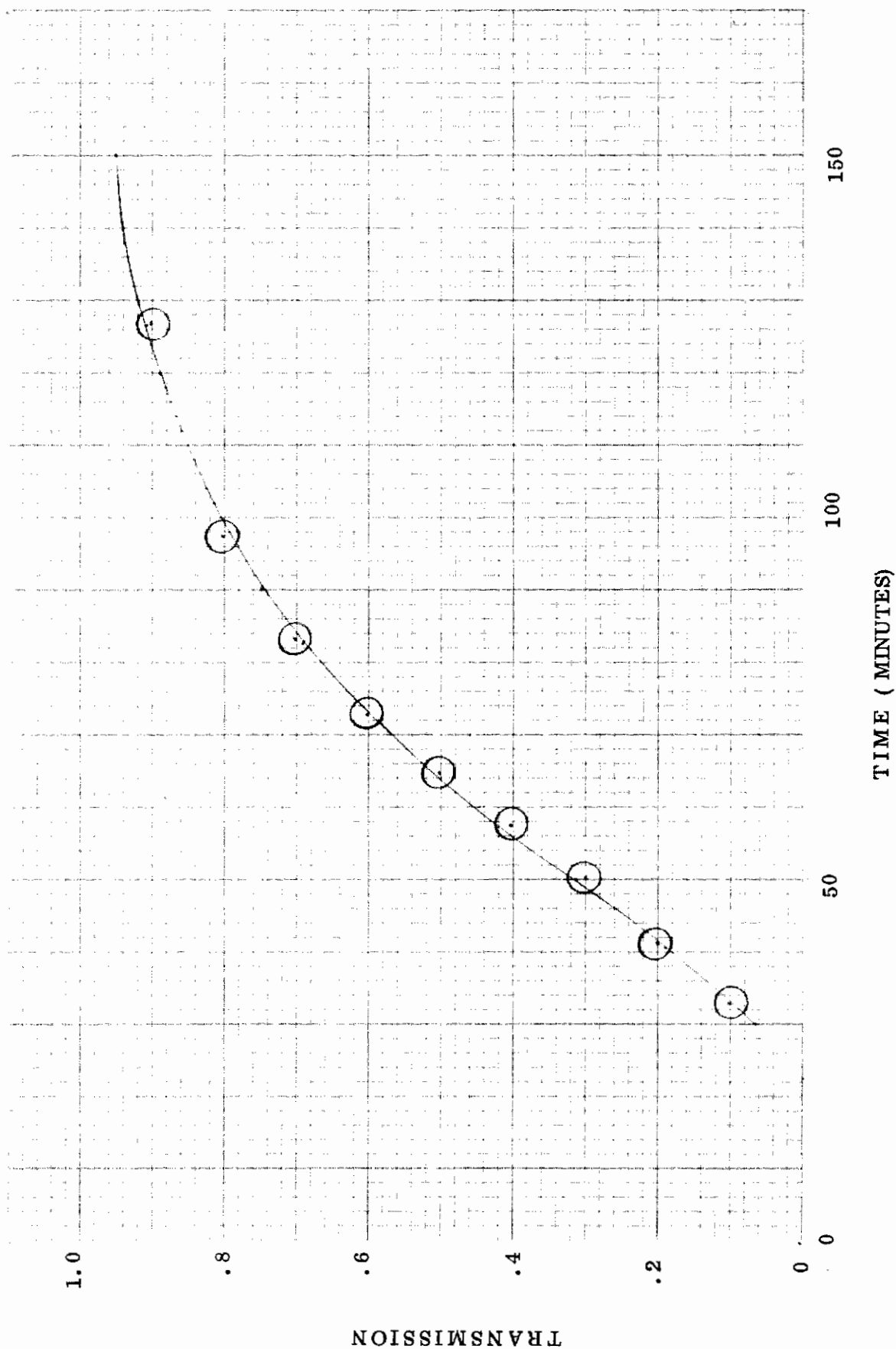
76

Figure 22.

Christensen Run 16
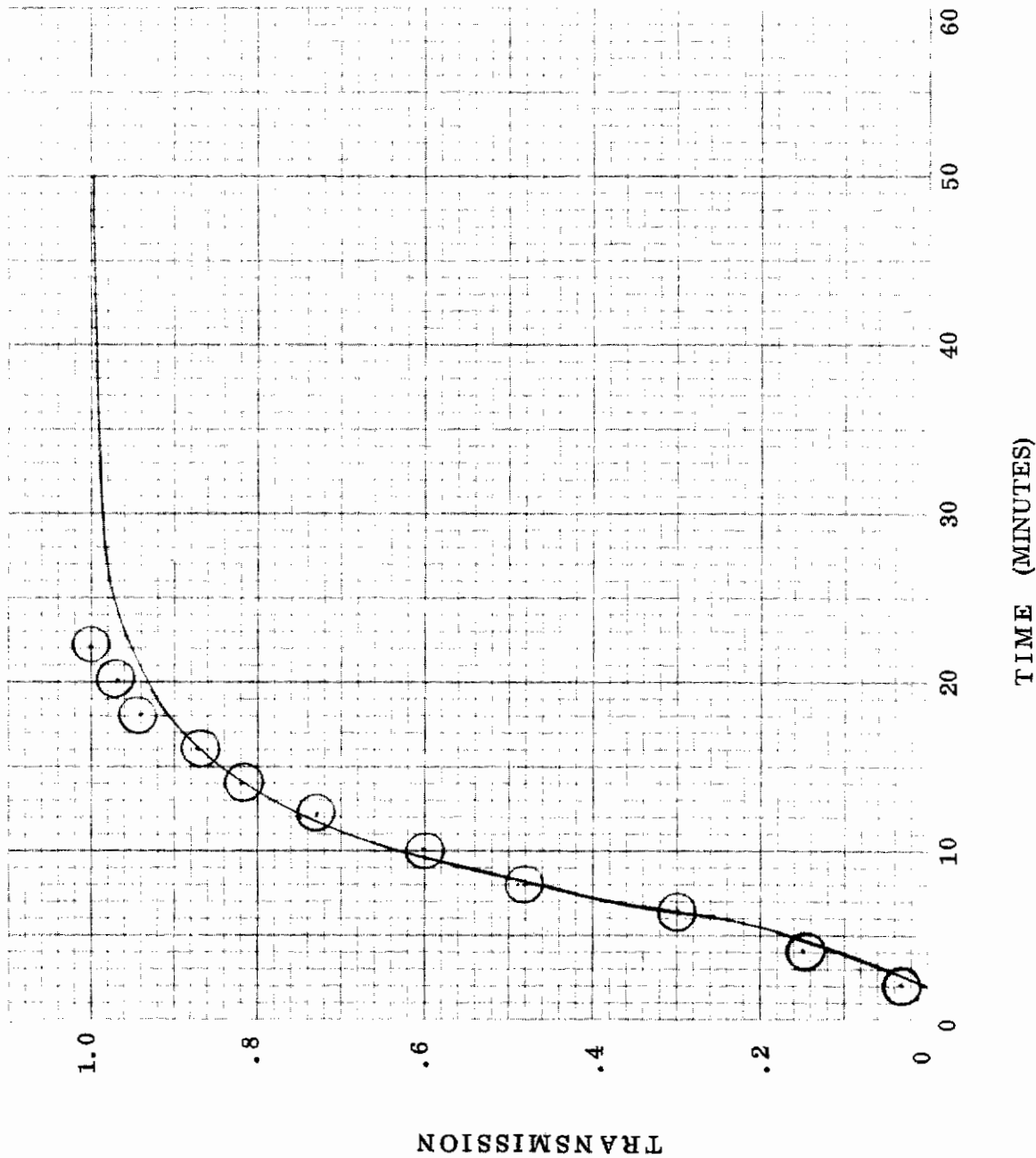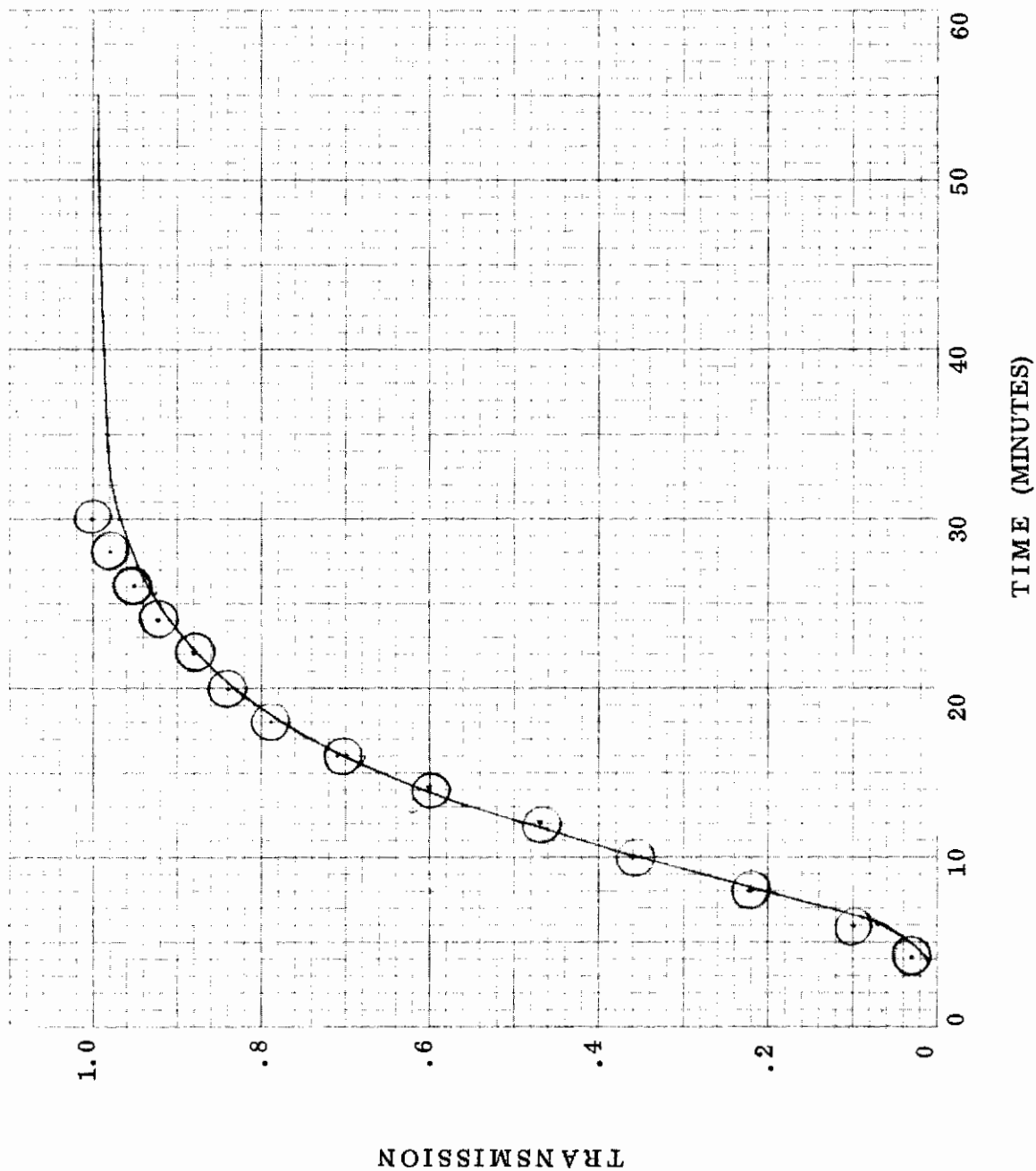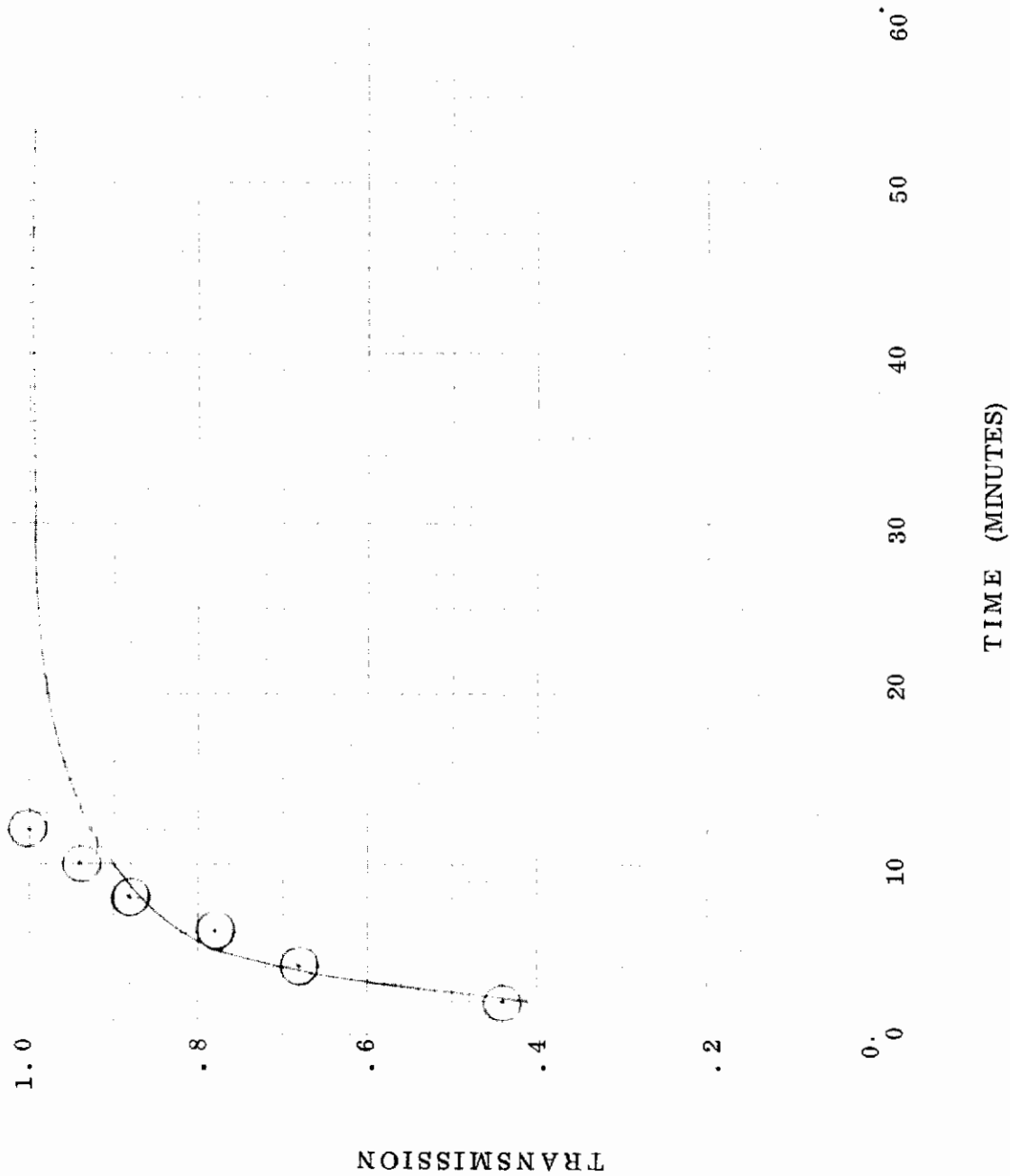
TIME (MINUTES)

TRANSMISSION

77

TRANSMISSION

TIME (MINUTES)

Fox Run 19F

Figure 23.

78

TIME (MINUTES)

TRANSMISSION

Fox Run 23F

Figure 24.

79

TIME (MINUTES)

TRANSMISSION

Fox Run 29 F

Figure 25.

80

TIME (MINUTES)

TRANSMISSION

Fox Run 1F

Figure 26.

81

Figure 27.

Fox Run 9F

82

TRANSMISSION

TIME (MINUTES)

Fox Run 5A

Figure 28.

83

TIME (MINUTES)

TRANSMISSION

Fox Run 6A

Figure 29.

84

TRANSMISSION vs TIME (MINUTES)

Figure 30.

Fox Run 10AA

TRANSMISSION

TIME (MINUTES)
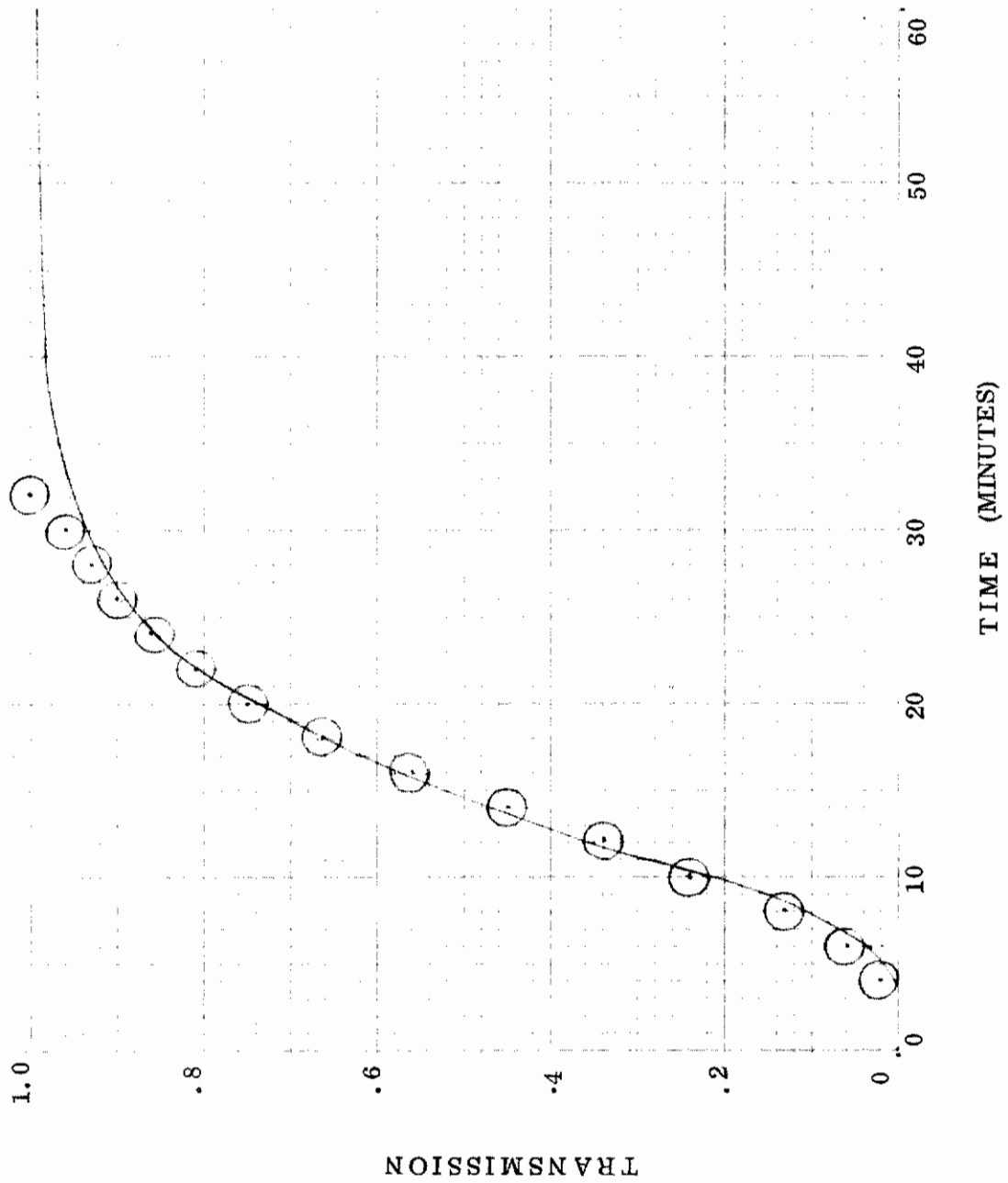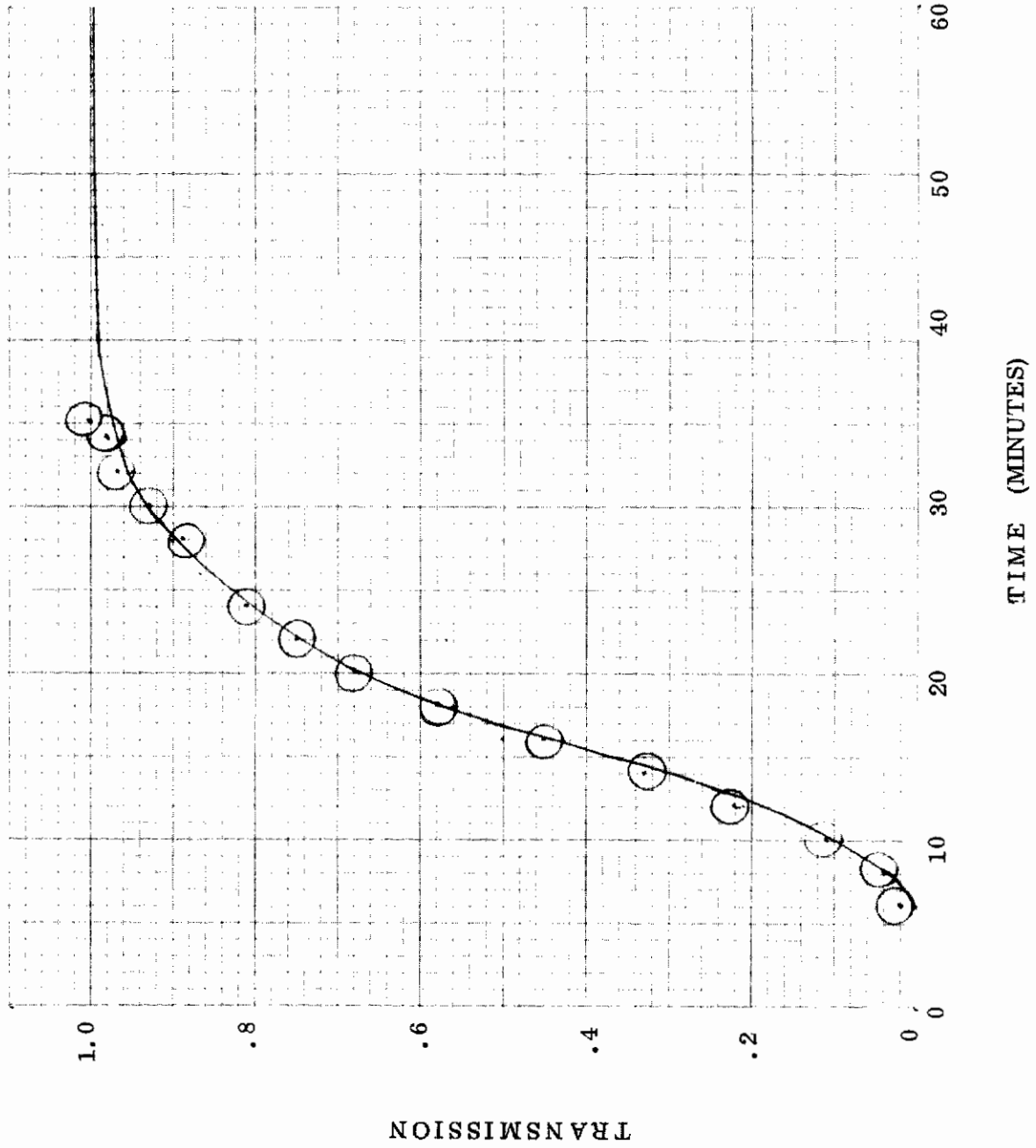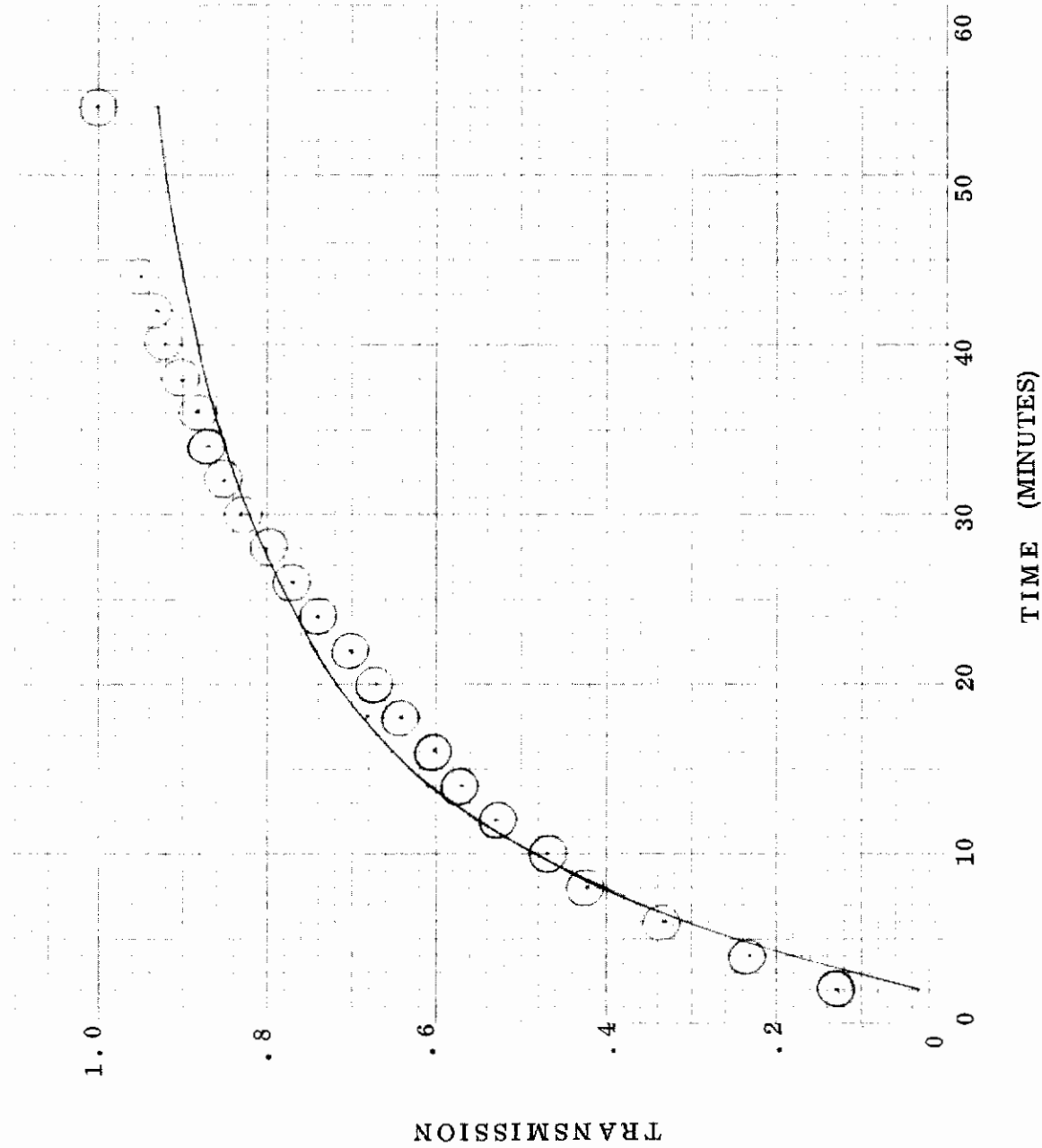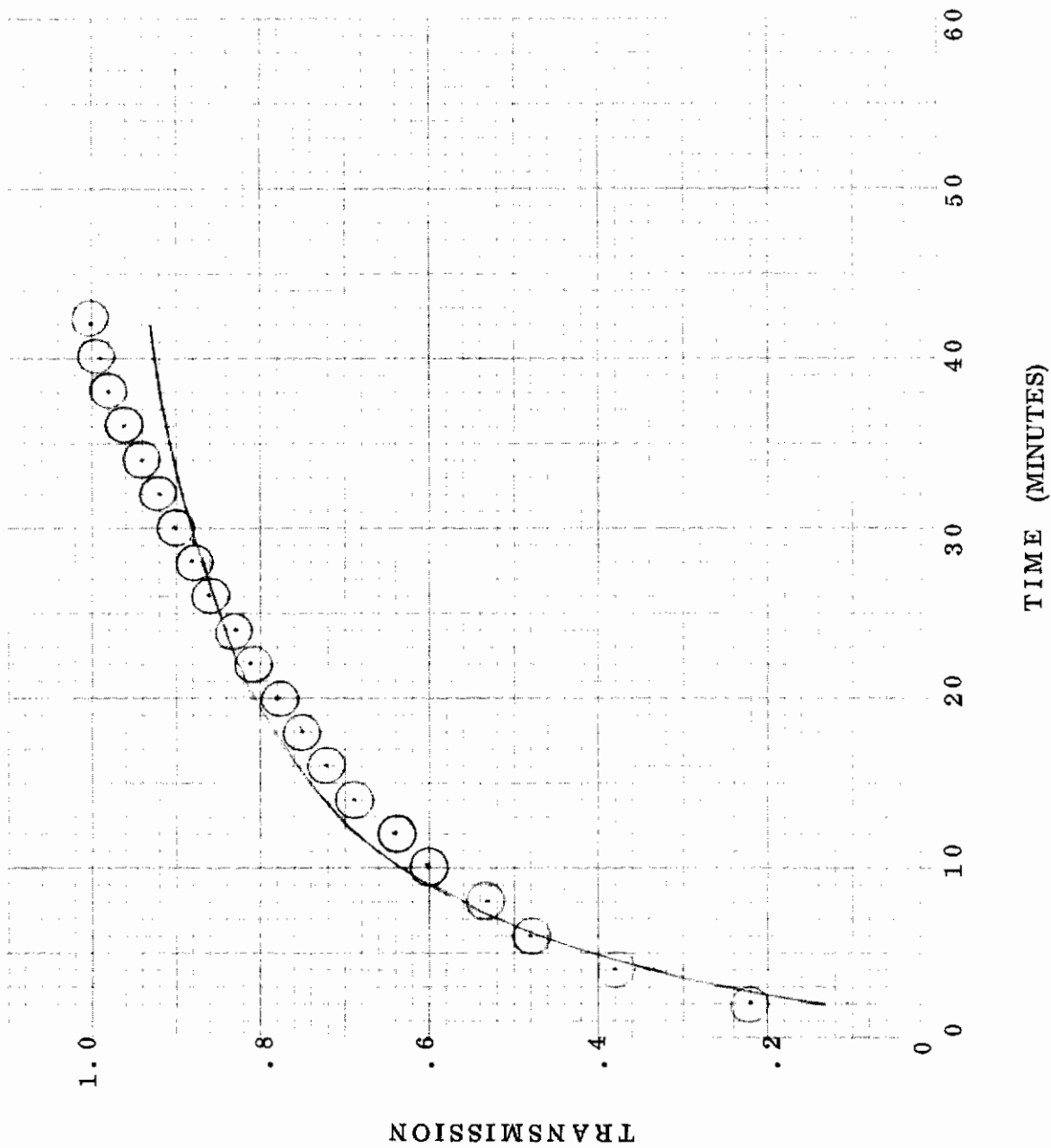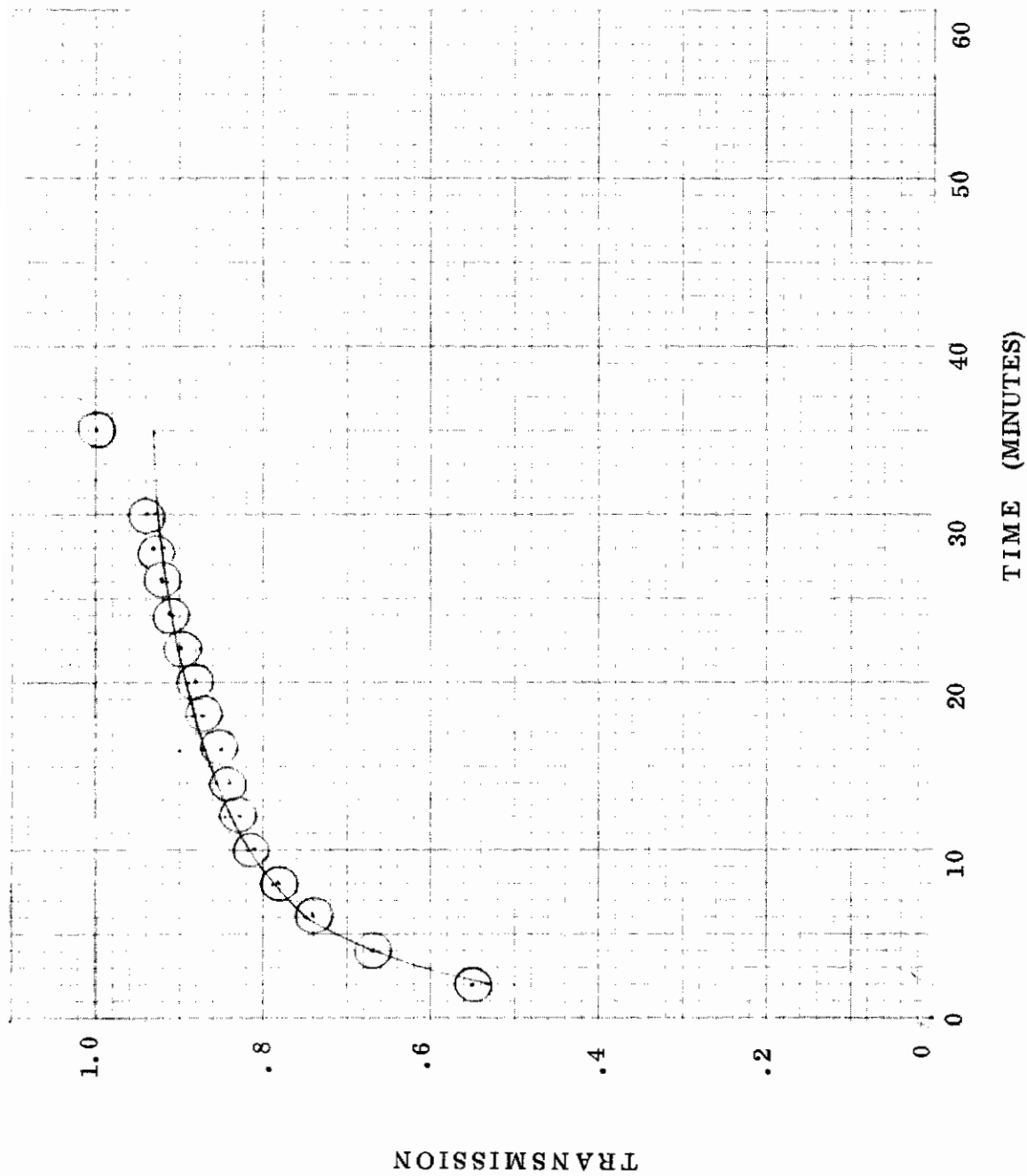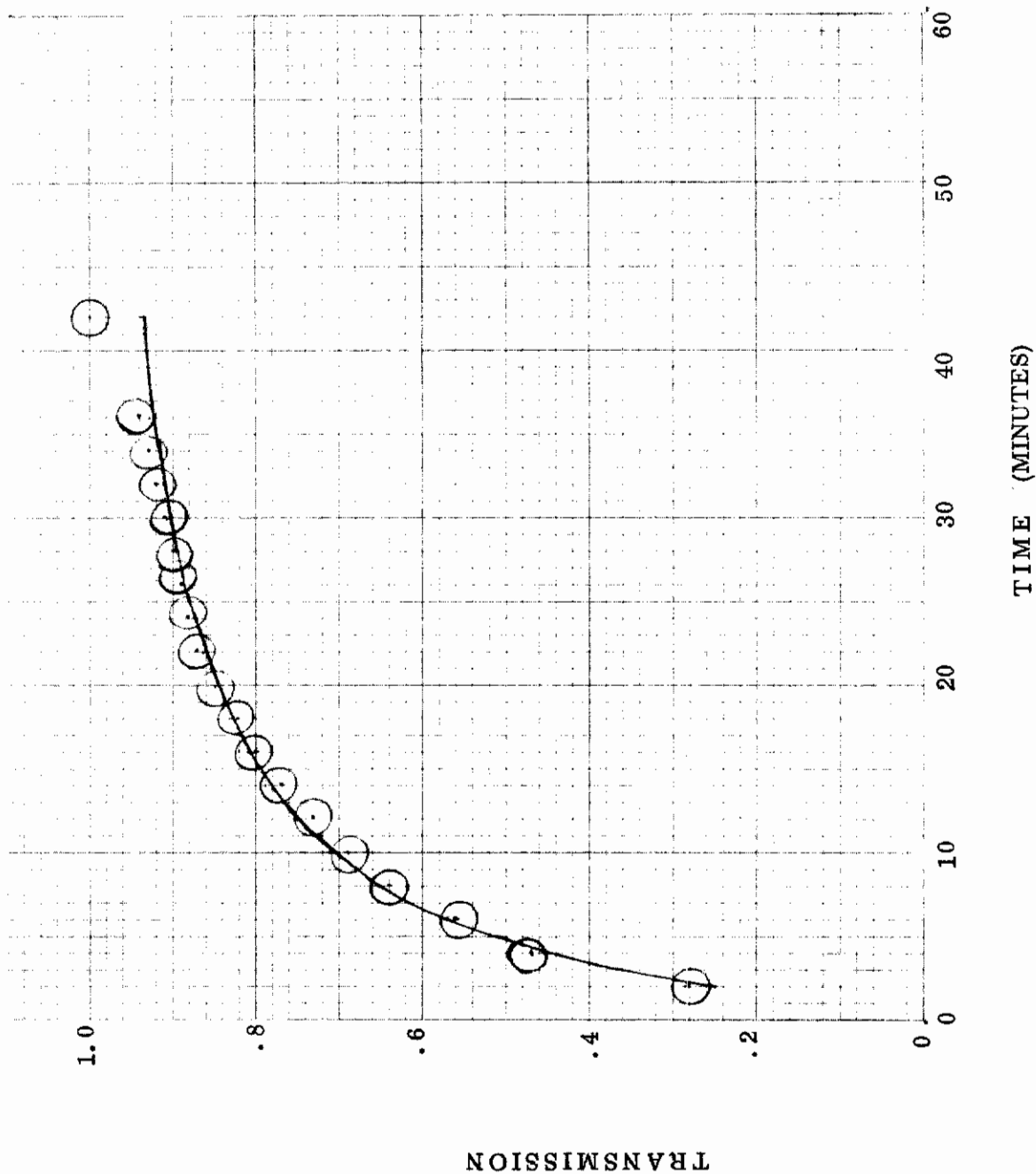
Fox Run 11AA

Figure 31.

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13. ABSTRACT

This study of the theoretical performance of gaseous adsorption systems is based on an equation for the time-dependent transmission of a gas through an adsorber bed of length, ℓ, and bulk density, ρ, and a gas-adsorber system characterized by an isothermal adsorption capacity, K, and a dispersivity, D. For a step-function gaseous input pulse injected into a stream of carrier gas which flows through the adsorber at a superficial flow velocity, u, the time-dependent expression for the transmission is a function only of the dimensionless dispersion number, $D/u\ell$, and the dimensionless time measured in units of the inflection time. A weighted least-squares analysis is developed and programmed on a digital computer to determine from an experimental transmission versus time curve the values of the two theoretical parameters (namely, the dispersivity and the adsorptivity) in the transmission equation. The errors in the values of the two theoretical parameters are evaluated also by propagating the errors in the experimental values of the transmission through the normal equations of the least-squares analysis. The Newton-Raphson method is used for obtaining the solution of the two simultaneous normal equations of the least-squares analysis. The theory is used to analyze experimental data on the transmission of carbon dioxide in air through molecular sieve adsorber beds.

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