8. APPENDIX

8.1 Hydrodynamic Experimental Procedure

The column pressure drop, expanded bed height, bubble column height, and total gas volume fraction were measured for each set of operating conditions. The column pressure drop was measured as a difference in water level between the sight tube and the column. Since the sight tube extended upward from the point at which the pressure drop of the column was measured, the elevation difference was eliminated and the level difference was the actual pressure drop. The expanded bed height was defined as the height at which the homogeneous, dense, three-phase region ended and the bubble column region with scattered particles started. The bubble column height was a measure from this point to the water level of the column. In most cases the two regions should be apparent. However, a measurement error due to poorly defined regions was substantial for high superficial velocities and for 3/32-in. Plexiglas cubes.

The total gas volume fraction was calculated from the drop in height of the column water level due to a simultaneous closing of both inlet gas and liquid flows. The drainage tube was closed to prevent water in the column from draining. Leakage of this tube and the closing of the valves were major sources of error.

Alumina beads which evolve heat when absorbing water were pre-treated with water. A known volume of dry Plexiglas or drained alumina was weighed, and water was then added to yield the void fraction. The particle density and the buoyant weight of the solid were then calculated.

Additional experiments without packings were performed for various superficial gas velocities (0.57, 1.51, 2.47, and 3.51 cm/sec) and for four heights (40.2, 65.7, 87.2, and 121.7 cm). Subtraction of the bubble column pressure drop from the total column pressure drop yields the pressure drop through the three-phase region.

A better procedure for determining the fluidized bed height would be to photograph the column during operation with a meter stick next to the column. By counting the spouting beads in the column, a height can be determined where 95 to 99% of the beads are in the lower part of the column. The heights obtained would be more accurate and consistent than those obtained by the current method, i.e., estimation through observation.

8.2 Mass Transfer Experimental Procedure

Predetermined water, air, and carbon dioxide flows were set on the rotameters. For high liquid flow rates, the water passed through a countercurrent air stripper and returned to the feed tank. Otherwise, the water

leaving the bed was sent to the drain. The aqueous carbon dioxide concentration was monitored until four consecutive samples at 10-min separations agreed within ± 0.05 ml acid in the titration.

When steady state was achieved, samples were taken from five ports and from the tank, if not done previously, to be titrated for carbon dioxide content. After the sample port hose was opened and filled, the 10-ml pipette was inserted and allowed to fill and then to overflow for about 20 sec. If an air bubble passed through, the 20-sec count was restarted. While this sample drained into a sample bottle containing sodium hydroxide solution, a second sample was taken with a second pipette. Both pipettes were rinsed with distilled water, and water drops were blown out with air. Samples were taken downward from top port to bottom, or tank, and were repeated four times.

After the column height and temperature were recorded, the water flow was stopped, the height lowered to prevent diffusion through the outlet port, and the column was monitored until equilibrium was reached. Again, four samples from the column consistent within 0.05-ml acid over about 45 min constituted equilibrium. The column temperature and height were again recorded.

Samples were titrated with a Radiometer Copenhagen automatic titrator. Each sample bottle was filled, under an argon blanket, with 10 ml of a sodium hydroxide solution of known normality and capped with a ground glass stopper. After the sample was added, the solution was titrated with hydrochloric acid, again under an argon blanket, to an 8.3 pH endpoint.

On the first day, a known 0.1 N hydrochloric acid solution was used to determine the normality of a prepared sodium hydroxide solution of about 0.01 N. This solution was then used to standardize a 0.01 N hydrochloric acid solution. On succeeding days the 0.01 N acid concentration was assumed constant and was used to re-standardize the basic solution.

8.3 Sample Calculations

8.3.1 Pressure Drop for the Three-Phase Region

Two sets of measurements were taken to derive the pressure drop, ΔP, for the three-phase region, the pressure drop for the entire column (both three-phase and bubble column region), and for the bubble column in a different experiment. Sufficient runs were taken to determine the bubble column pressure drop as a function of gas superficial velocity and the height of the bubble column. The operating conditions used in the bubble column correlation were similar to those of the fluidized bed. The pressure drop of the three-phase region was calculated by:

$$\Delta P_{three-phase} = \Delta P_{total\ column} - \Delta P_{bubble\ column} \tag{21}$$

For example, using the results from Run IV for U_G = 1.51 cm/sec and U_L = 2.53 cm/sec, one obtains

$$\Delta P_{three\ phase} = 1.3 - (-3.9) = 5.2\ gm/cm^2$$

8.3.2 Buoyant Solid Bed Weight Per Area

First the weight of a dry solid, W, was measured for a known volume of the solid, V_S. Then the volume of water, V_L, required to occupy the void fraction of the bed was measured. The density of the solid, ρ_S, was calculated from:

$$\rho_S = \frac{W}{V_S - V_L} \tag{22}$$

If the data from Run IV are used, then

$$\rho_S = \frac{1140\ gm}{1000\ cc - 408\ cc} = 1.93\ gm/cc$$

Since the buoyant force is defined as:

$$W_{buoyant} = \frac{W(\rho_S - \rho_L)}{\rho_S} \tag{23}$$

and the cross sectional area, A, of the column is:

$$A = \pi r^2 \tag{24}$$

then the buoyant pressure is:

$$\frac{W_{buoyant}}{A} = \frac{W(\rho_S - \rho_L)}{\pi r^2 \rho_S} \tag{25}$$

Thus, for Run IV,

$$\frac{W_{buoyant}}{A} = \frac{1142\ gm(1.93 - 1.00\ gm/cc)}{\pi(3.81\ cm)^2\ 1.93\ gm/cc} = 12.07\ gm/cm^2$$

8.3.3 Volume Fraction Determination

For the data from Run IV when U_G = 1.51 cm/sec and U_L = 3.14 cm/sec, the solid volume fraction is:

$$\epsilon_S = \frac{W}{\rho_S HA} = \frac{1142 \text{ gm}}{(1.93 \text{ gm/cc})(21.6 \text{ cm})(45.6 \text{ cc})} = 0.60 \qquad (2)$$

To determine the gas volume fraction in the three-phase region, experiments with the same packing but at different bed heights were performed for similar flow conditions. The gas phase volume fractions, ϵ_i, for the two columns shown in Fig. 18 with the same cross sectional areas, are:

$$\epsilon_{11}h_{11} + \epsilon_{12}h_{12} = \epsilon_1 H_1 = \Delta H_1 \text{ gas} \qquad (26)$$

$$\epsilon_{21}h_{21} + \epsilon_{22}h_{22} = \epsilon_2 H_2 = \Delta H_2 \text{ gas} \qquad (27)$$

where ϵ_{11} is the volume fraction of the three phase region and ϵ_{12} is the volume fraction of the bubble column region. If the gas volume fractions in each respective region are independent of the bed height, then

$$\epsilon_{11} = \epsilon_{21} \qquad (28)$$

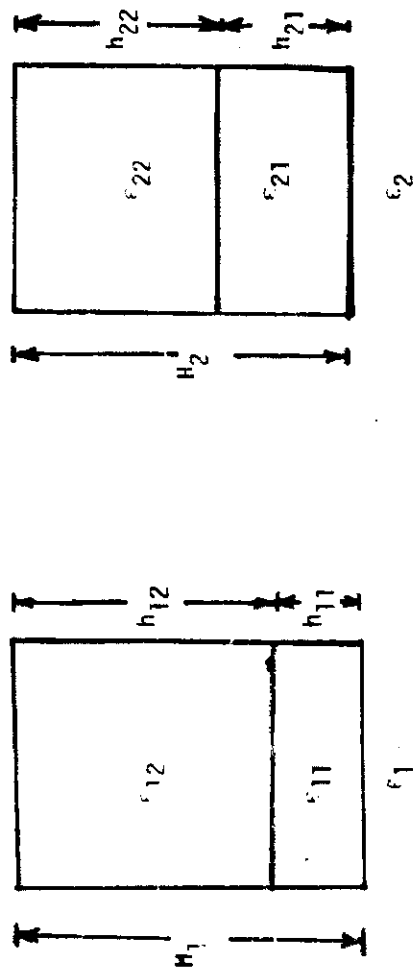$$\epsilon_{12} = \epsilon_{22} \qquad (29)$$

and Eqs. (26) and (27) may be solved simultaneously for ϵ_1 and ϵ_2:

$$\epsilon_{11} = \frac{\Delta H_1 h_{22} - \Delta H_2 h_{12}}{h_{11}h_{22} - h_{21}h_{12}} \qquad (30)$$

$$\epsilon_{12} = \frac{\Delta H_1 - \epsilon_{11}h_{11}}{h_{12}} \qquad (31)$$

If the results from Run IV (sets d and h) are substituted in Eqs. (30) and (31), then

h_{22}

h_{21}

ϵ_{22}

ϵ_{21}

ϵ_2

H_2

h_{12}

h_{11}

ϵ_{12}

ϵ_{11}

ϵ_1

H_1

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

SCHOOL OF CHEMICAL ENGINEERING PRACTICE

AT

OAK RIDGE NATIONAL LABORATORY

GAS VOLUME FRACTION DETERMINATION
FROM TWO BED HEIGHTS

| DATE 5-19-75 | DRAWN BY RM | FILE NO. CEPS-X-213 | FIG. 18 |

$$\varepsilon_{11} = \frac{(7.7 \text{ cm})(84.3 \text{ cm}) - (8.0 \text{ cm})(106.2 \text{ cm})}{(21.6 \text{ cm})(84.3 \text{ cm}) - (39.7 \text{ cm})(106.2 \text{ cm})} = 0.0837$$

$$\varepsilon_{12} = \frac{7.7 \text{ cm} - (0.0837)(21.6 \text{ cm})}{106.2 \text{ cm}} = 0.0555$$

Equation (3) is used to determine the liquid volume fraction.

$$\varepsilon_L = 1 - \varepsilon_S - \varepsilon_G = 1 - 0.60 - 0.084 = 0.32 \tag{3}$$

8.3.4 Determination of $U^\circ_{G_{mf}}$

For turbulent flow the Ergun equation reduces to the Blake-Plummer equation:

$$-\frac{\Delta P}{\rho h} \frac{g_c}{U^2_{G_{mf}}} \frac{D_p \varepsilon^3_{ns}}{(1-\varepsilon_{ns})} = 1.75 \tag{32}$$

Equation (32) is solved for $U^\circ_{G_{mf}}$:

$$U^\circ_{G_{mf}} = \sqrt{1.75 \frac{(1-\varepsilon_{ns})}{D_p \varepsilon^3_{ns}} \frac{1}{g_c} \frac{\rho h}{(-\Delta P)}} \tag{33}$$

At fluidization

$$\Delta P = \frac{W}{A} \tag{34}$$

For 4x8 mesh alumina,

$$\Delta P = 2.52 \text{ lb}/0.0491 \text{ ft}^2 = 51.3 \text{ lb/ft}^2$$

Substituting into Eq. (33),

$$U^\circ_{G_{mf}} = \sqrt{1.75 \frac{(1 - 0.408)}{0.208 \text{ ft}(0.408)^3} \frac{1}{32.17 \text{ ft/sec}^2} \frac{(0.0749 \text{ lb/ft}^3)(0.738 \text{ ft})}{51.3 \text{ lb/ft}^2}}$$

$$= 6.38 \text{ ft/sec} = 194 \text{ cm/sec}$$

Checking the Reynolds number to determine if the flow is turbulent:

$$Re = \frac{D\rho U_G}{\mu} = \frac{0.25 \text{ ft}(0.0749 \text{ lb/ft}^3)(5.4 \text{ ft/sec})}{1.08 \times 10^{-5} \text{ lb/ft-sec}} \tag{35}$$

$$= 11,000$$

The assumption of turbulent flow is valid.

8.3.5 Bubble Column Correlation for E_L

The axial dispersion coefficient, E_L, is determined from the Peclet number, Pe, which is defined as:

$$Pe = \frac{DU_G}{E_L} \tag{36}$$

The Peclet number is a function of bubbly or slugging flow. Correlations have been developed for each flow regime (3). For the bubbly flow regime,

$$Pe = 11.12 \, Re^{0.82} \, Ar^{-0.45} \tag{37}$$

where:

$$Re = \frac{DU_G}{\nu} \tag{38}$$

and

$$Ar = \frac{D^3 g}{\nu^3} \tag{39}$$

For the slugging flow regime,

$$Pe = 0.387 \, Re^{0.25} \, Su^{-0.13} \tag{40}$$

where:

$$Su = \frac{D\rho\sigma}{\mu^2} \qquad (41)$$

The transition between bubbly flow and slugging flow may be reliably predicted from the intersection of Eqs. (37) and (40). The observed Peclet number is usually the lower (greater axial mixing) value of the Peclet number across the transition (3). For Run C,

$$Re = \frac{(7.62 \text{ cm})(4.05 \text{ cm/sec})}{8.571 \times 10^{-3} \text{ cm}^2/\text{sec}} = 3.601 \times 10^3$$

$$Ar = \frac{(7.62 \text{ cm})^3(980.7 \text{ cm/sec}^2)}{(8.571 \times 10^{-3} \text{ cm}^2/\text{sec})^3} = 5.907 \times 10^9$$

$$Su = \frac{(7.62 \text{ cm})(0.997 \text{ gm/cm}^3)(71.66 \text{ gm/sec}^2)}{(8.545 \times 10^{-3} \text{ gm/cm-sec})^2} = 7.456 \times 10^6$$

If the flow regime is bubbly,

$$Pe = 11.12(3.601 \times 10^3)^{0.82}(5.907 \times 10^9)^{-0.45} = 0.3675$$

If the flow regime is slugging,

$$Pe = 0.387(3.601 \times 10^3)^{0.25}(7.456 \times 10^6)^{-0.13} = 0.3832$$

Since the Peclet number is smallest for bubbly flow, bubbly flow is the important flow regime. A Peclet number of 0.3675 is used in the calculation of the axial dispersion coefficient from Eq. (36) which was rearranged:

$$E_L = \frac{DU_G}{Pe} = \frac{(7.62 \text{ cm})(4.05 \text{ cm/sec})}{0.3675} = 84 \text{ cm}^2/\text{sec} \qquad (42)$$

The value of the experimental dispersion coefficient was 35 cm^2/sec.

8.4 Previous Mass Transfer Data

The mass transfer data collected by Saad et al. (1) were recalculated to correct for two errors and an assumption which could not be tested. First the stoichiometric amount of carbon dioxide neutralized by one mole of sodium hydroxide was 0.9975 as calculated by Reber et al. (4) rather than the unsupported value of 0.9998. Secondly the sample port heights were changed from the distance between the liquid disperser and the sample port to that between the gas disperser and the port, the actual height in which mass transfer may occur. Finally, the dispersion coefficient was determined by fitting the data experimentally with the use of the computer programs TPFBED and BLE. These changes were necessary for comparison of previous and current results.

8.5 Literature Value of Henry's Law Constant

The value of Henry's Law constant was obtained from:

$$m_{lit} = \frac{0.00459 \ (273 + T°C)}{1.2 + 0.044 \ (T°C - 15)} \tag{43}$$

This equation is plotted in Fig. 19.

8.6 Computer Calculations

Three computer programs, TPFXPM.F4, and the pair TPFBED.F4 and BLE.F4, were used to calculate the mass transfer data.

8.6.1 TPFXPM.F4

The program TPFXPM.F4 is the result of the combined efforts of the consultants, the previous group (1), and the work of Reber et al. (4). The computer program was modified for this project. The current logic diagram is shown in Fig. 20. The program accepts as input the experimental approach to equilibrium for each port during the steady state run, the extraction factor, and a value for Henry's Law constant from the equilibrium run. The overall mass transfer coefficient and numbered transfer units for the plug flow model are calculated. The dispersed model calculations, including the BLE subroutine, have been moved to a separate program so the dispersion coefficient may be easily varied. After the initial data have been processed, an additional loop added for this study accepts as input only port height and titration data for the calculations of the remaining ports in a run. To reduce printing time, much of the explanation in the computer output that was previously printed was transferred to comment statement, and the repetitive printout of experimentally determined constants was eliminated. The program listing of TPFXPM follows with sample input and outout for Run F.
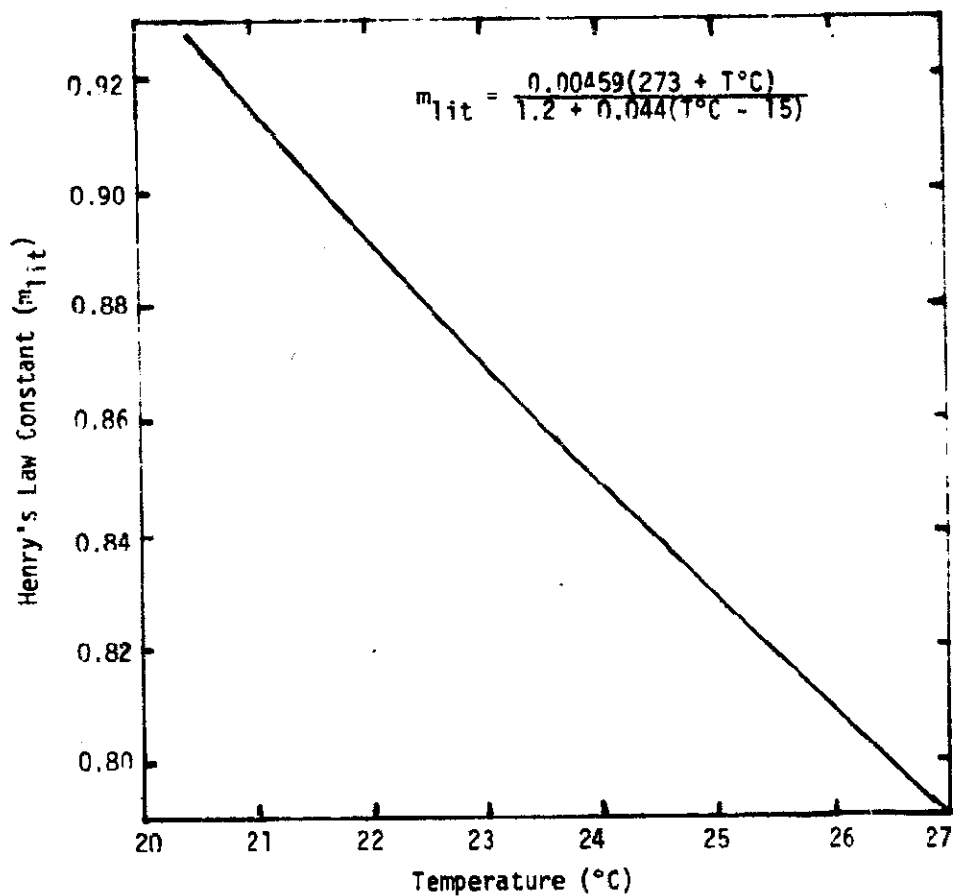
52

$$m_{lit} = \frac{0.00459(273 + T°C)}{1.2 + 0.044(T°C - 15)}$$

HENRY'S LAW CONSTANT VS TEMPERATURE

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
SCHOOL OF CHEMICAL ENGINEERING PRACTICE
AT
OAK RIDGE NATIONAL LABORATORY

DATE	DRAWN BY	FILE NO.	FIG.
5-19-75	RM	CEPS-X-213	19

Start

Accept as input:
    Operating Conditions
    Titration Data

Accept as input:
    Port Height
    Titration Data

Calculate:
    m, F, X, NTU_{pf}, $K_L a_{pf}$

More Sample Ports?

yes   no

New Data Set?

yes   no

Stop

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
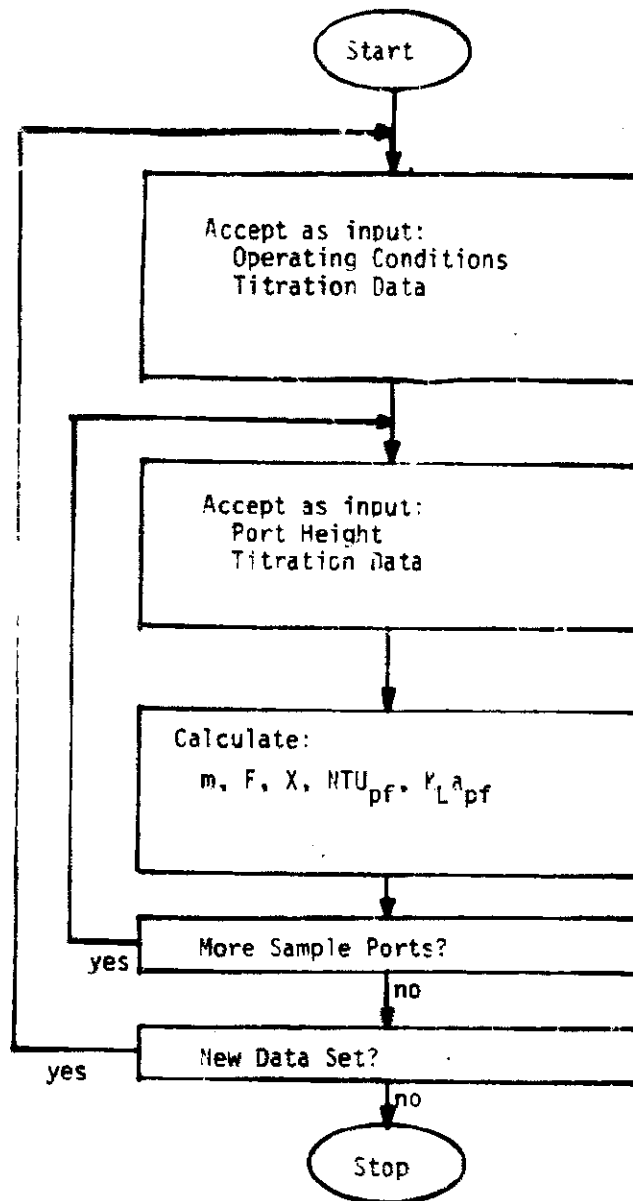SCHOOL OF CHEMICAL ENGINEERING PRACTICE
AT
OAK RIDGE NATIONAL LABORATORY

LOGIC DIAGRAM FOR
COMPUTER PROGRAM TPFXPM.F4

DATE	DRAWN BY	FILE NO.	FIG.
5-19-75	RM	CEPS-X-213	20

Program Listing of TPFXPM.F4

```
          REAL NTUPF,NB,MEXP,MLIT,KLAPF,NA
          DIMENSION DAT(4),VAL(25),ENT(17)
          DATA DAT/3HSTD, 2HTD, 3HTRD, 3HEQU/,
        *  ENT/4HVCO2, 4HVAIR, 2HDC, 4HVLIQ, 4HPATM, 4HTCOL, 2HDP,
        *  1HH, 4HRHOL, 2HNA, 4HHDEQ, 4HHSEQ, 5HSTOIC, 2HVB, 2HEX,
        *  2HVS, 3HHEP/
          JJ = 0
          TYPE 898
898       FORMAT(' DO YOU WANT A LISTING OF THE ABBREVIATIONS USED
        *  IN THIS PROGRAM?(YES = 1, NO = 0)'/)
          ACCEPT 899,RES
899       FORMAT(I2)
          IF(RES .EQ. 0  ) GO TO 9
          TYPE 900
          TYPE 999
900       FORMAT(' THE ABBREVS FOR REQUESTED DATA FOLLOW. /
        *  TYPE IN ONE VALUE PER LINE WHEN ITS ASKED FOR. /
        *  ALL VALUES MUST INCLUDE DECIMAL POINT.'/
        *  ' STD IS FOR ACID-BASE STANDARDIZATION'  /
        *  '  TD IS FOR TANK DATA'  /
        *  '  TRD IS FOR TITRATION RUN DATA'  /
        *  '  EQU IS FOR EQUILIBRIUM DATA'  /
        *  '  EX IS DISPERSION COEFFICIENT(SQCM/SEC)'  /
        *  '  VCO2 IS FOR VOLUMETRIC CO2(CC/SEC)'  /
        *  '  VAIR IS FOR AIR FLOW RATES(CC/SEC)'  /
        *  '  DC IS FOR COLUMN DIAMETER(CM)       '  /
        *  '  VLIQ IS FOR VOLUMETRIC WATER FLOW RATE(CC/SEC)'  /)
999       FORMAT('     PATM IS FOR ATMOSPHERIC PRESSURE(MMHG)'  /
        *  '  TCOL IS FOR COLUMN TEMPERATURE 0C'  /
        *  '  DP IS FOR PRESSURE DIFFERENCE(MMHG)'  /
        *  '  H IS HEIGHT OF SAMPLE PORT(CM)'  /
        *  '  RHOL IS FOR DENSITY OF LIQUID(G/CC)'  /
        *  '  NA IS FOR THE NORMALITY OF THE ACID'  /
        *  '  VB IS FOR THE VOLUME OF THE BASE(ML)'  /
        *  '  VS IS FOR THE VOLUME OF THE SAMPLE(ML)'  /
        *  '  HEP IS FOR SAMPLE PORT HEIGHT(EQUIL. RUN)(CM)'  /
        *  ' HSEQ IS FOR STATIC EQ. HEIGHT(CM)'  /
        *  'HDEQ IS FOR DYNAMIC EQ HEIGHT(CM)'  /
        *  ' STOIC IS STOICH.COEFF.'  /)
9         J=1
6          TYPE 901,DAT(J)
901       FORMAT('  TYPE IN THE NUMBER OF VALUES YOU HAVE FOR
        *  THE',2X,A4,'  (<=25),'/'  THEN TYPE IN THE VALUES.'/  )
          ACCEPT 902,N,(VAL(I),I=1,N+1)
902       FORMAT(I3,77X,(F14.7,66X))
          AV=0.
          SD=0.
          RN=N
          DO 10 I=2,N+1
```

```
10        AV=AV+VAL(I)/RN
          IF (RN.EQ.1.) GO TO 13
          TSD=0.
          DO 12 IJ=2,N+1
 12       TSD=TSD + (AV - VAL(IJ))**2
          SD=SQRT(TSD/(RN-1.))
13        GO TO (1,2,3,4)J
  1       VAA = AV
          GO TO 7
2         VAB=AV
          GO TO 7
3         VAC=AV
          GO TO 7
4         VAD=AV
7         TYPE 933,AV,SD
903       FORMAT(' AVERAGE = ',2X,E13.7,4X,' STAND DEV =',
     *    4X,E13.7)
          J=J+1
          IF(JJ.EQ.1) GO TO 11
          IF(J.LE.4) GO TO 6
          K=1
 11       TYPE 990,ENT(K)
990       FORMAT(' ENTER VALUE FOR',2X  ,A5/)
          ACCEPT 991,EVAL
991       FORMAT(F14.7)
          GO TO (111,112,113,114,115,116,117,118,119,120,123,
     *    124,125,121,126,127,128)K
111       VCO2=EVAL
          GO TO 122
112       VAIR=EVAL
          GO TO 122
113       DC=EVAL
          GO TO 122
114       VLIQ=EVAL
          GO TO 122
115       PATM=EVAL
          GO TO 122
116       TCOL=EVAL
          GO TO 122
117       DP=EVAL
          GO TO 122
118       H=EVAL
          IF(JJ.EQ.1) GO TO 50
          GO TO 122
119       RHOL=EVAL
          GO TO 122
120       NA=EVAL
          GO TO 122
123       HDEQ=EVAL
          GO TO 122
124       HSEQ=EVAL
          GO TO 122
```

```
125         STOIC=EVAL
            GO TO 122
121         VB=EVAL
            GO TO 122
126         EX = EVAL
            GO TO 122
127         VS = EVAL
            GO TO 122
123         HEP = EVAL
122         K=K+1
            IF(K.LE.17)GO TO 11
            NB=NA*VAA/VB
C           NB IS NORMALITY OF BASE
            CXTANK=(NB*VB-NA*VAB)/(STOIC*VS)
C           CXTANK IS CO2 CONCENTRATION IN FEED TANK
            CXEQBM=(NB*VB-NA*VAD)/(STOIC*VS)
C           CXEQBM IS CO2 CONCENTRATION IN LIQUID AT EQUIL
            VCO2=VCO2*SQRT(740./(PATM+DP))
            VAIR=VAIR*SQRT(740./(PATM+DP))
            CSA= 3.1416*DC*DC/4
            UY=(VCO2+VAIR)/CSA
C           UY IS GAS SUPERFICIAL VELOCITY(CM/SEC)
            YCO2=VCO2/(VCO2+VAIR)
C           YCO2 IS CO2 GAS MOLE FRACTION
            PEQB=(PATM+(HDEQ-HEP)*(HSEQ/HDEQ)*(10./13.5)*RHOL)
      *     /760.
            CY=YCO2*PEQB/(0.08205*(TCOL+273.))
C           CY IS CO2 CONCENTRATION IN GAS
            MEXP=CXEQBM/CY
C           MEXP IS EXPERIMENTAL HENRYS LAW CONSTANT
            MLIT=(.00459*(273.16+TCOL))/(1.2+0.044*(TCOL-15.))
C           MLIT IS THE CORRESPONDING LITERATURE VALUE
            UX=VLIQ/CSA
            F=MEXP*UX/UY
C           F IS THE EXTRACTION FACTOR
   50       CXO=(NB*VB-NA*VAC)/(STOIC*VS)
C           CXO IS CO2 CONC. IN LIQUID SAMPLE
            X=(CXEQBM-CXO)/(CXEQBM-CXTANK)
C           X IS DIMENSIONLESS APPROACH TO EQUILIBRIUM
            NTUPF=ALOG(1./(X-F+(X*F)))/(F+1.)
C           NTU IS NUMBER OF TRANSFER UNITS
C           PF IS FOR PLUG FLOW
            HTUPF=H/NTUPF
C           HTU IS HEIGHT OF A TRANSFER UNIT
            KLAPF=UX/HTUPF
C           KLA IS VOLUMETRIC MASS TRANSFER COEFFICIENT
            IF(JJ.EQ.1) GO TO 5
            TYPE 925,NB,CXTANK,CXEQBM,UY,MEXP,MLIT,YCO2,CY,UX,F
   5        TYPE 926,CXO,X,NTUPF,HTUPF,KLAPF
```

```
     925        FORMAT(' NB = ',E13.7/' CXTANK = ',E13.7/
          *    ' CXEQ3M = ',E13.7/ ' UY = ',E13.7/
          *    ' MEXP = ',E13.7/ ' MLIT = ',E13.7/
          *    ' YCO2 = ',E13.7/ ' CY = ', E13.7/
          *    ' UX = ',E13.7/ ' F = ', E13.7 )
     926        FORMAT(' CXO = ',E13.7/' X = ',E13.7/
          *    ' NTUPF = ',E13.7/' HTUPF = ',E13.7/
          *    ' KLAPF = ',E13.7/)
               TYPE 997
     997        FORMAT(' ARE THERE ADDITIONAL SAMPLE PORT DATA
          *    TO BE'/' ENTERED?(YES = 1,NO = 0)'/)
               ACCEPT 899,ANSW
               IF (ANSW.EQ.0  ) GO TO 76
               J = 3
               JJ = 1
               K = 8
               GO TO 6
      76       JJ = 0
               TYPE 995
     995        FORMAT(' DO YOU WANT TO CONTINUE WITH THIS PROGRAM
          *    BY ENTERING A'/' NEW SET OF DATA?(YES=1,NO=0)'/)
               ACCEPT 899, ANSW
               IF (ANSW.NE. 0  ) GO TO 9
               STOP
```

Sample Input and Output from TPFXPM.F4 Using Data from Run F

```
DO YOU WANT A LISTING OF THE ABBREVIATIONS USED  IN THIS PROGRAM?(YES =
1, NO = 0)

0
 TYPE IN THE NUMBER OF VALUES YOU HAVE FOR  THE   STD   (<=25),
 THEN TYPE IN THE VALUES.

4
9.52
9.54
9.55
9.50
AVERAGE =    .9527500E+01     STAND DEV =    .2217354E-01
 TYPE IN THE NUMBER OF VALUES YOU HAVE FOR  THE   TD   (<=25),
 THEN TYPE IN THE VALUES.

4
8.93
8.95
8.85
8.91
AVERAGE =    .8910000E+01     STAND DEV =    .4320493E-01
 TYPE IN THE NUMBER OF VALUES YOU HAVE FOR  THE   TRD   (<=25),
 THEN TYPE IN THE VALUES.
```

```
4
7.93
7.97
7.99
7.92
AVERAGE =     .7965000E+01     STAND DEV =     .3189126E-01
 TYPE IN THE NUMBER OF VALUES YOU HAVE FOR   THE   EQU   (<=25),
 THEN TYPE IN THE VALUES.

4
6.63
6.59
6.56
6.60
AVERAGE =     .6595000E+01     STAND DEV =     .2886751E-01
ENTER VALUE FOR   VCO2

19.2
ENTER VALUE FOR   VAIR

275.
ENTER VALUE FOR   DC

7.62
ENTER VALUE FOR   VLIQ

139.
ENTER VALUE FOR   PATM

739.
ENTER VALUE FOR   TCOL

22.4
ENTER VALUE FOR  .DP

84
ENTER VALUE FOR   H

48.
ENTER VALUE FOR   RHOL

0.998
ENTER VALUE FOR   NA

0.01038
ENTER VALUE FOR   HDEQ

129.5
ENTER VALUE FOR   KSEQ

105.
ENTER VALUE FOR   STOIC

0.9975
ENTER VALUE FOR   VB
```

```
10.0
ENTER VALUE FOR   EX

8.5
ENTER VALUE FOR   VS

10.0
ENTER VALUE FOR   HEP

48.
MB =   .9889545E-02
CXTANK =   .6425714E-03
CXEQBM =   .3051564E-02
NY =   .6455583E+01
MEXP =   .1093257E+01
MLIT =   .8892373E+00
YCO2 =   .6526173E-01
CY =   .2791258E-02
NX =   .3047993E+01
F =   .5161797E+00
CXO =   .1625940E-02
X =   .5917927E+00
NTUPF =   .6362930E+00
HTUPF =   .7543694E+02
KLAPF =   .4040452E-01

ARE THERE ADDITIONAL SAMPLE PORT DATA   TO BE
ENTERED?(YES = 1,NO = 0)

1
 TYPE IN THE NUMBER OF VALUES YOU HAVE FOR   THE   TRD   (<=25),
 THEN TYPE IN THE VALUES.

4
8.3
8.13
8.24
8.05
AVERAGE =   .8180000E+01   STAND DEV =   .1116542E+00
ENTER VALUE FOR   H

17.7
CXO =   .1402210E-02
X =   .6846652E+00
NTUPF =   .4288985E+00
HTUPF =   .4126850E+02
KLAPF =   .7385761E-01

ARE THERE ADDITIONAL SAMPLE PORT DATA   TO BE
ENTERED?(YES = 1,NO = 0)

0
DO YOU WANT TO CONTINUE WITH THIS PROGRAM   BY ENTERING A
 NEW SET OF DATA?(YES=1,NO=0)

0
STOP
```

8.6.2 TPFBED.F4 and BLE.F4

The subroutine BLE written by the previous group (1), who used the technique used by Reber et al. (4), was transferred to a separate program. An iterative technique was used to perform the inverse calculation of Eqs. (5) and (6) The number of plug flow transfer units are accepted as input and the corresponding number of backmix transfer units are calculated. The program TPFBED.F4 was written with the BLE.F4 routine to determine the best dispersion coefficient for each experimental concentration profile. The logic diagram is shown in Fig. 21. With the experimental outlet concentration, a value of the dispersion coefficient, and flow variables, an initial backmix profile is determined. The dispersion coefficient can then be varied so that the model profile will best approximate the experimental profile. The overall mass transfer coefficients for the three models are calculated for comparison. The program listing is presented on the following pages with a sample output from Run F.

Program Listing of TPFBED.F4 and BLE.F4

```
          DIMENSION PORT(10)
          REAL KLABM,KLACST,KLAPF
           REAL*8 DF,DX,DPE,DNTUPF,DZ
3         TYPE 901
          L = 0
901       FORMAT(' TYPE NO. OF PORTS')
          ACCEPT 902,N1
902       FORMAT(I2)
          TYPE 903
903       FORMAT(' ENTER PORT HTS IN INCREASING ORDER')
          ACCEPT 904, (PORT(I),I=1,N1)
904       FORMAT((F14.7,66X))
           TYPE 905
905       FORMAT(' ENTER XEXP FROM TOP PORT')
          ACCEPT 906,XEXP
906       FORMAT(F14.7)
1         TYPE 907
          M = 0
907       FORMAT(' ENTER VALUE OF EX')
          ACCEPT 906,EX
          IF(L.EQ.1) GO TO 4
          TYPE 908
908       FORMAT(' ENTER F AND UX, ONE PER LINE')
          ACCEPT 909, F,UX
909       FORMAT((F14.7,66X))
          DNTUPF=ALOG(1./(XEXP-F+(XEXP*F)))/(F+1.)
          KLAPF = (DNTUPF*UX)/PORT(N1)
          KLACST=UX*ALOG(XEXP/(XEXP*F+XEXP-F))/(F*PORT(N1))
          TYPE 915,KLAPF,KLACST
```

Logic Diagram for Programs TPFBED.F4 and BLE.F4
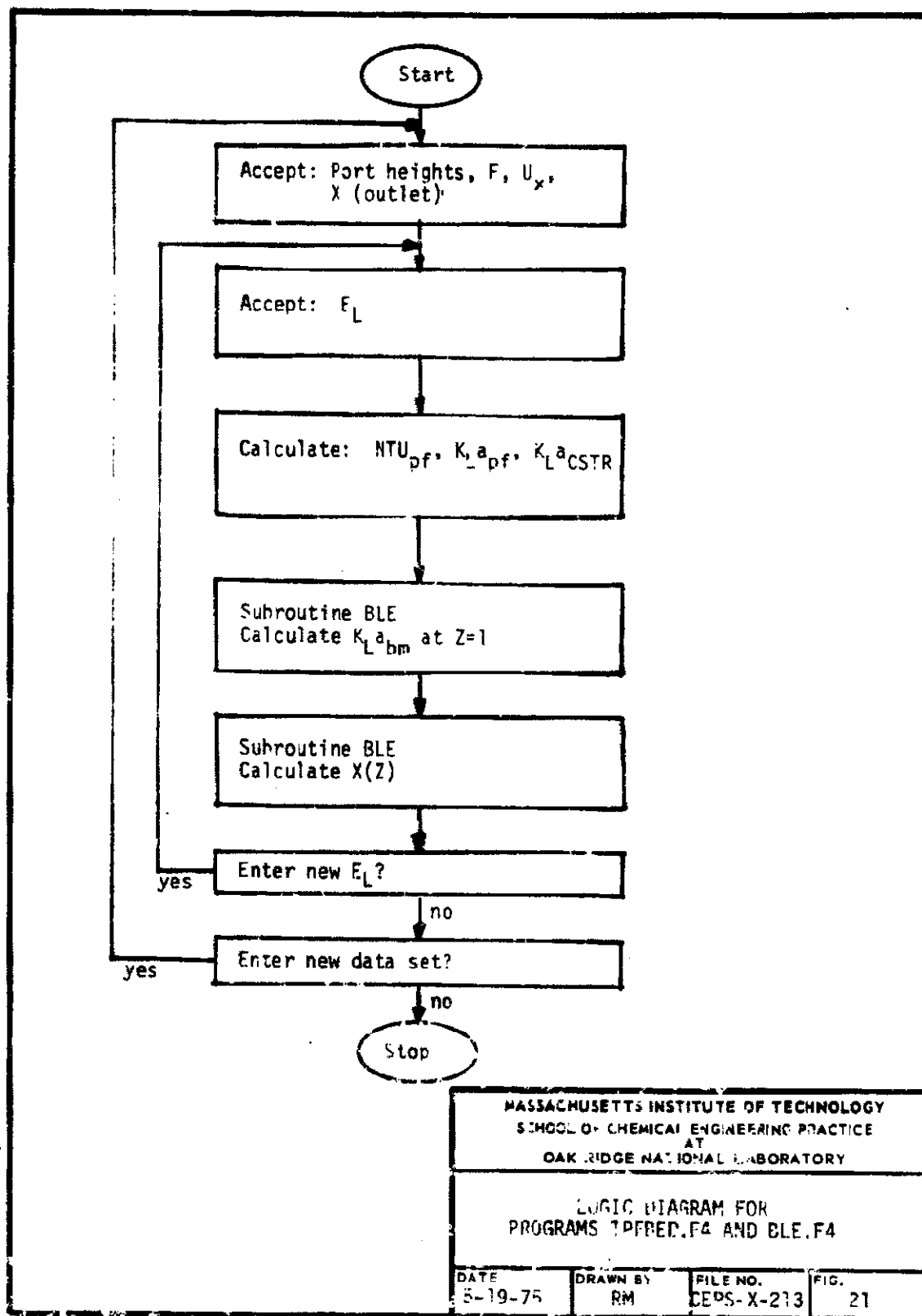
```
915     FORMAT(' KLAPF =    ',F14.7/' KLACST =     ',F14.7)
  4     DPE = PORT(N1)*UX/EX
        DF = F
        DX = XEXP
        DZ = 1.
        N5 = 0
        CALL BLE(DF,DX,DPE,DNTUPF,DZ,N5)
        KLABM = DNTUPF*UX/PORT(N1)
        TYPE 914,KLABM
914     FORMAT('  KLABM =     ',F14.7)
        DO 2 I = 1,N1
        DZ    = PORT(I)/PORT(N1)
        N5 = 1
        CALL BLE(DF,DX,DPE,DNTUPF,DZ,N5)
        IF(M.EQ.1) GO TO 5
        TYPE  916
916     FORMAT(8X, 'Z', 12X, 'X')
        M = 1
  5     TYPE 910,DZ,DX
910     FORMAT(F14.7,E14.7)
  2     CONTINUE
        L = 1
        TYPE 911
911     FORMAT(' ENTER NEW EX?(YES=1,NO=0)')
        ACCEPT 902, N3
        IF (N3.EQ.1) GO TO 1
        TYPE 913
913     FORMAT(' DATA FOR NEW RUN?(YES=1,NO=0)')
        ACCEPT 902,N4
        IF(N4.EQ.1) GO TO 3
        STOP
        END
        SUBROUTINE BLE (F,LHS,PE,NOX,Z,X)
C
C   THIS PROGRAM CALCULATES "TRUE" NOX BASED ON THE MATHEMATICAL
C   MODEL THAT INCLUDES AXIAL MIXING IN THE LIQUID PHASE,X.
C
C   CALCULATION OF NOX:   FIRST NOX IS BOUNDED
C   NTU1=LOWER BOUND,NTU PLUG FLOW NTU2=UPPER BOUND,ARBITRARY
C   THE MIDPOINT OF THE INTERVAL IS USED TO EVALUATE THE RHS OF
C   THE EQUATION WHICH IS COMPARED TO THE CONSTANT LHS.
C   THE INTERVAL IS THEN UPDATED AND A NEW MIDPOINT CHOSEN.
C   THE PROCESS IS REPEATED 20 TIMES TO INSURE THE RHS = LHS
C
        IMPLICIT DOUBLE PRECISION (A-H,L-Z)
        IF(X.EQ.1) GO TO 111
        J=0
        NTU1=NOX
        NTU2=15.D0
100     CONTINUE
        J=J+1
        IF (J-20)    110,1000,1000
```

```
110      NOX=(NTU1+NTU2)/2.0D0
 111     A  =((NOX/PE)-(1.0D0/F))**2.0D0
         B  =(4.0D0/(F*PE))*((NOX/F)+NOX)
         C  =DSQRT(A+B)
         R1 =(-((NOX/PE)-(1.0D0/F))+C)/(2.0D0/(F*PE))
         R2 =(-((NOX/PE)-(1.0D0/F))-C)/(2.0D0/(F*PE))
         E1 =DEXP(R1)
         E2 =DEXP(R2)
         H1 =1.0D0-(R1/PE)
         H2 =1.0D0-(R2/PE)
         T1 = DEXP(R2*Z)/(R2*DEXP(R2))
         T2 = DEXP(R1*Z)/(R1*DEXP(R1))
         D1 =H2/(R2*E2)
         D2 =H1/(R1*E1)
         DN =(T1-T2)/(D1-D2)
         F1 =1.0D0/(F+1.0D0)
         RHS=1.0D0-F1+(F1*DN)
         IF(K.EQ.0) GO TO 4
         LHS=RHS
         GO TO 1000
    4    IF (RHS-LHS) 1,2,2
 1       NTU2=NOX
         GO TO 100
 2       NTU1=NOX
         GO TO 100
1000     CONTINUE
C        PROGRAM BY BURKE
         RETURN
          END
```

Sample Input and Output from TPFBED.F4 and BLE.F4

```
TYPE NO. OF PORTS
6
ENTER PORT HTS IN INCREASING ORDER
00.0
 5.7
17.7
26.7
38.7
48.0
ENTER XEXP FROM TOP PORT
0.5913
ENTER VALUE OF EX
70.
ENTER F AND UX, ONE PER LINE
0.5446
3.043
```

```
KLAPF =          0.0409309
KLACST =         0.0549222
 KLABM =         0.0479743
       Z              X
    0.0000000  0.8055103E+00
    0.1812500  0.7385155E+00
    0.3437500  0.6824176E+00
    0.5562500  0.6390454E+00
    0.8062500  0.6017340E+00
    1.0000000  0.5918056E+00
ENTER NEW EX?(YES=1,NO=0)
1
ENTER VALUE OF EX
50.
 KLABM =          0.0479760
       Z              X
    0.0000000  0.8212513E+00
    0.1812500  0.7493493E+00
    0.3437500  0.6833985E+00
    0.5562500  0.6417701E+00
    0.8062500  0.6005563E+00
    1.0000000  0.5893199E+00
ENTER NEW EX?(YES=1,NO=0)
0
DATA FOR NEW RUN?(YES=1,NO=0)
0
STOP
```

8.7 Location of Original Data

The original data are located in ORNL Databook A-7219-G, pp. 1-84,
on file at the MIT School of Chemical Engineering Practice, Bldg. 3001,
ORNL.

8.8 Nomenclature

A   cross-sectional area of column, cm^2

Ar   Archimedes number, $D^3 g/\nu$

a   interfacial area/volume of equipment, cm^{-1}

C   concentration, $gmole/cm^3$

D_p particle diameter, cm

E dispersion coefficient, cm^2/sec

F extraction factor, mU_L/U_G, except in Sect. 4.1.7 where it is Fisher F, used in the variance test

g_c acceleration due to gravity, cm/sec^2

H height of column or bed, cm

h height of column or bed, cm

K overall mass transfer coefficient, cm/sec

m Henry's Law constant, $C_{L_{eq}}/C_G$

Pe Peclet number, $U_L H/E_L$

ΔP pressure drop, gm/cm^2

Re Reynolds number, DU_G/ν

Su Suratman number, $D\rho\sigma/\mu^2$

U velocity, cm/sec

V volume, cm^3

W weight of solids in a column, gm

X dimensionless approach to equilibrium

Z dimensionless column height, h/H

ϵ volume fraction

ρ density, gm/cm^3

ϕ shape factor

σ surface tension, dynes/cm

ν liquid kinematic viscosity, cm^2/sec

μ liquid viscosity, gm/cm-sec

$\mu_{1,2}$ solution of Eq. (6) for constants for Eq. (5)

Subscripts

b   corrected for buoyancy

bm   backmix or dispersed

CSTR   continuously stirred tank reactor; well-mixed

eq   equilibrium

exp   experimental value

G   gas phase

in   inlet

L   liquid phase

lit   literature value

mf   minimum fluidization

ns   non-solid phases

pf   plug flow

S   solid phase

Superscripts

°   evaluated at $U_L=0$ for subscript G; evaluated at $U_G=0$ for subscript L

'   normalized on a solid-free basis

8.9 Literature References

1. Saad, E.T., et al., "Cocurrent Three Phase Fluidized Bed, Part I," ORNL-MIT-209 (1975).

2. Michelson, M.L., and K. Ostergaard, "Holdup and Fluid Mixing in Gas-Liquid Fluidized Beds," Chem. Eng. J., 1, 37 (1970).

3. Chemical Technology Division Annual Progr. Rept. Mar. 31, 1974, ORNL-4966, pp. 54-56.

4. Reber, S.A., et al., "The Effects of Liquid Flow Rate and Viscosity on Mass Transfer in Open Bubble Columns," ORNL-MIT-201 (1974).

5. Ho., A.S.Y., et al., "Axial Mixing in Open Bubble Columns, Part VII: Mass Transfer Effects," ORNL-MIT-183 (1974).