

must be solved in such a way as to ensure that s is a minimum.
This requires that parameter values which ensure that

$$\frac{\partial s^2}{\partial b_p} = 0 \quad \text{for } p = 1(1)p$$

must be found.

Thus

$$-2 \sum_{i=1}^n (y_i - \phi_i) \frac{\partial \phi_i}{\partial b_p} = 0$$

Let

$$f_p = \sum_{i=1}^n (y_i - \phi_i) \frac{\partial \phi_i}{\partial b_p}$$

Hence

$$f_1 = (\ln AR_a - \ln AR_T) \frac{\partial \ln AR_T}{\partial D} + (\tan \phi_a - \tan \phi_T) \frac{\partial \tan \phi_T}{\partial D} = 0$$

(A.3.3)

and

$$f_2 = (\ln AR_a - \ln AR_T) \frac{\partial \ln AR_T}{\partial u} + (\tan \phi_a - \tan \phi_T) \frac{\partial \tan \phi_T}{\partial u} = 0$$

(A.3.4)

Continued/...A12

The procedure for solving these two equations is to make an initial guess at u and D and then to use an iterative procedure to converge on the solution.

The changes to be made to u and D after each iteration phase are evaluated by solving

$$\frac{\partial f_1}{\partial D} \cdot \Delta D + \frac{\partial f_1}{\partial u} \cdot \Delta u = -f_1 \quad (\text{A.3.5})$$

$$\frac{\partial f_2}{\partial D} \cdot \Delta D + \frac{\partial f_2}{\partial u} \cdot \Delta u = -f_2 \quad (\text{A.3.6})$$

and the improved approximations are then given by

$$D^{(i+1)} = D^{(i)} + \Delta D \quad (\text{A.3.7})$$

$$u^{(i+1)} = u^{(i)} + \Delta u \quad (\text{A.3.8})$$

The partial derivatives of the functions f_p to be used in equations (A.3.5) and (A.3.6) can be obtained from

$$\frac{\partial f_p}{\partial b_j} = - \sum_{i=1}^n \frac{\partial \phi_i}{\partial b_p} \cdot \frac{\partial \phi_i}{\partial b_j} + \sum_{i=1}^n (y_i - \phi_i) \frac{\partial^2 \phi_i}{\partial b_p \partial b_j} \quad (\text{A.3.9})$$

Continued/...A13

The second series of terms in this equation is always sufficiently small to be ignored,

$$\frac{\partial f_p}{\partial b_j} = - \sum_{i=1}^n \frac{\partial \phi_i}{\partial b_p} \cdot \frac{\partial \phi_i}{\partial b_j} \quad (\text{A.3.10})$$

Thus

$$\begin{aligned} \frac{\partial f_1}{\partial D} &= - \frac{\partial \ln AR_T}{\partial D} \cdot \frac{\partial \ln AR_T}{\partial D} - \frac{\partial \tan \phi_T}{\partial D} \cdot \frac{\partial \tan \phi_T}{\partial D} \\ \frac{\partial f_2}{\partial D} &= - \frac{\partial \ln AR_T}{\partial D} \cdot \frac{\partial \ln AR_T}{\partial u} - \frac{\partial \tan \phi_T}{\partial D} \cdot \frac{\partial \tan \phi_T}{\partial u} \quad (\text{A.3.11}) \\ \frac{\partial f_1}{\partial u} &= - \frac{\partial \ln AR_T}{\partial D} \cdot \frac{\partial \ln AR_T}{\partial u} - \frac{\partial \tan \phi_T}{\partial D} \cdot \frac{\partial \tan \phi_T}{\partial u} \\ \frac{\partial f_2}{\partial u} &= - \frac{\partial \ln AR_T}{\partial u} \cdot \frac{\partial \ln AR_T}{\partial u} - \frac{\partial \tan \phi_T}{\partial u} \cdot \frac{\partial \tan \phi_T}{\partial u} \end{aligned}$$

where

$$\begin{aligned} \ln AR_T &= \left[\frac{uL}{2D} - L \left(\frac{u^4}{16D^4} + \frac{w^2}{D^2} \right)^{1/4} \cos \left(\frac{1}{2} \arctan \frac{4wD}{u^2} \right) \right] \\ &\quad (\text{A.3.12}) \\ \tan \phi_T &= \frac{-1}{\tan \left[L \left(\frac{u^4}{16D^4} + \frac{w^2}{D^2} \right)^{1/4} \sin \left(\frac{1}{2} \arctan \frac{4wD}{u^2} \right) \right]} \end{aligned}$$

Continued/...A14

The partial derivatives required in equations (A.3.11) can now be evaluated. (SEE SECTION 2).

To ensure convergence of the iteration procedure the proposals of Law and Bailey will be adopted.

Since the solution is approaching a minimum in s^2 , its total derivative must be negative.

$$\therefore ds^2 = -2 \sum_{k=1}^2 db_k \cdot \sum_{j=1}^2 s_j \frac{\partial \phi_j}{\partial b_k} < 0$$

Hence when evaluating the Δb_k 's the criterion

$$D_T > 0 \quad (3.13)$$

must be satisfied.

Thus

$$\begin{aligned} D_T = & \left[\left(\ln AR_a - \ln AR_T \right) \frac{\partial \ln AR_T}{\partial D} + \left(\tan \phi_a - \tan \phi_T \right) \frac{\partial \tan \phi_T}{\partial D} \right] \Delta D \\ & + \left[\left(\ln AR_a - \ln AR_T \right) \frac{\partial \ln AR_T}{\partial u} + \left(\tan \phi_a - \tan \phi_T \right) \frac{\partial \tan \phi_T}{\partial u} \right] \Delta u \\ & > 0 \end{aligned}$$

Now if $D_T \not> 0$, then the signs of all the b_k 's must be changed and the calculation resumed.

This condition in itself is not sufficient to ensure convergence and a further condition must be imposed.

$$\Delta s^2 = (s^2) + 1 - (s^2)^i < 0$$

This can be achieved after (A.3.13) is satisfied if all the Δb_k 's are restricted so that

$$\left(\Delta b_k \right)_r = a \Delta b_k$$

where a is a positive fraction.

Faster convergence is in fact obtained if a is made small enough to satisfy

$$\Delta s^2 = -b(a^2 - 2a) D_T$$

where b is a fraction in the range

$$0.1 \leq b \leq 0.25$$

A better estimate of the parameters is then obtained from

$$b_k^{(i+1)} = b_k^{(i)} + a \Delta b_k$$

Finally, convergence is obtained when all the Δb_k 's become as small as desired.

EVALUATION OF THE PARTIAL DERIVATIVES (MODEL 2)

The partial derivatives for use in equations (A.3.11) are shown below.

$$\frac{\partial p}{\partial D} = - \frac{u^2 L^2}{2D^3}$$

$$\frac{\partial q}{\partial D} = - \frac{wL^2}{D^2}$$

$$\frac{\partial p}{\partial u} = \frac{2uL^2}{4D^2}$$

$$\frac{\partial q}{\partial u} = 0$$

$$\frac{\partial k}{\partial D} = \frac{1}{1 + \left(\frac{q}{p}\right)^2} \cdot \left[\frac{1}{p} \cdot \frac{\partial q}{\partial D} - \frac{q}{p^2} \cdot \frac{\partial p}{\partial D} \right]$$

$$\frac{\partial j}{\partial D} = \frac{1}{4} (p^2 + q^2)^{-3/4} \cdot \left[2p \frac{\partial p}{\partial D} + 2q \frac{\partial q}{\partial D} \right]$$

$$\frac{\partial k}{\partial u} = \frac{1}{1 + \left(\frac{q}{p}\right)^2} \cdot \left[\frac{1}{p} \cdot \frac{\partial q}{\partial u} - \frac{q}{p^2} \cdot \frac{\partial p}{\partial u} \right]$$

$$\frac{\partial j}{\partial u} = \frac{1}{4} (p^2 + q^2)^{-3/4} \cdot \left[2p \frac{\partial p}{\partial u} + 2q \frac{\partial q}{\partial u} \right]$$

$$\frac{\partial y}{\partial D} = - \frac{uL}{2D^2} + j \sin k \cdot \frac{\partial k}{\partial D} - \cos k \cdot \frac{\partial j}{\partial D}$$

Continued/...A17

$$\frac{\partial Z}{\partial D} = -j \cos k \cdot \frac{\partial k}{\partial D} - \sin k \frac{\partial j}{\partial D}$$

$$\frac{\partial y}{\partial u} = \frac{L}{2D} + j \sin k \frac{\partial k}{\partial u} - \cos k \frac{\partial j}{\partial u}$$

$$\frac{\partial Z}{\partial u} = -j \cos k \frac{\partial k}{\partial u} - \sin k \frac{\partial j}{\partial u}$$

$$\frac{\partial \ln AR}{\partial D} = \frac{\partial y}{\partial D}, \quad \frac{\partial \ln AR}{\partial u} = \frac{\partial y}{\partial u}$$

$$\frac{\partial \tan \phi}{\partial D} = -\frac{1}{\sin^2 Z} \cdot \frac{\partial Z}{\partial D}$$

$$\frac{\partial \tan \phi}{\partial u} = -\frac{1}{\sin^2 Z} \cdot \frac{\partial Z}{\partial u}$$

Continued/...A18

APPENDIX IV

SOLUTION OF THE EQUATIONS BY THE METHOD OF LAW AND BAILEY (6) (MODEL I)

The method outlined in APPENDIX III may be used for evaluating k and M knowing u and D . Only the relevant equations are listed below.

$$s^2 = (\ln AR_a - \ln AR_T)^2 + (\tan \phi_a - \tan \phi_T)^2$$

$$0 = (\ln AR_a - \ln AR_T) \frac{\partial \ln AR_T}{\partial M} + (\tan \phi_a - \tan \phi_T) \frac{\partial \tan \phi_T}{\partial M}$$

$$0 = (\ln AR_a - \ln AR_T) \frac{\partial \ln AR_T}{\partial k_2} + (\tan \phi_a - \tan \phi_T) \frac{\partial \tan \phi_T}{\partial k_2}$$

$$\frac{\partial f_1}{\partial k_2} \cdot \Delta k_2 + \frac{\partial f_1}{\partial M} \cdot \Delta M = -f_1$$

$$\frac{\partial f_2}{\partial k_2} \cdot \Delta k_2 + \frac{\partial f_2}{\partial M} \cdot \Delta M = -f_2$$

$$k_2^{(i+1)} = k_2^{(i)} + \Delta k_2 \quad (A.41)$$

$$M^{(i+1)} = M^{(i)} + \Delta M$$

$$\frac{\partial f_1}{\partial k_2} = - \frac{\partial \ln AR_T}{\partial k_2} \cdot \frac{\partial \ln AR_T}{\partial k_2} - \frac{\partial \tan \phi_T}{\partial k_2} \cdot \frac{\partial \tan \phi_T}{\partial k_2}$$

Continued/...A19

$$\frac{\partial f_2}{\partial k_2} = - \frac{\partial \ln AR_T}{\partial k_2} \cdot \frac{\partial \ln AR_T}{\partial M} - \frac{\partial \tan \phi_T}{\partial k_2} \cdot \frac{\partial \tan \phi_T}{\partial M}$$

$$\frac{\partial f_1}{\partial M} = \frac{\partial f_2}{\partial k_2}$$

$$\frac{\partial f_2}{\partial M} = - \frac{\partial \ln AR_T}{\partial M} \cdot \frac{\partial \ln AR_T}{\partial M} - \frac{\partial \tan \phi_T}{\partial M} \cdot \frac{\partial \tan \phi_T}{\partial M}$$

$$\ln AR_T = \frac{uL}{2D} - (U^2 + v^2)^{1/4} \cos \frac{\theta}{2}$$

$$\partial \tan \phi_T = \frac{-1}{\tan \left[- (U^2 + v^2)^{1/4} \sin \frac{\theta}{2} \right]}$$

EVALUATION OF THE PARTIAL DERIVATIVES (MODEL I)

The partial derivatives for use in equations (A.4.1) are presented below.

$$\frac{\partial Y}{\partial k_2} = \frac{M^2 w^2}{k_2^3} \cdot Y^3$$

$$\frac{\partial Y}{\partial M} = - \frac{M w^2}{k_2^2} \cdot Y^3$$

Continued/...A20

$$\frac{\partial \beta}{\partial k_2} = \frac{MwY^2}{k_2^2}$$

$$\frac{\partial \beta}{\partial M} = -\frac{wY^3}{k_2}$$

$$\frac{\partial U}{\partial k_2} = \frac{L^2 F}{D} \left[k_2 \left(Y \sin \beta \frac{\partial \beta}{\partial k_2} - \cos \beta \frac{\partial Y}{\partial k_2} \right) + 1 - Y \cos \beta \right]$$

$$\frac{\partial U}{\partial M} = -\frac{L^2 k_2 F}{D} \left[-Y \sin \beta \frac{\partial \beta}{\partial M} + \cos \beta \frac{\partial Y}{\partial M} \right]$$

$$\frac{\partial v}{\partial k_2} = -\frac{L^2}{\Gamma} \cdot F \left[\frac{MwY^3}{k_2} \cdot \cos \beta + \left(\frac{M^2 w^2}{k_2^2} \cdot Y^3 + Y \right) \sin \beta \right]$$

$$\frac{\partial v}{\partial M} = \frac{L^2 F Y^3 w}{D} \left[\cos \beta + \frac{Mw}{k_2} \sin \beta \right]$$

$$\frac{\partial \theta}{\partial k_2} = \frac{1}{(U^2 + v^2)} \cdot \left(U \frac{\partial v}{\partial k_2} - v \frac{\partial U}{\partial k_2} \right)$$

$$\frac{\partial \theta}{\partial M} = \frac{1}{(U^2 + v^2)} \left(U \frac{\partial v}{\partial M} - v \frac{\partial U}{\partial M} \right)$$

$$\frac{\partial \ln AR_1}{\partial k_2} = -\frac{1}{2} \left[\cos \frac{\theta}{2} \cdot (U^2 + v^2)^{-3/4} \left(U \frac{\partial U}{\partial k_2} + v \frac{\partial v}{\partial k_2} \right) - (U^2 + v^2)^{1/4} \cdot \sin \frac{\theta}{2} \cdot \frac{\partial \theta}{\partial k_2} \right]$$

$$\frac{\partial \ln AR_1}{\partial M} = -\frac{1}{2} \left[\cos \frac{\theta}{2} (U^2 + v^2)^{-3/4} \left(U \frac{\partial U}{\partial M} + v \frac{\partial v}{\partial M} \right) - (U^2 + v^2)^{1/4} \sin \frac{\theta}{2} \cdot \frac{\partial \theta}{\partial M} \right]$$

$$\frac{\partial \tan \phi_T}{\partial k_2} = \frac{-1}{\sin^2 \left[(U^2 + v^2)^{1/4} \sin \frac{\theta}{2} \right]} \left[\frac{1}{2} (U^2 + v^2)^{-3/4} \left(U \frac{\partial U}{\partial M} + v \frac{\partial v}{\partial k_2} \right) \right. \\ \left. + \sin \frac{\theta}{2} + \frac{1}{2} (U^2 + v^2)^{1/4} \cos \frac{\theta}{2} \cdot \frac{\partial \theta}{\partial k_2} \right]$$

$$\frac{\partial \tan \phi_T}{\partial M} = \frac{-1}{\sin^2 \left[(U^2 + v^2)^{1/4} \sin \frac{\theta}{2} \right]} \left[\frac{1}{2} (U^2 + v^2)^{-3/4} \left(u \frac{\partial U}{\partial M} + v \frac{\partial v}{\partial M} \right) \right. \\ \left. + \sin \frac{\theta}{2} + \frac{1}{2} (U^2 + v^2)^{1/4} \cos \frac{\theta}{2} \cdot \frac{\partial \theta}{\partial M} \right]$$

APPENDIX V

Consider MODEL 2 in which no interphase mass transfer occurs.
Equation (2.5) represents the transfer function.

$$F(s) = \exp \left[\frac{ux}{2D} - \left(\frac{u^2 x^2}{4D^2} + \frac{x^2 s}{D} \right)^{\frac{1}{2}} \right]$$

$$\therefore \ln F(s) = \frac{ux}{2D} - \left(\frac{u^2 x^2}{4D^2} + \frac{x^2 s}{D} \right)^{\frac{1}{2}}$$

$$\text{and } \ln F(s) = \ln \alpha_0 - T_m s + \frac{T_s^2}{2} s^2 + \dots$$

(A.5.1)

also

$$\ln f(s) \Big|_{s \rightarrow 0} = \ln \alpha_0$$

$$\frac{\partial \ln f(s)}{\partial s} \Big|_{s \rightarrow 0} = -T_m$$

$$\frac{\partial^2 \ln f(s)}{\partial s^2} \Big|_{s \rightarrow 0} = T_s^2$$

(A.5.2)

Thus

Continued/...A23

$$\alpha_0 = 1$$

$$T_{m1} = \frac{x}{u}$$

$$T_{s1}^2 = \frac{2Dx}{u^3}$$

(A.5.3)

Equations (A.5.3) represent two simultaneous equations in the two unknowns u and D . Solving at $x = L$

$$u = \frac{L}{T_{m1}}$$

$$D = \frac{L^2 T_{s1}^2}{2T_m}$$

(A.5.4)

Consider now MODEL 1 in which interphase mass transfer occurs. Equation (2.4) represents the transfer function.

$$F(s) = \exp \left[\frac{ux}{2D} - \left(\frac{u^2 x^2}{4D^2} - \left(\frac{k_1}{\frac{M}{k_2} \cdot s + 1} - k_1 - s \right) \right)^{\frac{1}{2}} \right]$$

Using equations (A.5.2)

Continued/...A24

$$\alpha_0 = 1$$

$$T_{m2} = \frac{(MF + 1) x}{u}$$

$$T_{s2}^2 = \frac{2M^2 Fx}{uk_2} + \frac{2x(MF + 1)^2 D}{u^3}$$

(A.5.5)

and solving at $x = L$

$$M = \frac{(uT_{m2} - L)}{FL}$$

$$k_2 = \frac{2M^2 FLu^2}{u^3 T_{s2}^2 - 2L (MF + 1)^2 D}$$

(A.5.6)

APPENDIX VI

COMPARISON OF REPORTED AND DETERMINED M VALUES.

Partition coefficients are customarily determined by static vapour-liquid equilibrium measurements. A method using corrected gas chromatographic retention volumes has been investigated by Mellado and Kobayashi (8). They found that values consistent with static measurements were obtained. The system n-dodecane/n-butane was extensively studied and curves of K-values as a function of temperature and pressure produced.

The relationship between K and the partition coefficient at infinite dilution M^0 is

$$M^0 = \frac{1}{K} \cdot \frac{d}{p} \cdot \frac{RT}{W}$$

where

p is the total pressure

d is the density of the stationary phase

R is the gas constant

T is the temperature

W is the molecular weight of the stationary phase

Under the applicable experimental conditions $M^0 = 53.2$.

Thus the values calculated using this method are not inconsistent with values reported in the literature.

Continued/... A26

APPENDIX VII

INVEISION TECHNIQUE.

By definition

$$\begin{aligned} F(s) &= \int_0^{\infty} e^{-st} f(t) dt \\ &= \sum_{M=0}^{\infty} \int_{2MT}^{2(M+1)T} e^{-st} f(t) dt \end{aligned} \quad (A.7.1)$$

where T is a positive constant.

Now let s take on values of $\alpha + iw$, where α and w are real and positive, also let $e^{-\alpha t} f(t) = g(t)$, a function which can be described by a non-periodic full range Fourier Series.

$$\text{i.e. } g(t) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi t}{T} + \sum_{n=0}^{\infty} b_n \cos \frac{n\pi t}{T}$$

$$\text{for } 0 \leq t \leq 2T$$

$$g(t) = 0$$

$$\text{for } 2T < t < 0$$

Continued /...A27

The use of this functional form requires that

- (a) $e^{-st}f(t)$ can be adequately described by a Fourier Series in the interval $0 \leq t \leq 2T$ where a_n and b_n tend to zero as n tends to infinity.
- (b) $e^{-st}f(t)$ at $t < 0$ be zero. This can usually be arranged by suitable choice of base line.
- (c) $e^{-at}f(t)$ at $t > 2T$ be zero. This will in most cases be only approximately satisfied.

This provides a proposal for the selection of the parameters a and T .

(4)

For the particular case of an impulse system, $a = 0$ if T is chosen with care.

$$\text{Now } F(s) = \int_0^{2T} e^{at}, e^{-i\omega t} f(t) dt$$

$$= \int_0^{2T} e^{-i\omega t} g(t) dt$$

$$\text{Let } \omega = \frac{n\pi}{T}, \text{ where } n \text{ is a positive integer.}$$

Continued/...A28

$$\begin{aligned}
 F(s) &= F\left(\alpha + \frac{in\pi}{T}\right) \\
 &= \int_0^{2T} \left(\cos \frac{n\pi t}{T} - i \sin \frac{n\pi t}{T}\right) g(t) dt \\
 &= Tb_n - iTa_n \qquad n = 1(1)\infty
 \end{aligned}$$

$$\text{and } F(\alpha) = 2Tb_0 \qquad n = 0$$

$$\text{Thus } b_0 = \frac{1}{2T} F(\alpha)$$

$$b_n = \frac{1}{T} \operatorname{Re} \left[F\left(\alpha + \frac{in\pi}{T}\right) \right] \qquad (A.7.2)$$

$$a_n = -\frac{1}{T} \operatorname{IM} \left[F\left(\alpha + \frac{in\pi}{T}\right) \right]$$

DYNAMIC DESCRIPTION OF A GAS CHROMATOGRAPHIC COLUMN.

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OCTOBER 1969.

M.A.GREENBERG

REMOTE PRINT/DISPLAY FOR USER NO 20

FILE NAME MG51

DEPT OF CHEM ENG

DATE= 69-279

L.0001 ZFTG

L.0002 C

ANALYSIS OF D AND U ----- INERT SOLUTE

DOUBLE PRECISION W,D,U,X,THETA,SS,RR,RD,RU,AL,PT,PHT,AD,AU,PV,PD,PU,PI,F,CONST,ANG1,ANG2

DOUBLE PRECISION BAP,DAR,TOR,AR,PAR,PL,PHL,SA,SB,TTI,ATI,TE,DI,UI,F1,F2,F1D,F1U,F2D,F2U,D0,DU,DT

DOUBLE PRECISION C(300),A(2,40),B(2,40),AN(40),BN(40),AREA(2),TM(2),VAR(2)

L.0006 C

INPUT AND OUTPUT

L.0007 C

200 FORMAT(13,F6.0)

L.0008

TT=1.D-12

L.0010 201 FORMAT(8H RUN NO=,I3,5X,10H FLOWRATE=,F6.3,13H LITRES PER MINUTE/)

L.0011 202 FORMAT(4I4,2F6.0)

L.0012 203 FORMAT(' START POINT NUMBER =',I4,5X,'FINISH POINT NUMBER =',I4,5X,'TIME AXIS INTERVAL =',F5.3/)

L.0013 204 FORMAT(16F4.0)

L.0014 205 FORMAT(16F6.1)

L.0015 206 FORMAT(73H U=,F8.3,11H CM PER SEC,5X,5H TMF=,F8.3,4H SEC,5X,4H D=,F8.3,14H SQ CM PER SEC,5X,6H VAR1=,F8.3)

L.0016 207 FORMAT(1X,2H N,9X,5H A(N),14X,5H B(N),14X,2H W,9X,16H AMPLITUDE RATIO,4X,10H PHASE LAG,8X,2H D,9X,2H U)

L.0017 208 FORMAT(13,23X,E14.8)

L.0018 209 FORMAT(F8.0,4E20.8,12X,F8.3)

L.0019 210 FORMAT(' N',6X,'A(INPUT)',7X,'B(INPUT)',7X,'AR(INPUT)',5X,'FREQUENCY',6X,'A(OUTPUT)',7X,'AR(OUTPUT)')

L.0020 211 FORMAT(F4.0,7E15.8)

L.0021 212 FORMAT(//17H INPUT AND OUTPUT/)

L.0022 213 FORMAT(//7H SYSTEM/)

L.0023 214 FORMAT(//)

L.0024 215 FORMAT(F4.0,5E18.8,2F10.3)

L.0025 216 FORMAT(4E20.8)

L.0026 217 FORMAT(6E18.8)

L.0027 218 FORMAT(2E20.8)

L.0028 219 FORMAT(2Y,13)

L.0029 220 FORMAT(14)

L.0030 221 FORMAT(2D20.15,10X,3E10.3)

L.0031 225 FORMAT(' INPUT CURVE.'/)

L.0032 226 FORMAT(' CONCENTRATION PROFILE.'/)

L.0033 227 FORMAT(' OUTPUT CURVE.'/)

L.0034 228 FORMAT(//)' MOMENT ANALYSIS.'/)

L.0035 229 FORMAT(' FREQUENCY ANALYSIS.'/)

L.0036 C

READING IN OF DATA

L.0037 C

READ(9,220)IDUM

L.0038

PI=4.*DATAN(1.)

L.0039

X=183.0

L.0040 49 READ 200,NRUN,FLO

L.0041

IF(NRUN-30)50,50,74

L.0042

L=0

L.0043

PRINT 21

L.0044

PRINT 201,NRUN,FLO

L.0045

READ 202,J11,JF1,J12,JF2,DELTI,DELT2

L.0046

PRINT 214

L.0047

PRINT 225

L.0048

PRINT 203,J11,JF1,DELT1

L.0049

PRINT 226

L.0050

L=L+1

L.0051

IF(L-2)52,53,53

L.0052

52 J1=J11

L.0054

```

L.0055 JF=JF1
L.0056 DELT=DELT1
L.0057 GO TO 54
L.0058 53 JI=J12
L.0059 JF=JF2
L.0060 DELT=DELT2
L.0061 54 I=J1
L.0062 IF(L-2)47,46,47
L.0063 46 PRINT 214
L.0064 PRINT 227
L.0065 PRINT 203,J12,JF2,DELT2
L.0066 PRINT 226
L.0067 47 DO 55 J=J1,JF,16
L.0068 READ 204,(C(I+M),M=1,16)
L.0069 IF(IIDUM-0)55,222,55
L.0070 222 PRINT 205,(C(I+M),M=1,16)
L.0071 55 I=I+16
L.0072 EVALUATION OF MOMENTS USING SIMPSONS RULE FOR INTEGRATION
L.0073 EVALUATION OF AREAS FOR NORMALIZATION OF INPUT AND OUTPUT
L.0074 C *****
L.0075 SUM1=0.
L.0076 SUM2=0.
L.0077 SUM3=0.
L.0078 JI=J1+1
L.0079 J11=J1+1
L.0080 JF1=JF-1
L.0081 DO 56 J=J11,JF1,2
L.0082 SUM1=SUM1+C(J)*4.+C(J+1)*2.
L.0083 SUM2=SUM2+C(J)*DELT+J*4.+C(J+1)*DELT*(J+1)*2.
L.0084 AREA(L)=(SUM1+C(J1)+C(JF))*DELT/3.
L.0085 TM(L)=(SUM2+C(J1)*DELT+J1+C(JF)*DELT*JF)*DELT/(3.*AREA(L))
L.0086 I=J1
L.0087 DO 57 J=J1,JF
L.0088 T=J
L.0089 T=T*DELT
L.0090 I=I+1
L.0091 57 SUM3=SUM3+(T-TM(L))*(T-TM(L))*C(I)*DELT
L.0092 VAR(L)=SUM3/AREA(L)
L.0093 IF(L-2)51,58,58
L.0094 58 VAR1=VAR(2)-VAR(1)
L.0095 TME=TM(2)-TM(1)
L.0096 U=X/TME
L.0097 DV=VAR1*X**3/(2.*TME**3)
L.0098 WRITE(9,221)DV,U
L.0099 PRINT 228
L.0100 PRINT 206,U,TME,DV,VAR1
L.0101 PRINT 240
L.0102 240 FORMAT('+TOR = ')
L.0103 READ(9,2+1)TOR,TTS
L.0104 241 FORMAT(Y,A4)
L.0105 READ(9,220)KOUM
L.0106 L=0
L.0107 60 L=L+1
L.0108 IF(L-2)61,62,62
L.0109 61 JI=J11+1
L.0110 JF=JF1
L.0111 DELT=DELT1
L.0112 GO TO 63
L.0113 62 JI=J12+1

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Author Greenberg M A

Name of thesis Dynamic sescription of a gas chromatographic column. 1969

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