APPENDIX

BCSR Model 1

The user has to supply the operating parameters, the design parameters and the pertinent physico-chemical properties to the simulator. This is done via an interactive program, SIM.FOR. Following is the list of variables, which the user has to provide, prior to the execution of the main simulator:

Design and Operating Conditions:

Operating temperature (K)

Operating Pressure (Atm)

Reactor Diameter (cm)

Reactor Height (cm)

Weight of Catalyst Charged (gm)

Weight of Suspension (gm)

Particle Diameter (cm)

Inlet Feed Conditions:

Inlet gas velocity (cm/sec)

CO/H_2 molar ratio

Inlet H_2 mole fraction

Physico-Chemical Properties:

Catalyst Density (gm/cm^3)

Kinetic Parameters:

Activation Energy (kJ/gmol)

Pre-Exponential factor $(sec\ \%\ Fe)^{-1}$

CO/H_2 usage ratio

Volumetric contraction factor

All the data provided by the user is stored in a data file and retrieved by the main simulator, during execution. Once the data is supplied, the main simulator, FISHER.FOR can be executed.

The output from FISHER.FOR is stored in a result file, and can be accessed by the user. The result file includes all the input data supplied by the user, along with the variation of syn-gas conversion, the concentration of H_2 in the gas and the liquid phase, along the reactor. The variation of superficial gas velocity along the reactor, is also indicated in the result file.

Following is a list of subroutines used in the main simulator:

Subroutine Name	Purpose
INPUT	Retrieves of input data from the data file
HOLDUP	Computes the gas holdup
MASTRN	Computes $k_L a$ for the reactor
LIQDEN	Computes the density of the liquid phase
LIQVIS	Computes the viscosity of the liquid phase
SLUVIS	Computes the viscosity of the slurry
SLUDEN	Computes the density of the slurry
VOLFRA	Computes the volume fraction of the catalyst phase
GASDIF	Computes the dispersion coefficient in the gas phase
LIQDIF	Computes the dispersion coefficient in the liquid phase
SOLDIF	Computes the solid dispersion coefficient
TERVEL	Computes the terminal settling velocity
CATCON	Computes the catalyst concentration along the reactor
LIQSOL	Computes the $K_s a_{SL}$ for the reactor

The user can update any of the above subroutines, by making appropriate changes in the correlations presently used.

Case Study

The program was used to predict the performance of a large scale BCSR. The data generated at the Rheinpreussen-Koppers plant, as reported by Kolbel and Ralek (1980), was used. Similar prediction of the performance has been reported by Deckwer et al. (1980).

The design parameters used include an effective diameter of 129 cm and a suspension height of 7.7 m. The operating temperature was assumed to be 273°C, with an inlet CO/H_2 ratio of 1.5. Kinetic parameters, as reported by Deckwer (1980), were used. The data required for the simulator is input via SIM.FOR. A typical input sample is as shown. The main simulator, FISHER.FOR is executed in a batch mode with a core requirement of 80 K. The execution statement to be used is, .EX FISHER.FOR,MTH:COLSYS.REL. The output files obtained are as indicated. The results agree satisfactorily with those reported by Deckwer et al. (1980). The variation of syngas conversion along the reactor length is as indicated in Figure A-B-1. Variation of H_2 concentration in the gas and the liquid phase and the superficial gas velocity along the reactor length are as shown in Figure A-B-2 and Figure A-B-3 respectively.

The dispersion in the liquid phase is large for the above operating conditions, which can be appreciated from the relatively flat catalyst concentration profile as shown in Figure A-B-4 . An outlet conversion of CO + H_2 of 87 percent is predicted as against 88 percent, reported by Kolbel and Ralek (1980).

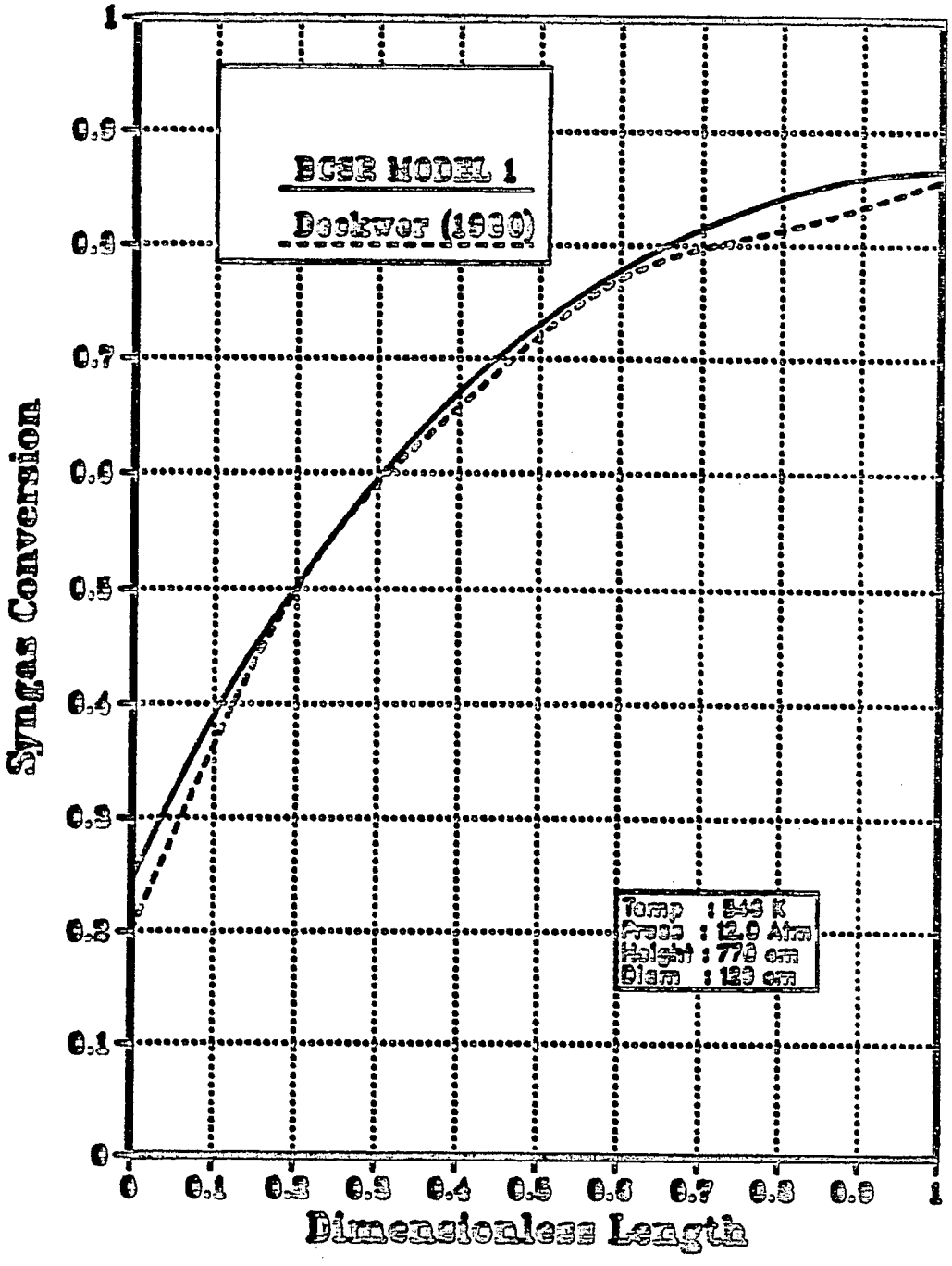

Figure A-B-1: Variation of Syngas Conversion along length

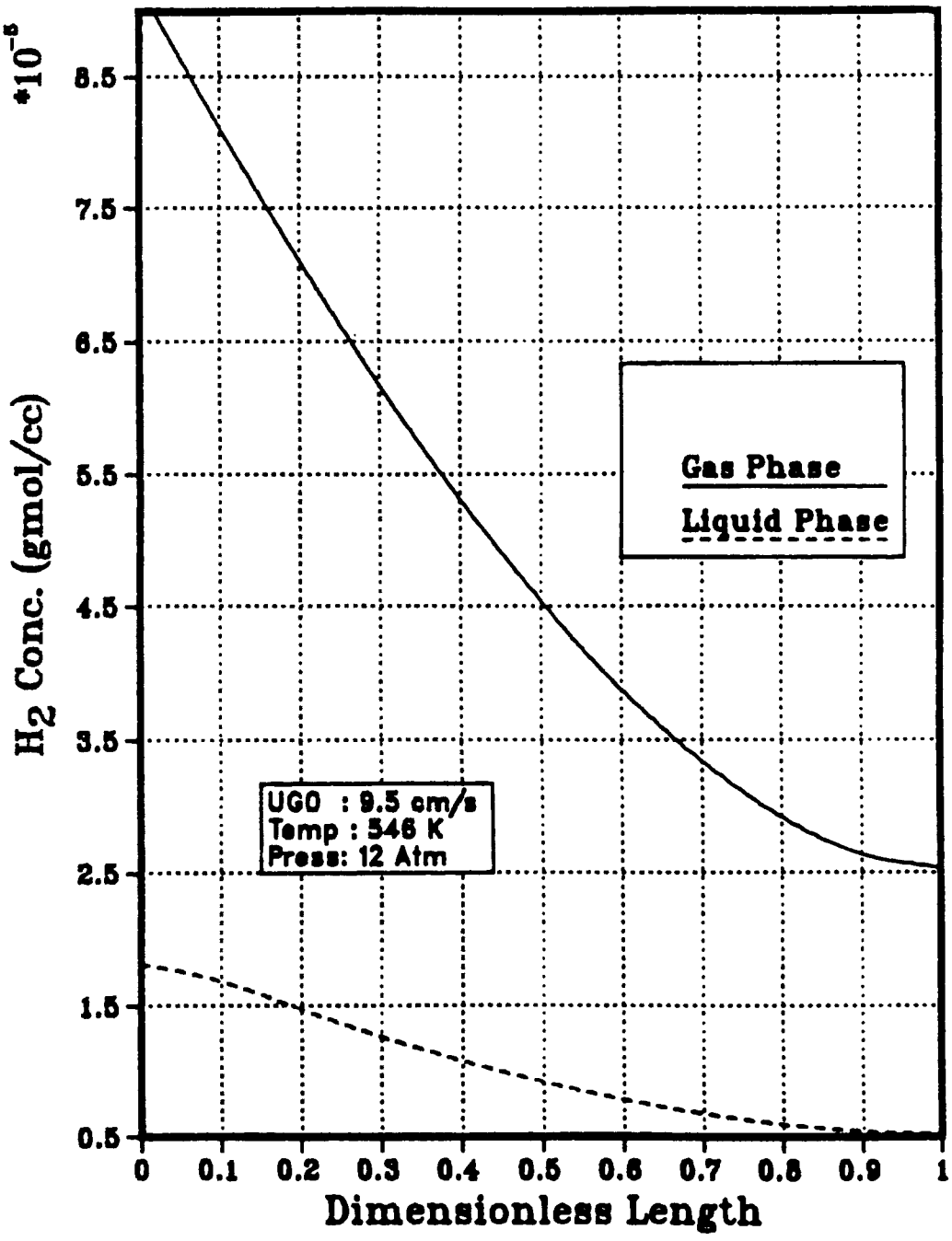

Figure A-B-2: Variation of H_2 concentration along length

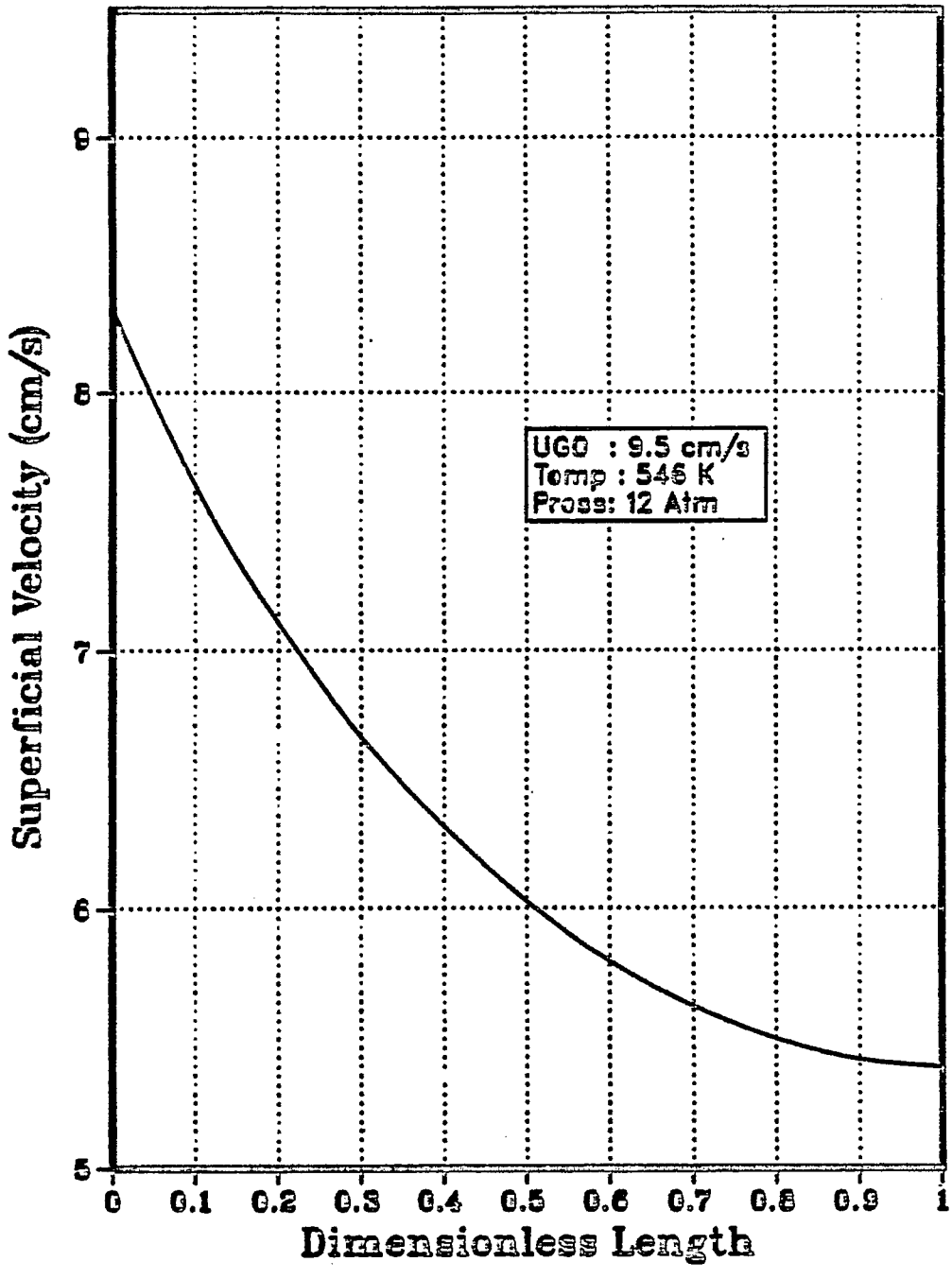

Figure A-B-3: Variation of superficial gas velocity along length

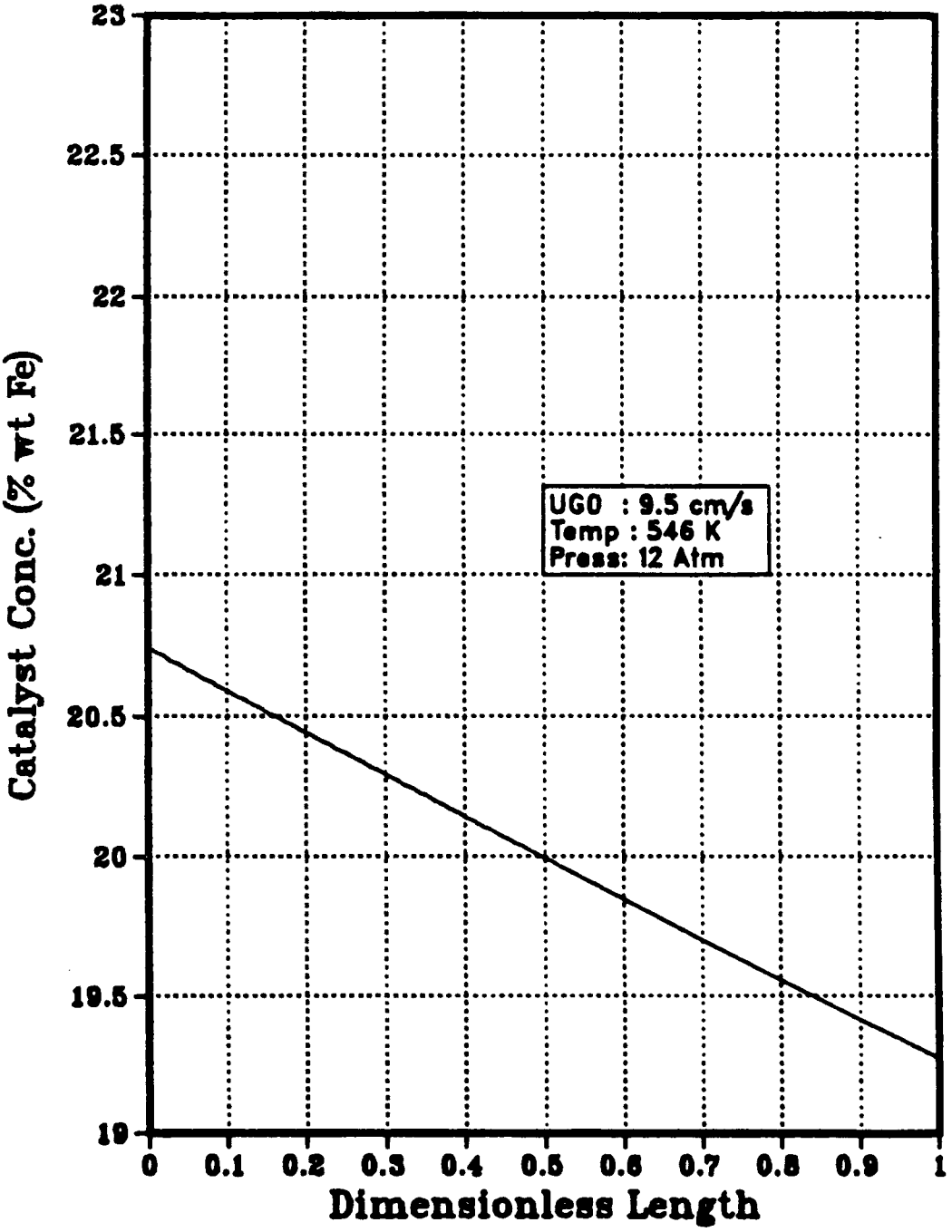

Figure A-B-4: Catalyst concentration profile along length

TYPICAL INPUT SAMPLE: SIM.FOR

```
THIS IS AN INTERACTIVE PROGRAM
IT WILL ASSIST YOU TO INPUT THE REQUISITE VARIABLES
INPUT ALL THE DATA IN FREE FORMAT
-------------------------------------------------
FOLLOWING ARE THE OPERATING VARIABLES

OPERATING TEMP.(DEG.K)=?
>546
OPERATING PRESS.(ATM)=?
>12
REACTOR DIAM (CM)=?
>129
REACTOR HEIGHT (CM)=?
>770
WT. OF CATALYST (GM)=?
>20
WT. OF SUSPENSION (GM)=?
>100
PARTICLE DIAMETER (CM)=?
>0.005
-------------------------------------------------
FOLOWING ARE THE FEED CONDITIONS

INPUT THE INLETGAS VELOCITY(CM/SEC)
>9.5
INPUT THE INLET CO/H2 MOLAR RATIO
>1.5
INPUT THE INLET H2 MOLE FRACTION
>0.4
-------------------------------------------------
FOLLOWING ARE THE PHYSICOCHEMICAL PROPERTIES

WHAT IS THE CATALYST DENSITY (GM/CM**3)=?
>5.0
-------------------------------------------------

THIS SIMULATOR CAN HANDLE THE FOLLOWING MODEL
1.....FIRST ORDER IN HYDROGEN CONC.
-------------------------------------------------
 INPUT THE ACTIVATION ENERGY (kJ/mol)
>70
 INPUT THE PRE-EXPONENTIAL FACTOR (per sec %Fe)
>1.12E5
INPUT THE CO/H2 USAGE RATIO
>1.5
INPUT THE CONTRACTION FACTOR
>-0.5
-------------------------------------------------
ALL THE DATA HAS BEEN TRANSFERED TO SIM.DAT

CHECK THE DATA IN FILE: SIM.DAT

OTHERWISE PROCEED TO THE SIMULATOR
```

OUTPUT FILE: RESULT.DAT

FISCHER-TROPSCH SYNTHESIS IN BUBBLE COLUMN REACTOR

DESIGN PARAMETERS :

REACTOR DIAMETER : 129.000 Cm
REACTOR HEIGHT : 770.000 Cm

OPERATING PARAMETERS :

REACTOR TEMPERATURE : 273.000 Deg.C
REACTOR PRESSURE : 12.000 Atm.

FEED CONDITIONS :

INLET GAS VELOCITY : 9.500 Cm/sec
INLET CO/H2 MOLAR RATIO : 1.50
INLET H2 MOLE FRACTION : 0.40
CATALYST LOADING : 0.200
CATALYST PARTICLE SIZE : 0.005 Cm
DENSITY OF THE CATALYST : 5.000 Gm/cc

KINETIC PARAMETERS :

A FIRST ORDER KINETIC EXPRESSION IN H2 CONC. IS USED

CO/H2 USAGE RAT : 1.50
RATE CONST. : 0.009 1/Sec
CONTRACTION FACTOR : -0.50

LEN cm	CGH mol/cc	CLH mol/cc	SUP V cm/s	CONSYN %
0.000	.9216E-04	.1810E-04	8.33497	24.52701
77.000	.8120E-04	.1681E-04	7.84813	38.98678
154.000	.7120E-04	.1475E-04	7.11393	50.23296
231.000	.6180E-04	.1271E-04	6.67521	59.46928
308.000	.5316E-04	.1086E-04	6.31735	67.00309
385.000	.4547E-04	.9243E-05	6.02962	73.08080
462.000	.3886E-04	.7873E-05	5.80227	77.84702
539.000	.3341E-04	.6765E-05	5.62737	81.52915
616.000	.2921E-04	.5933E-05	5.49975	84.21571
693.000	.2642E-04	.5404E-05	5.41817	85.93327
770.000	.2537E-04	.5219E-05	5.38788	86.57145

WHSV = 2.635 STY=.144E-04

PROGRAM LISTING: SEM.FOR

```
C       THIS INTERACTIVE PROGRAM WOULD ASSIST YOU IN USING THE SIMULATOR
C       IT IS DEVISED TO HELP IN INPUTING THE REQUISITE DATA TO THE SIMULATOR
C       THE DATA IS DIVIDED INTO THE FOLLOWING GROUPS:
C       1 FEED AND OPERATING CONDITIONS
C       2 PHYSICOCHEMICAL PROPERTIES
C       3 KINETIC PARAMETERS
C       ------------------------------------------------------------------
C       FOLLOWING IS THE LIST OF TYPE 1 SYMBOLS USED IN THE SIMULATOR
C       DIAM = REACTOR DIAMETER(CM)
C       L = REACTOR HEIGHT(CM)
C       Z = DIMENSIONAL AXIAL DISTANCE
C       T = OPERATING TEMPERATURE (DEG. K)
C       P = OPERATING PRESSURE (ATM)
C       UG = SUPERFICIAL VELOCITY OF GAS (CM/SEC)
C       UL = SUPERFICIAL VELOCITY OF SLURRY (CM/SEC)
C       MCAT = WEIGHT OF THE CATALYST (GM)
C       MSUS = WEIGHT OF THE SUPENSION(GM)
C       CGHO =INLET H2 MOLE FRACTION
C       UGO =INLET SUPERFICIAL VELOCITY(CM/SEC)
C       RAT =INLET CO/H2 MOLAR RATIO
C       ------------------------------------------------------------------
C       FOLLOWING IS THE LIST OF TYPE 2 SYMBOLS USED IN THE SIMULATOR
C       DENCAT= DENSITY OF THE CATALYST (GM/CM**3)
C       ------------------------------------------------------------------
C       FOLLOWING IS THE LIST OF TYPE 3 SYMBOLS USEDIN THE SIMULATOR
C       K = KINETIC CONSTANT FOR FIRST ORDER KINETIC EXPRESSION
C       USE=USAGE RATIO
C       ALPHA= CONTRACTION FACTOR
C       ==================================================================
        REAL T,P,QGAS,QSLUR,DIAM,L,MCAT,MSUS,K,FN,AN,BN
        INTEGER CHOICE
        OPEN(UNIT=1,FILE='FORO1.DAT')
        WRITE*,'THIS IS AN INTERACTIVE PROGRAM'
        WRITE*,'IT WILL ASSIST YOU TO INPUT THE REQUISITE VARIABLES'
        WRITE*,'INPUT ALL THE DATA IN FREE FORMAT'
        WRITE*,'-----------------------------------------------------'
        WRITE*,'FOLLOWING ARE THE OPERATING VARIABLES'
        WRITE*
        WRITE*,'OPERATING TEMP.(DEG.K)=?'
        READ*,T
        WRITE(1,200)T
        WRITE*,'OPERATING PRESS.(ATM)=?'
        READ*,P
        WRITE(1,200)P
        WRITE*,'REACTOR DIAM (CM)=?'
        READ*,DIAM
        WRITE(1,200)DIAM
        WRITE*,'REACTOR HEIGHT (CM)=?'
        READ*,L
        WRITE(1,200)L
        WRITE*,'WT. OF CATALYST (GM)=?'
        READ*,MCAT
        WRITE(1,200)MCAT
        WRITE*,'WT. OF SUSPENSION (GM)=?'
        READ*,MSUS
        WRITE(1,200)MSUS
        WRITE*,'PARTICLE DIAMETER (CM)=?'
        READ*,DP
        WRITE(1,200)DP
        WRITE*,'-----------------------------------------------'
```

```
      WRITE*,'FOLOWING ARE THE FEED CONDITIONS'
      WRITE*,'INPUT THE INLET GAS VELOCITY(CM/SEC)'
      READ*,UGO
      WRITE(1,200)UGO
      WRITE*,'INPUT THE INLET CO/H2 MOLAR RATIO'
      READ*,RAT
      WRITE(1,200)RAT
      WRITE*,'INPUT THE INLET H2 MOLE FRACTION'
      READ*,CGHO
      WRITE(1,200)CGHO
      WRITE*,'------------------------------------------------'
      WRITE*,'FOLLOWING ARE THE PHYSICOCHEMICAL PROPERTIES'
      WRITE*
      WRITE*,'WHAT IS THE CATALYST DENSITY (GM/CM**3)=?'
      READ*,DENCAT
      WRITE(1,200)DENCAT
      WRITE*,'------------------------------------------------'
      WRITE*
      WRITE*,'THIS SIMULATOR CAN HANDLE THE FOLLOWING MODEL '
      WRITE*,'1.....FIRST ORDER IN HYDROGEN CONC.'
      WRITE*,'------------------------------------------------'
      WRITE*,' INPUT THE ACTIVATION ENERGY (kJ/mol)'
      READ*,EA
      WRITE(1,200)EA
      WRITE*,' INPUT THE PRE-EXPONENTIAL FACTOR (per sec %Fe)
      READ*,PF
      WRITE(1,200)PF
      WRITE*,'INPUT THE CO/H2 USAGE RATIO'
      READ*,USE
      WRITE(1,200)USE
      WRITE*,'INPUT THE CONTRACTION FACTOR'
      READ*,ALPHA
      WRITE(1,200)ALPHA
      WRITE*,'------------------------------------------------'
      WRITE*,'ALL THE DATA HAS BEEN TRANSFERED TO FORO1.DAT'
      WRITE*
      WRITE*
      WRITE*,'OTHERWISE PROCEED TO THE SIMULATOR'
200   FORMAT(F15.5)
300   FORMAT(I2)
      CLOSE(UNIT=1)
      STOP
      END
```

PROGRAM LISTING: FISHER.FOR

```
C       ------------------------------------------------------------------
C       THIS IS THE MAIN SIMULATOR FOR FT SYNTHESIS IN A BUBBLE COLUMN REACTOR
C       FOR A GIVEN SET OF OPERATING AND DESIGN PARAMETERS IT EVALUATES THE
C       SYN GAS CONVERSION ALONG THE REACTOR HEIGHT.
C       THE REQUISITE DATA IS RETRIEVED FROM SIM.FOR
C      ------------------------------------------------------------------

C       FOLLOWING IS A LIST OF THE MAJOR VARIABLES USED :

C       T        :TEMPERATURE (DEG K)
C       P        :PRESSURE (ATM)
C       DIAM     :REACTOR DIAMETER (CM)
C       AL       :REACTOR HEIGHT (CM)
C       AMCAT    :WT. OF CATALYST (GM)     ¦ This ratio should be equal
C       AMSUS    :WT. OF SUSPENSION (GM)   ¦ to the catalyst loading.
C       DP       :DIAMETER OF PARTICLE (CM)
C       UGO      :INLET GAS VELOCITY (CM/SEC)
C       RAT      :INLET CO/H2 MOLAR RATIO
C       CGHO     :INLET MOLE FRACTION OF H2
C       DENCAT   :DENSITY OF CATALYST (GM/CC)
C       EA       :ACTIVATION ENERGY (kJ/MOL)
C       PF       :FREQUENCY FACTOR (per sec,%Fe)
C       USE      :USAGE RATIO
C       ALPHA    :VOLUMETRIC CONTRACTION FACTOR

C       ------------------------------------------------------------------


C       THIS IS THE MAIN PROGRAM


        IMPLICIT REAL*8(A-H,O-Z)

        DIMENSION M(2),ZETA(4),IPAR(11),LTOL(2),TOL(2),Z(4),S(100)
        DIMENSION ISPACE(800),FSPACE(15000),B(15)

        COMMON/PAR2/AL,CGHO,AM
        COMMON/PAR3/ALPHA,CONSYN,USE,RAT
        COMMON/PAR4/UG,PEG,STG,EG,EL,PEL,AKLA
        COMMON/PAR1/UGO,CCAT,AK,UGB,NITER
        COMMON/PAR5/EGO,DGHO,DLHO
        COMMON/PAR6/T,DENSL,VISSL,VISL
        COMMON/PAR7/DIAM,P
        COMMON/PAR8/DENL,AMCAT,AMSUS,DENCAT,DP,VCAT,WCAT
        COMMON/COEF/ AAST

        EXTERNAL FSUB,DFSUB,GSUB,DGSUB

        OPEN (UNIT=3,FILE='OUT.DAT')

        CALL INPUT

        AREA=(22.0/(7.0*4.0))*(DIAM**2.0)
        VFR=AREA*UGO
        DEN1=CGHO*P*2.0/(82.05*T)
        DEN2=(1.0-CGHO)*P*28.0/(82.05*T)
        DENM=DEN1+DEN2
        WTSOL=800000.0

        WHSV=VFR*DENM*3600.0/WTSOL
```

```
      CIN=P*CGHO/(82.05*T)



      WRITE(3,*)' FISCHER-TROPSCH SYNTHESIS IN BUBBLE COLUMN REACTOR'

      WRITE(3,*)
      WRITE(3,*)' DESIGN PARAMETERS :'
      WRITE(3,*)' -------------------'
      WRITE(3,*)
      WRITE(3,270)' REACTOR DIAMETER                    :',DIAM,' Cm'
      WRITE(3,270)' REACTOR HEIGHT                   :',AL,' Cm'
      WRITE(3,*)
      WRITE(3,*)' OPERATING PARAMETERS :'
      WRITE(3,*)' ----------------------'
      WRITE(3,*)
      WRITE(3,270)' REACTOR TEMPERATURE                 :',T-273,' Deg.C'
      WRITE(3,270)' REACTOR PRESSURE                    :',P,' Atm.'
      WRITE(3,*)
      WRITE(3,*)' FEED CONDITIONS :'
      WRITE(3,*)' -----------------'
      WRITE(3,*)
      WRITE(3,270)' INLET GAS VELOCITY                  :',UGO,' Cm/sec'
      WRITE(3,280)' INLET CO/H2 MOLAR RATIO             :',RAT
      WRITE(3,280)' INLET H2 MOLE FRACTION              :',CGHO
      WRITE(3,270)' CATALYST LOADING                    :',AMCAT/AMSUS
      WRITE(3,270)' CATALYST PARTICLE SIZE              :',DP,' Cm'
      WRITE(3,270)' DENSITY OF THE CATALYST             :',DENCAT,' Gm/cc'
      WRITE(3,*)
      WRITE(3,*)' KINETIC PARAMETERS :'
      WRITE(3,*)' --------------------'
      WRITE(3,*)
      WRITE(3,*)' A FIRST ORDER KINETIC EXPRESSION IN H2 CONC. IS USED'
      WRITE(3,*)
      WRITE(3,280)' CO/H2 USAGE RAT                     :',USE
      WRITE(3,270)' RATE CONST.                         :',AK,' 1/Sec'
      WRITE(3,280)' CONTRACTION FACTOR                  :',ALPHA
      WRITE(3,*)
      WRITE(3,*)
      WRITE(3,*)
      WRITE(3,*)
      WRITE(3,300)

      WRITE(3,260)'LEN',' CGH','CLH','SUP V','CONSYN'
      WRITE(3,260)'cm','mol/cc','mol/cc','cm/s','%'
      WRITE(3,300)

      WRITE(8,220)' X','SUPVEL','GAS HOLDUP'
      WRITE(9,220)' X','SUPVEL','MASTRN COEF'
      WRITE(10,220)' X','SUPVEL','CAT. CONC.'

      R=82.056

C     CT= TOTAL GAS CONCENTRATION

      CT=P/(R*T)

C     FOLLOWING SET OF STATEMENTS SPECIFY THE COLSYS CHOICES USED
```

```
      NCOMP=2
      M(1)=2
      M(2)=2
      ALEFT=0.D0
      ARIGHT=1.D0
      ZETA(1)=0.D0
      ZETA(2)=0.D0
      ZETA(3)=1.D0
      ZETA(4)=1.D0

      DO 11 I=1,11
11    IPAR(I)=0
      IPAR(1)=1
      IPAR(4)=2
      IPAR(5)=15000
      IPAR(6)=800
      IPAR(7)=1
      LTOL(1)=1
      LTOL(2)=3
      TOL(1)=1.D-3
      TOL(2)=1.D-3
      L=1

15    CALL COLSYS(NCOMP,M,ALEFT,ARIGHT,ZETA,IPAR,LTOL,TOL,FIXPNT,
     *  ISPACE,FSPACE,IFLAG,FSUB,DFSUB,GSUB,DGSUB,DUMMY)

      WRITE(3,*)' IFLAG=',IFLAG
      IF(IFLAG.NE.1) STOP


      X=0.D0

C     FOLLOWING DO LOOP EVALUATES THE FINAL RESULTS

      DO 20 J=1,11
      CALL APPSLN(X,Z,FSPACE,ISPACE)

      AAST=ALPHA*((1.+USE)/(1.+RAT))
      CONVH=1.-Z(1)*((1.+AAST)/(1.+AAST*Z(1)))
      CONSYN=((1.+USE)*CONVH)/(1.+RAT)
      UG=UGO*((1.+AAST)/(1.+AAST*Z(1)))


      WRITE(3,250)X*AL,Z(1)*CGHO*CT,Z(3)*CGHO*CT/AM,
     *  UGO*(1.+ALPHA*CONSYN),CONSYN*100.0
      CALL HOLDUP(EG,UG)
      CALL MASTRN(UG,AKLA)

      WRITE(8,210)X,UG,EG
      WRITE(9,210)X,UG,AKLA
      CALL CATCON(DIAM,DENSL,DENL,VISL,AMCAT,AMSUS,DENCAT,CCAT,X,
     *  T,DP)
      WRITE(10,*)X,UG,CCAT


      X=X+0.1D0

20    CONTINUE
```

```
25      WRITE(3,300)
        UOUT=UGO*(1.0+ALPHA*CONSYN)
        COUT=Z(1)*CGHO*CT
        GARY=((UGO*CIN)-(UOUT*COUT))*AREA
        STY=GARY/WTSOL

        WRITE(3,310)' WHSV =',WHSV,'STY=',STY

        WRITE(3,*)'1'
200     FORMAT(F12.5)
210     FORMAT(X,3(F7.5,3X))
220     FORMAT(5X,3(A,5X))
250     FORMAT(X,F8.3,2X,2(E9.4,3X),2(F8.5,5X))
260     FORMAT(5X,5(A,7X))
270     FORMAT(X,A,F8.3,A)
280     FORMAT(X,A,F6.2)
300     FORMAT(65('-'))
310     FORMAT(2X,A,F6.3,3X,A,E8.3)

        STOP
        END
C       ------------------------------------------------------------------
        SUBROUTINE FSUB(X,Z,F)

C       THIS SUBROUTINE DEFINES THE DIFFERENTIAL EQNS. AS PER COLSYS


        IMPLICIT REAL*8(A-H,O-Z)

        DIMENSION F(2),Z(4),SUP(50)

        COMMON/PAR1/ UGO,CCAT,AK,UGB,NITER
        COMMON/PAR2/ AL,CGHO,AM
        COMMON/PAR3/ALPHA,CONSYN,USE,RAT
        COMMON/PAR4/UG,PEG,STG,EG,EL,PEL,AKLA
        COMMON/PAR5/EGO,DGHO,DLHO
        COMMON/PAR6/T,DENSL,VISSL,VISL
        COMMON/PAR7/DIAM,P
        COMMON/PAR8/DENL,AMCAT,AMSUS,DENCAT,DP,VCAT,WCAT
        COMMON/COEF/ AAST

        AAST=ALPHA*((1.+USE)/(1.+RAT))
        CONVH=1.-Z(1)*((1.+AAST)/(1.+AAST*Z(1)))
        CONSYN=(1.+USE)*CONVH/(1.+RAT)
        UG=UGO*((1.+AAST)/(1.+AAST*Z(1)))

        IF(NITER.NE.2) GOTO 30
        UGA=UGB
        GOTO 40

30      UGA=UG
40      CALL HOLDUP(EG,UGA)
        CALL GASDIF(UGA,EG,DGH)
        PEG=(UGO*AL)/DGH
        CALL MASTRN(UGA,AKLA)
        STG=(AKLA*AL)/(AM*UGO)
        CALL LIQDIF(UGA,DLH)
        PEL=(UGO*AL)/DLH
        EL=1.-EG
        CALL CATCON(DIAM,DENSL,DENL,VISL,AMCAT,AMSUS,DENCAT,CCAT,X,
```

```
     *  T,DP,UGA)

        CALL LIQSOL(UGA,EL,DLH,AS,AKS,DENCAT,DP,WCAT,DENL,VISL,DENSL)

        BETA=(1./(AK*CCAT*EL))/((1./AKLA)+(1./(AK*CCAT*EL)))

        EFF=1.D0/(1.D0+(AK*CCAT*EL/(AKS*AS)))

        BL=(1.+AAST)/((1.+AAST*Z(1))**2.)

        F(1)=(BL*Z(2)+STG*(Z(1)-Z(3)))*PZG/EG
        F(2)=((CCAT*EFF*AK*EL*AL*Z(3)/UG0)-STG*AH*(Z(1)-Z(3)))*PZL/EL


        RETURN
        END
C       ------------------------------------------------------------

        SUBROUTINE DFSUB(X,Z,DF)

C       THIS IS A SUPPORTING SUBROUTINE TO COLSYS

        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION Z(4),DF(2,4),WORK1(2),WORK2(2)

        EPS=1.0E-7
        DO 10 J=1,4
        Z(J)=Z(J)+EPS
        CALL FSUB(X,Z,WORK1)
        Z(J)=Z(J)-2.*EPS
        CALL FSUB(X,Z,WORK2)
        Z(J)=Z(J)+EPS
        DO 10 I=1,2
 10     DF(I,J)=(WORK1(I)-WORK2(I))*.5/EPS
        RETURN
        END
C       ------------------------------------------------------------------
        SUBROUTINE GSUB(I,Z,G)

C       THIS SUBROUTINE DEFINES THE BOUNDARY CONDITIONS

        IMPLICIT REAL*8(A-H,O-Z)

        COMMON/PAR1/ UG0,CCAT,AK
        COMMON/PAR2/ AL,CGH0,AH
        COMMON/PAR3/ EG0,DGH0,DLH0
        COMMON/COEF/ AAST

        DIMENSION Z(4)

        GOTO(1,2,3,4),I
1       G=(EG0*DGH0/(AL*UG0))*Z(2)-((1.+AAST)*Z(1)/(1.+AAST*Z(1)))+1.D0
        RETURN
3       G=Z(2)-0.0
        RETURN
2       G=Z(4)-0.0
        RETURN
4       G=Z(4)-0.0
        RETURN
        END
```

```
C     ------------------------------------------------------------------
      SUBROUTINE DGSUB(I,Z,DG)

C     THIS IS A SUPPORTING SUBROUTINE

      IMPLICIT REAL*8(A-H,O-Z)

      COMMON/PAR1/ UGO,CCAT,AK
      COMMON/PAR2/ AL,CGHO,AM
      COMMON/PAR5/ EGO,DGHO,DLHO
      COMMON/COEF/ AAST

      DIMENSION DG(4),Z(4)

      DO 11 J=1,4
 11   DG(J)=0.0

      GOTO(1,2,3,4),I
1     DG(1)=-(1.+AAST)/((1.+AAST*Z(1))**2.0)
      DG(2)=EGO*DGHO/(AL*UGO)
      RETURN
3     DG(2)=1.D0
      RETURN
2     DG(4)=1.D0
      RETURN
4     DG(4)=1.D0

      RETURN
      END
C     ------------------------------------------------------------------
      SUBROUTINE DUMMY
      RETURN
      END
C     ------------------------------------------------------------------
      SUBROUTINE HOLDUP(EG,UGA)
      IMPLICIT REAL*8(A-H,O-Z)

C     THIS SUBROUTINE EVALUATES THE GAS PHASE HOLDUP
C     IT USES THE CORRELATION PROPOSED BY DECKWER

C     FOLLOWING ARE THE INPUT VARIABLES:
C     UGA=SUPERFICIAL VELOCITY (Cm/sec)
C     FOLLOWING IS THE OUTPUT VARIABLE:
C     EG= GAS HOLD UP

      EG=0.053D0*(UGA**1.1D0)
      RETURN
      END
C     ------------------------------------------------------------------
      SUBROUTINE MASTRN(UGA,AKLA)


      IMPLICIT REAL*8(A-H,O-Z)

      COMMON/PAR6/T,DENSL,VISSL,VISL

C     THIS SUBROUTINE EVALUATES THE KLA (1/sec)
C     INPUT VARIABLES;
C     UG= SUPERFICIAL VELOCITY
C     DENSL= DENSITY OF SLURRY (gm/cm**3)
```

```
C       VISSL= VISCOSITY OF SLURRY (gm/cm/sec)
C       T= TEMPERATURE (Deg. K)
C       OUTPUT VARIABLES:
C       AKLA= MASS TRANSFER COEFF. (1/sec)

        A=4.5D0*(UGA**1.1D0)

        AKL=0.116ED0*(((DENSL*EXP(-4570.D0/T))/VISSL)**(0.333D0))
        AKLA=AKL*A

        RETURN
        END
C       ------------------------------------------------------
        SUBROUTINE LIQDEN(DENL)

        IMPLICIT REAL*8(A-H,O-Z)

        COMMON/PARS/T,DENSL,VISSL,VISL

C       THIS SUBROUTINE EVALUATES THE DENSITY OF THE LIQ. PHASE
C       IT USES THE CORRELATION PROPOSED BY DECKWER (1980)

C       INPUT VARIABLES:
C       T= TEMPERATURE (Deg. K)
C       OUTPUT VARIABLES:

        DENL=0.758D0-(0.555D-3*(T-373.0D0))

        RETURN
        END
C       ------------------------------------------------------------
        SUBROUTINE LIQVIS(VISL)

        IMPLICIT REAL*8(A-H,O-Z)

        COMMON/PARS/T,DENSL,VISSL

C       THIS SUBROUTINE EVALUATES THE VISCOSITY OF THE LIQ. PHASE
C       IT USES THE CORRELATION PROPOSED BY DECKWER

C       INPUT VARIABLES :
C       T= TEMPERATURE (Deg. K)
C        OUTPUT VARIABLES:
C       VISL= LIQUID VISCOSITY (gm/cm/sec)

        VISL=0.052D0*EXP(-6.905D0+3286.D0/T)

        RETURN
        END
C       ------------------------------------------------------------------
        SUBROUTINE SLUVIS(VISL,VCAT,VISSL)
        IMPLICIT REAL*8(A-H,O-Z)

C       THIS SUBROUTINE EVALUATES THE VISCOSITY OF THE SLURRY

C       INPUT VARIABLES;
C       VISL= VISCOSITY OF LIQUID (gm/cm/sec)
C       VCAT=VOLUME FRACTION OF CAT IN SLURRY
C       OUTPUT VARIABLES :
C       VISSL= VISCOSITY OF SLURRY (gm/cm/sec)
```

```
      VISSL=VISL*(1.0D0+4.5D0*VCAT)

      RETURN
      END
C     ------------------------------------------------------------
      SUBROUTINE SLUDEN(VCAT,DENCAT,DENL,DENSL)

      IMPLICIT REAL*8(A-H,O-Z)

C     THIS SUBROUTINE EVALUATES THE DENSITY OF THE SLURRY

C     INPUT VARIABLES:
C     VCAT= VOLUME FRACTION OF THE CATALYST IN THE SLURRY
C     DENCAT= DENSITY OF THE CATALYST
C     DENL= DENSITY OF THE LIQUID (gm/cm**3)
C     OUTPUT VARIABLES:
C     DENSL= DENSITY OF THE SLURRY (gm/cm**3)

      DENSL=VCAT*DENCAT+(1.D0-VCAT)*DENL

      RETURN
      END
C     ------------------------------------------------------------
      SUBROUTINE VOLFRA(AMCAT,AMSUS,DENL,DENCAT,WCAT,VCAT)

      IMPLICIT REAL*8(A-H,O-Z)

C     THIS SUBROUTINE EVALUATES THE VOLM. FRACTION OF THE CATALYST

C     INPUT VARIABLES:
C     AMCAT= WT. OF THE CATALYST (gm)
C     AMSUS= WT. OF THE SUSPENSION (gm)
C     DENL= DENSITY OF THE LIQUID (gm/cm**3)
C     DENCAT= DENSITY OF THE CATALYST (gm/cm**3)
C     OUTPUT VARIABLES :
C     WCAT= CATALYST LOADING
C     VCAT= VOLUME FRACTION OF THE CATALYST

      WCAT=AMCAT/AMSUS
      VCAT=(DENL*WCAT)/(DENCAT-WCAT*(DENCAT-DENL))

      RETURN
      END
C     ------------------------------------------------------------
      SUBROUTINE SUPVEL(DIAM,QGAS,QSLUR,S,UG,UL)

      IMPLICIT REAL*8(A-H,O-Z)

C     THIS SUBROUTINE EVALUATES THE SUPERFICIAL VELOCITY OF THE GAS
C     AND THE LIQUID PHASE

C     INPUT VARIABLES:
C     DIAM= DIAMETER OF THE REACTOR (cm)
C     QGAS= VOLM. FLOW RATE OF GAS (Ccm*3/sec)
C     QSLUR= VOLM. FLOW RATE OF THE SLURRY (cm**3/sec)
C     OUTPUT VARIABLES:
C     S= CROSS SECTIONAL AREA (cm**2)
C     UG= SUPERFICIAL VELOCITY OF THE GAS (cm/sec)
C     UL= SUPERFICIAL VELOCITY OF THE SLURRY (cm/sec)
      S=(3.14159D0*(DIAM**2.D0))/4.D0
```

```
      UG=QGAS/S
      UL=QSLUR/S

      RETURN
      END
C     ------------------------------------------------------------
      SUBROUTINE GASDIF(UGA,EG,DGH)

      IMPLICIT REAL*8(A-H,O-Z)

      COMMON/PAR7/DIAM,P

C     THIS SUBROUTINE EVALUATES THE GAS PHASE DIFFUSIVITY
C     INPUT VARIABLES:
C     UG= SUPERFICIAL VELOCITY (cm/sec)
C     EG= GAS PHASE HOLD UP
C     DIAM= REACTOR DIAMETER (cm)
C     OUTPUT VARIABLES:
C     DGH= GAS PHASE DIFFUSIVITY OF H2 (cm**2/sec)

      DGH=(5.D-4)*((UGA/EG)**3.DO)*(DIAM**1.5DO)

      RETURN
      END
C     ------------------------------------------------------------
      SUBROUTINE LIQDIF(UGA,DLH)

      IMPLICIT REAL*8(A-H,O-Z)

      COMMON/PAR7/DIAM,P

C     THIS SUBROUTINE EVALUATES THE LIQ. PHASE DIFFUSIVITY

C     INPUT VARIABLES:
C     UG= SUPERFICIAL GAS VELOCITY (Cm/sec)
C     DIAM= REACTOR DIAMETER (cm)
C     OUTPUT VARIABLES:
C     DLH= LIQ. PHASE DIFFUSIVITY OF H2 (cm**2/sec)

      DLH=3.676DO*(UGA**0.32DO)*(DIAM**1.34DO)
      RETURN
      END
C     ------------------------------------------------------------
      SUBROUTINE SOLDIF(UGA,DIAM,DSOL)

      IMPLICIT REAL*8(A-H,O-Z)

C     THIS SUBROUTINE EVALUATES THE DIFFUSION OF THE SOLID PHASE

C     INPUT VARIABLES:
C     UG=SUPERFICIAL VELOCITY OF THE GAS
C     DIAM= DIAMETER OF THE REACTOR (cm)
C     OUTPUT VARIABLES:
C     DSOL= DIFFUSIVITY OF THE SOLIDS
C     G= GRAVITATIONAL ACCELERATION
C     FR= FROUDE NUMBER
C     BOC= BODENSTIEN NUMBER FOR SOLIDS

      G=980.
      FR=UGA/(G*DIAM)**0.5
```

```
      BOC=(13.DO*FR)/(1.DO+8.DO*(FR**0.85DO))
      DSOL=(UGA*DIAM)/BOC

      RETURN
      END
C     ------------------------------------------------------------
      SUBROUTINE TERVEL(DENSL,DENL,VISL,AMCAT,AMSUS,UT,UGA,T,DENCAT,DP)

      IMPLICIT REAL*8(A-H,O-Z)

C     THIS SUBROUTINE EVALUATES THE TERMINAL VELOCITY OF SOLIDS

C     INPUT VARIABLES:
C     DENSL= DENSITY OF THE SLURRY
C     DP= PARTICLE SIZE (cm)
C     VISL= VISCOSITY OF THE LIQUID (gm/cm/sec)
C     OUTPUT VARIABLES: -
C     UT= TERMINAL VELOCITY (Cm/sec)

      AMCAT1=AMCAT
      AMSUS1=AMSUS
      AMCAT=0.1DO/DENSL
      AMSUS=1.DO
      CALL VOLFRA(AMCAT,AMSUS,DENL,DENCAT,WCAT,VCAT)
      VAST= VCAT
      G=980.DO
      AR=(DENL*(DENCAT-DENL)*G*(DP**3.DO))/((VISL)**2.DO)
      RE=AR/18.0
      UT=(RE*VISL)/(DP*DENL)
      AMCAT=AMCAT1
      AMSUS=AMSUS1
      CALL VOLFRA(AMCAT,AMSUS,DENL,DENCAT,WCAT,VCAT)
      UT=1.2DO*UT*((UGA/UT)**0.25DO)*(((1.DO-VCAT)/(1.DO-VAST))**2.5DO)

      RETURN
      END
C     ------------------------------------------------------------
      SUBROUTINE CATCON(DIAM,DENSL,DENL,VISL,AMCAT,AMSUS,DENCAT,CCAT,X,
     *  T,DP,UGA)

      IMPLICIT REAL*8(A-H,O-Z)

C     THIS SUBROUTINE EVALUATES THE CATALYST CONC. AT A AXIAL POSN.

      COMMON/PAR2/AL,CGHO,AM
      COMMON/PAR4/UG,PEG,STG,EG,EL,PEL

      CALL SOLDIF(UGA,DIAM,DSOL)
      CALL TERVEL(DENSL,DENL,VISL,AMCAT,AMSUS,UT,UGA,T,DENCAT,DP)

      AVCON=0.2*DENSL

      CALL VOLFRA(AMCAT,AMSUS,DENL,DENCAT,WCAT,VCAT)

      SIL=1.0-VCAT

      ACAT=-(SIL*UT*AL)/DSOL
      CSO=(AVCON*ACAT)/(EXP(ACAT)-1.0)
      CCAT=CSO*EXP((-SIL*UT*AL*X)/DSOL)
```

```
      CCAT=(CCAT/DENSL)*100.0


      RETURN
     *END
C     ------------------------------------------------------------------
      SUBROUTINE LIQSOL(UGA,EL,DLH,AS,AKS,DENCAT,DP,WCAT,DENL,VISL,
     *DENSL)

      IMPLICIT REAL*8(A-H,O-Z)

C     THIS SUBROUTINE EVALUATES THE LIQ-SOL MASS TRNF COEFF.

      AS=(6.DO*WCAT*EL*DENSL)/(DP*DENCAT)
      IF(UGA.LE.6.0) GOTO 10
      EP=5885.DO
      GOTO 20
 10   EP=UGA*980.DO
 20   AKS=(DLH/DP)*(2.DO+0.545*((VISL/(DENL*DLH))**(0.333))*
     *((EP*(DP**4.0)*(DENL**3.0))/(VISL**3.0)))

      RETURN
      END
C     ------------------------------------------------------------------
      SUBROUTINE INPUT

      IMPLICIT REAL*8(A-H,O-Z)

      DIMENSION DAT(17)

C     THIS SUBROUTINE READS THE REQUISITE DATA FROM FORO1.DAT

      COMMON/PAR1/UGO,CCAT,AK
      COMMON/PAR2/AL,CGHO,AM
      COMMON/PAR3/ALPHA,CONSYN,USE,RAT
      COMMON/PAR5/EGO,DGHO,DLHO
      COMMON/PAR6/T,DENSL,VISSL,VISL
      COMMON/PAR7/DIAM,P
      COMMON/PAR8/DENL,AMCAT,AMSUS,DENCAT,DP,VCAT,WCAT

      DO 10 J=1,15
      READ (1,200)DAT(J)
10    CONTINUE
      T=DAT(1)
      P=DAT(2)
      DIAM=DAT(3)
      AL=DAT(4)
      AMCAT=DAT(5)
      AMSUS=DAT(6)
      DP=DAT(7)
      UGO=DAT(8)
      RAT=DAT(9)
      CGHO=DAT(10)
      DENCAT=DAT(11)
      EA=DAT(12)
      PF=DAT(13)
      USE=DAT(14)
      ALPHA=DAT(15)
      AM=4.3E
200   FORMAT(F15.5)
```

```
      AK=(PF/(1.+USE))*EXP(-EA*1.E3/(8.314*T))

      CALL HOLDUP(EGO,UGO)
      CALL GASDIF(UGO,EGO,DGHO)
      CALL LIQDIF(UGO,DLHO)
      CALL LIQDEN(DENL)
      CALL LIQVIS(VISL)
      CALL VOLFRA(AMCAT,AMSUS,DENL,DENCAT,WCAT,VCAT)
      CALL SLUDEN(VCAT,DENCAT,DENL,DENSL)
      CALL SLUVIS(VISL,VCAT,VISSL)

      RETURN
      END
C     ------------------------------------------------------------

C     END OF PROGRAM !
```

BCSR MODEL 2

Although equations based on both the plug flow and the axial dispersion assumptions have been developed in the present work, the computer program incorporating the latter assumption which is more general is included in the report. The program using the plug flow assumption has not been included for being concise, besides the axial dispersion model could be very easily adapted to assess the plug flow assumption by appropriate adjustment in the Peclet numbers for the gas and the liquid phase. However, the results obtained through both the programs have been counterchecked.

As described earlier for Model 1, the user has to supply the operating and the design parameters along with the pertinent physico-chemical properties to the simulator. This is done via an interactive program, INTER.FOR. Following is the list of variables which the user has to provide prior to the execution of the main simulator.

Design and Operating Conditions:

Operating Temperature (K)

Operating Pressure (Atm.)

Reactor Height (cm.)

Reactor Diameter (cm.)

Inlet Partial Pressure of H_2 (atm)

Inlet Partial Pressure of CO (atm)

Catalyst Loading

Physico Chemical Properties:

Solubility Coefficient for H_2O

Solubility coefficient for H_2

Solubility Coefficient for CO

Solubility Coefficient for Hydrocarbons

Density of the Catalyst (gm/cc)

Density of the Liquid Phase (gm/cc)

The kinetic parameters used in the simulator are provided via the interactive program ALPHA.FOR. The kinetic parameters include the activation energy (Kcal/mol), pre-exponential factor (gmol (gm of cat. sec. $atm^{a+b})^{-1}$), and the power law indices a_n and b_n for carbon numbers 1 to 4. The parameters used in the present work are listed in Table I-B-3. The data provided by the user is stored in two data files and is retrieved by the main simulator upon execution. The main simulator comprises of various subroutines, some of which define the boundary value problem to be solved using COLSYS, while the other subroutines incorporate the various correlations used for property estimation.

The following is a list of the subroutines used in the main simulator and their purpose:

Subroutine Name	Purpose
SIGMA	Evaluates the net depletion of components from the gas phase.
RHOH	Evaluates the kinetic contribution towards H_2 depletion.
RHON	Evaluates the kinetic contribution towards hydrocarbon formation.
INPUT	Retrieves the data supplied by the User.
CATCON	Evaluates the average catalyst concentration.
HOLDUP	Evaluates the gas phase holdup.

MASTRN	Evaluates the gas-liquid mass-transfer coefficient.
SLUDEN	Evaluates the density of the slurry.
VOLFRA	Evaluates the volume fraction of the solids.
VALUE	Evaluates the value of α as a function of temperature.
GASDIF	Evaluates the gas phase dispersion coefficient.
LIQDIF	Evaluates the liquid phase dispersion coefficient.
SUPER	Evaluates the superficial gas velocity along the reactor axis.

Besides these subroutines, other subroutines such as FSUB, DFSUB, GSUB, DGSUB, and SOLUTN have been used to define the problem as per the algorithm, COLSYS (Ascher et al., 1981).

On execution, the simulator generates results which are stored in files. The file specifications is as given below:

CONV.DAT	Stores all the input data provided by the user along with the concentration of the components and the syngas conversion along the reactor height.
SUP.DAT	Stores the values of superficial gas velocity along the reactor height.
LCON.DAT	Stores the concentrations of the components in the liquid phase along the reactor height.

Besides, output in the form of ratio ($RC_n/RC1$) along the reactor height can also be obtained from the simulator. These values are required to confirm the evidence that the product slate approximates to a Schulz-Flory distribution.

Case Study:

The program was used to predict the performance of a BCSR used on a laboratory scale, i.e., with a diamter of 2.6 cm and a suspension height of 180 cm. This column employed Ru/Al_2O_3 catalyst in order to bring about the F-T synthesis (Stern et al., 1984). Prediction of the syn-gas conversion and the usage ratio across the BCSR was made using both the plug flow model as well as the axial dispersion model. Based on the values of the Peclet numbers for the gas and the liquid phase, the performance can be satisfactorily explained using the plug flow assumption. The results obtained using both the assumptions tally very well with each other and also with the experimentally reported values.

The requisite input data was provided via INTER.FOR and ALPHA.FOR. Typical input samples of both the programs are as shown. The output files, viz., CONV.DAT, SUP.DAT and LCON.DAT obtained from the run are also shown herewith. Fig. A-B-5 and A-B-6 show the variation of the H_2 and CO concentration along the length in the gas and the liquid phases.

As indicated earlier, F-T synthesis over Ru catalyst can result in products ranging from methane to high molecular weight hydrocarbons depending upon the operating temperature and pressure. In this present case, since the operating pressure is moderately low, the amount of methane formed is significant. Furthermore, since the reaction stoichiometry assumed is the one for paraffin formation along with water, the amount of water formed is also significant, in fact from the stoichiometry, it is equal to the moles of CO

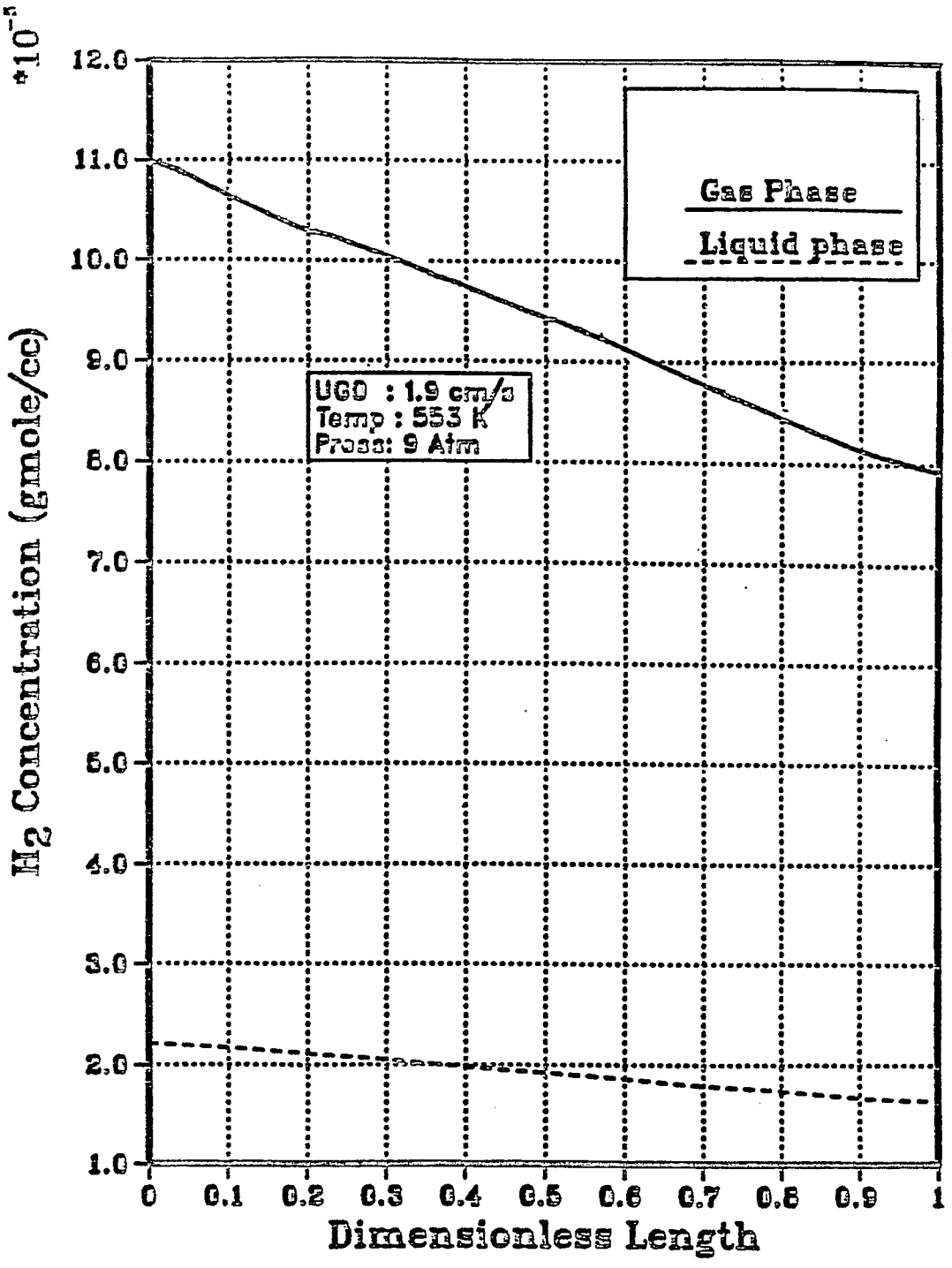

Figure A-B-5. Variation of H_2 Concentration in the Gas and the Liquid Phase

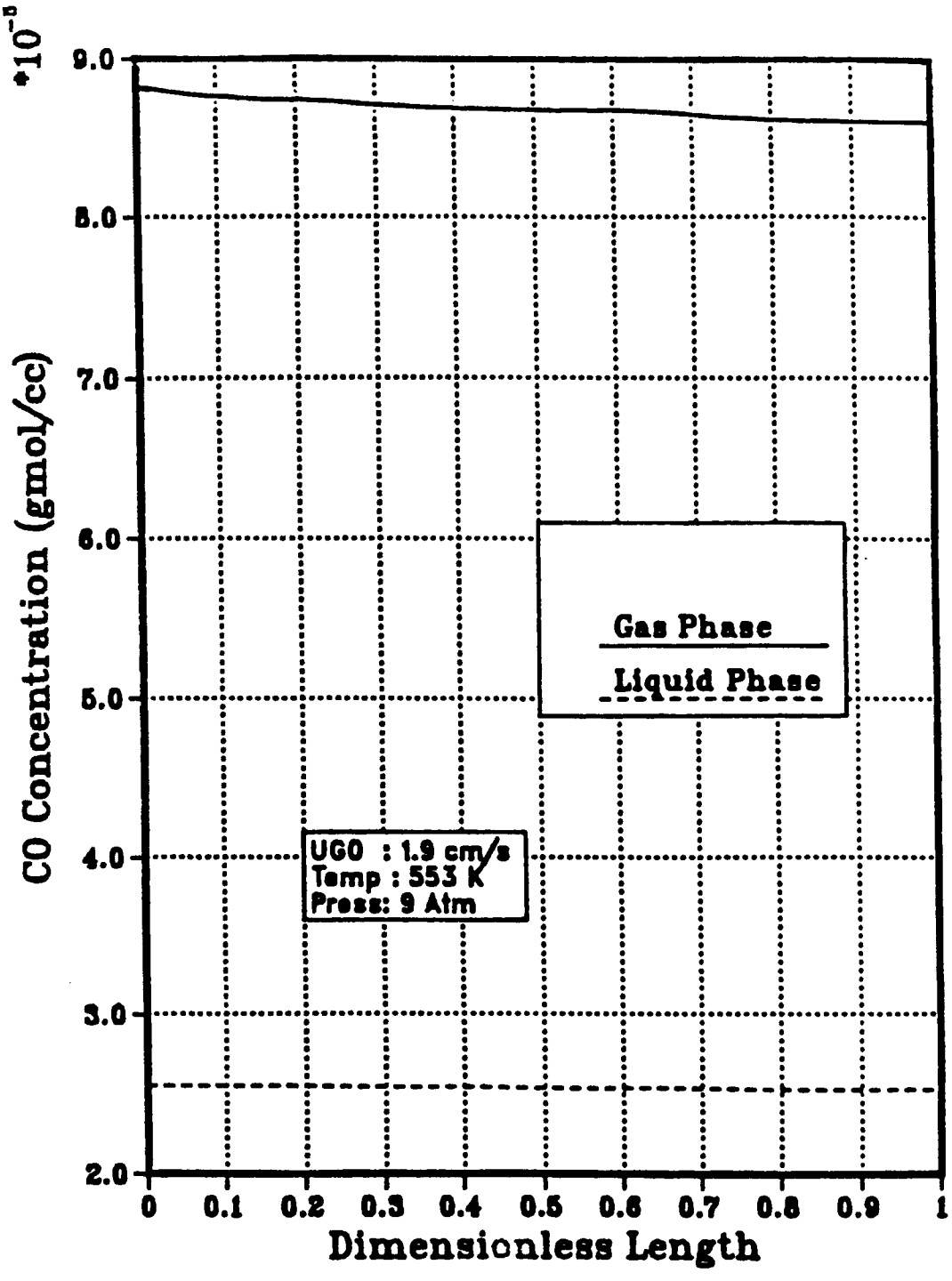

Figure A-B-6. Variation of CO Concentration in the Gas and the Liquid Phase

consumed. Fig. A-B-7 shows a plot of (Rcn/Rc1) v/s the carbon number. As seen in the plot, the products with carbon numbers above 4 lie on a straight line whose intercept lies below 1, a point corresponding to CH_4 and furthermore, products with carbon numbers 2,3 fail to lie on the line, a phenomenon observed experimentally (Stern et al., 1984b). The straight line dependence for higher hydrocarbons supports the evidence that the product slate follows the Schulz-Flory distribution.

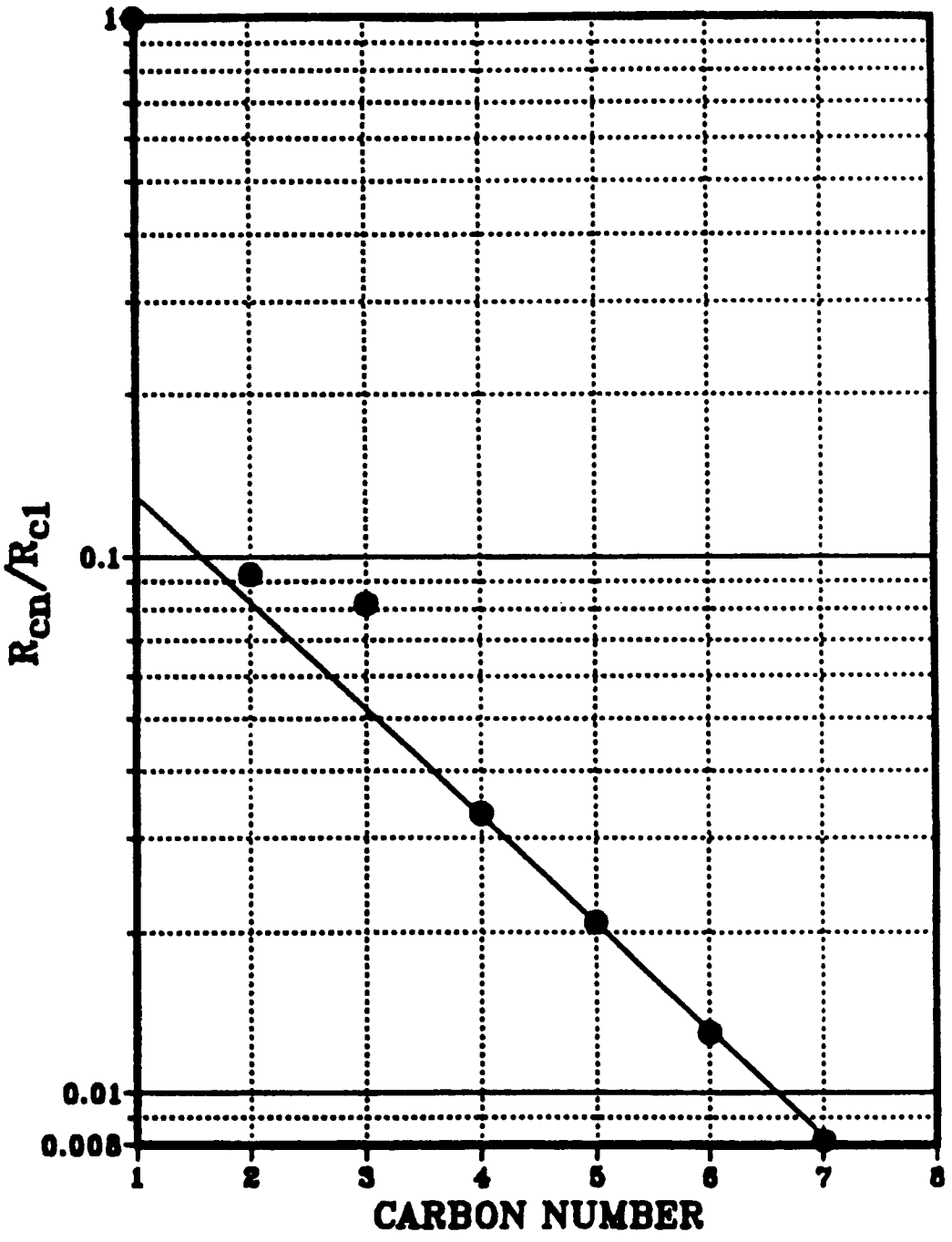

Figure A-B-7: R_{cn}/R_{c1} v/s carbon number

TYPICAL INPUT SAMPLE: INTER.FOR

```
THIS IS AN INTERACTIVE PROGRAM

PLEASE ENTER THE DATA ASKED FOR IN FREE FORMAT

-----------------------------------------------
REACTION TEMPERATURE (deg.K) =?
>553.0
REACTION PRESSURE (atm) =?
>9.0
REACTOR LENGTH (cm)=?
>180.0
REACTOR DIAMETER (cm)=?
>2.6
INLET GAS VELOCITY (cm/sec)=?
>1.9
WT. OF CATALYST (gm)=?
>41.3
WT. OF SUSPENSION (gm)=?
>272.0
SOLB. COEFF. FOR H2O=?
>1.17
SOLB.COEFF.FOR H2=?
>4.35
SOLB.COEFF. FOR CO=?
>3.30
SOLB. COEFF. FOR HYDROCARBON=?
>2.42
DENSITY OF CATALYST (gm/c.c) =?
>5.00
DENSITY OF LIQ. (gm/c.c) =?
>0.7
INLET PARTIAL PRESSURE OF H2 (atm) =?
>5.0
INLET PARTIAL PRESSURE OF CO (atm) =?
>8.0
-----------------------------------------------

ALL THE REQUIRED DATA HAS BEEN PROVIDED

PROCEED TO ALPHA.FOR TO ENTER THE KINETIC PARAM.
```

TYPICAL INPUT SAMPLE: ALPHA.FOR

```
 INPUT ALL THE VALUES IN FREE FORMAT

 ------------------------------------------------
 INPUT THE DATA FOR C1 HYDROCARBON
 ------------------------------------------------

 PRE-EXPONENTIAL FACTOR (An)
>92000.0
 ACTIVATION ENERGY (En)
>28.0
 EXPONENT FOR HYDROGEN (an)
>1.37
 EXPONENT FOR CARBON MONOXIDE (bn)
>-0.84

 ------------------------------------------------
 INPUT THE DATA FOR C2 HYDROCARBON
 ------------------------------------------------

 PRE-EXPONENTIAL FACTOR (An)
>6700.0
 ACTIVATION ENERGY (En)
>27.0
 EXPONENT FOR HYDROGEN (an)
>0.88
 EXPONENT FOR CARBON MONOXIDE (bn)
>-0.73

 ------------------------------------------------
 INPUT THE DATA FOR C3 HYDROCARBON
 ------------------------------------------------

 PRE-EXPONENTIAL FACTOR (An)
>2300.0
 ACTIVATION ENERGY (En)
>27.0
 EXPONENT FOR HYDROGEN (an)
>1.04
 EXPONENT FOR CARBON MONOXIDE (bn)
>-0.35

 ------------------------------------------------
 INPUT THE DATA FOR C4 HYDROCARBON
 ------------------------------------------------

 PRE-EXPONENTIAL FACTOR (An)
>0.97
 ACTIVATION ENERGY (En)
>20.0
 EXPONENT FOR HYDROGEN (an)
>1.11
 EXPONENT FOR CARBON MONOXIDE (bn)
>-0.05

 ************************************************


 ALL THE DATA HAS BEEN OBTAINED
 PROCEED TO THE MAIN SIMULATOR
```

OUTPUT FILES: CONV.DAT

SUP.DAT

LCON.DAT

****
FISCHER TROPSCH SYNTHESIS IN SLURRY BUBBLE COLUMN REACTOR
****

DESIGN PARAMETERS :

REACTOR DIAMETER : 2.600 cm
REACTOR HEIGHT :180.000 cm

OPERATING PARAMETERS :

REACTOR TEMPERATURE :553.000 Deg.K
REACTOR PRESSURE : 9.000 Atm.

FEED CONDITIONS :

INLET GAS VELOCITY : 1.900 cm/sec
INLET P.P OF H2 : 5.000 atm.
INLET P.P OF CO : 4.000 atm.

KINETIC PARAMETERS :

A POWER LAW RATE EXP : An*(PH2**an)*PCO**bn) IS USED

CHAIN GROWTH PROB. FACTOR : 0.825

OUTPUT FILE 1 GAS PHASE COMPOSITIONS :-

X	C1	C2	C3	C4	C5	C6	H2O	H2	CO	% CONV.
0.00	.103E-07	.185E-08	.682E-09	.180E-09	.113E-09	.704E-10	.235E-07	.110E-03	.881E-04	0.02
0.10	.125E-05	.232E-06	.840E-07	.221E-07	.138E-07	.865E-08	.247E-05	.107E-03	.877E-04	4.53
0.20	.236E-05	.441E-06	.159E-06	.418E-07	.261E-07	.163E-07	.436E-05	.103E-03	.876E-04	7.02
0.30	.340E-05	.640E-06	.230E-06	.604E-07	.378E-07	.236E-07	.628E-05	.101E-03	.872E-04	10.28
0.40	.458E-05	.875E-06	.312E-06	.818E-07	.511E-07	.320E-07	.826E-05	.970E-04	.872E-04	13.62
0.50	.549E-05	.105E-05	.374E-06	.981E-07	.614E-07	.384E-07	.101E-04	.945E-04	.867E-04	15.74
0.60	.670E-05	.130E-05	.460E-06	.120E-06	.753E-07	.471E-07	.121E-04	.909E-04	.866E-04	19.10
0.70	.778E-05	.153E-05	.536E-06	.140E-06	.877E-07	.548E-07	.140E-04	.877E-04	.865E-04	21.81
0.80	.858E-05	.170E-05	.593E-06	.155E-06	.969E-07	.606E-07	.156E-04	.854E-04	.861E-04	22.66
0.90	.992E-05	.199E-05	.690E-06	.180E-06	.113E-06	.704E-07	.179E-04	.815E-04	.860E-04	26.98
1.00	.106E-04	.216E-05	.743E-06	.194E-06	.121E-06	.757E-07	.190E-04	.793E-04	.860E-04	30.62

H2/CO USAGE RATIO =2.8677989146785425

OUTPUT FILE 2 VARIATION OF SUP. GAS VELOCITY :

X	GAS VEL.
0.0000	1.9000
0.1000	1.8520
0.2000	1.8352
0.3000	1.8016
0.4000	1.7677
0.5000	1.7526
0.6000	1.7174
0.7000	1.6913
0.8000	1.6992
0.9000	1.6429
1.0000	1.5809

OUTPUT FILE 4 LIQUID PHASE COMPOSITIONS :

X	C1	C2	C3	C4	C5	C6	H2O	H2	CO
0.00	.295E-08	.536E-07	.196E-07	.517E-08	.323E-08	.202E-08	.142E-05	.221E-04	.256E-04
0.10	.567E-08	.105E-06	.381E-07	.100E-07	.628E-08	.392E-08	.235E-05	.217E-04	.256E-04
0.20	.107E-05	.201E-06	.722E-07	.190E-07	.119E-07	.743E-08	.415E-05	.211E-04	.255E-04
0.30	.149E-05	.282E-06	.101E-06	.266E-07	.166E-07	.104E-07	.576E-05	.205E-04	.255E-04
0.40	.197E-05	.377E-06	.134E-06	.352E-07	.220E-07	.138E-07	.742E-05	.198E-04	.255E-04
0.50	.235E-05	.453E-06	.161E-06	.421E-07	.263E-07	.165E-07	.897E-05	.192E-04	.254E-04
0.60	.284E-05	.555E-06	.195E-06	.511E-07	.320E-07	.200E-07	.107E-04	.186E-04	.254E-04
0.70	.328E-05	.647E-06	.226E-06	.592E-07	.370E-07	.231E-07	.123E-04	.179E-04	.254E-04
0.80	.362E-05	.720E-06	.251E-06	.655E-07	.410E-07	.256E-07	.137E-04	.174E-04	.253E-04
0.90	.416E-05	.838E-06	.290E-06	.755E-07	.472E-07	.295E-07	.155E-04	.167E-04	.253E-04
1.00	.445E-05	.902E-06	.311E-06	.810E-07	.506E-07	.316E-07	.164E-04	.164E-04	.253E-04

FOLLOWING TABLE GIVES THE RATIO OF RCn/RC1

X	R1	R2	R3	R4	R5	R6	R7
0.10	1.0000	0.0748	0.0744	0.0311	0.0194	0.0121	0.0076
0.20	1.0000	0.0764	0.0751	0.0313	0.0196	0.0122	0.0076
0.30	1.0000	0.0780	0.0758	0.0315	0.0197	0.0123	0.0077
0.40	1.0000	0.0798	0.0766	0.0317	0.0198	0.0124	0.0078
0.50	1.0000	0.0817	0.0774	0.0320	0.0200	0.0125	0.0078
0.60	1.0000	0.0837	0.0782	0.0322	0.0202	0.0126	0.0079
0.70	1.0000	0.0858	0.0791	0.0325	0.0203	0.0127	0.0079
0.80	1.0000	0.0881	0.0800	0.0328	0.0205	0.0128	0.0080
0.90	1.0000	0.0904	0.0809	0.0331	0.0207	0.0129	0.0081
1.00	1.0000	0.0930	0.0819	0.0334	0.0209	0.0130	0.0082

OUTPUT FILE: PLUG FLOW MODEL

FISCHER-TROPSCH SYNTHESIS IN BUBBLE COLUMN REACTOR

DESIGN PARAMETERS :

REACTOR DIAMETER :2.800000Cm
REACTOR HEIGHT :180.0000Cm

OPERATING PARAMETERS :

REACTOR TEMPERATURE :553.0000Deg.C
REACTOR PRESSURE :9.000000Atm.

FEED CONDITIONS :

INLET GAS VELOCITY :1.900000cm/sec
INLET P.P OF H2 :5.000000Atm.
INLET P.P OF CO :4.000000Atm.

KINETIC PARAMETERS :

A POWER LAW RATE EXP : An(PH2**an)(PCO**bn) IS USED

CHAIN GROWTH PROB. FACTOR :0.6251534

X	C1	C2	C3	C4	C5	C6	C7	H2O	H2	CO	% CONV.
0.00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.00E+00	.110E-03	.882E-04	0.000
0.10	.11E-05	.20E-08	.74E-07	.19E-07	.12E-07	.76E-08	.48E-08	.19E-05	.107E-03	.879E-04	3.585
0.20	.22E-05	.41E-08	.15E-08	.39E-07	.24E-07	.15E-07	.95E-08	.39E-05	.104E-03	.877E-04	7.061
0.30	.33E-05	.62E-08	.22E-08	.59E-07	.37E-07	.23E-07	.14E-07	.59E-05	.101E-03	.875E-04	10.427
0.40	.44E-05	.84E-08	.30E-08	.79E-07	.49E-07	.31E-07	.19E-07	.79E-05	.975E-04	.873E-04	13.683
0.50	.55E-05	.11E-05	.38E-08	.99E-07	.62E-07	.39E-07	.24E-07	.98E-05	.943E-04	.871E-04	16.827
0.60	.66E-05	.13E-05	.45E-08	.12E-08	.74E-07	.46E-07	.29E-07	.12E-04	.911E-04	.868E-04	19.860
0.70	.77E-05	.15E-05	.53E-08	.14E-08	.87E-07	.54E-07	.34E-07	.14E-04	.879E-04	.866E-04	22.781
0.80	.87E-05	.17E-05	.61E-08	.16E-08	.99E-07	.62E-07	.39E-07	.16E-04	.847E-04	.864E-04	25.592
0.90	.98E-05	.20E-05	.68E-08	.18E-08	.11E-08	.70E-07	.44E-07	.18E-04	.815E-04	.862E-04	28.293
1.00	.11E-04	.22E-05	.76E-08	.20E-08	.12E-08	.77E-07	.48E-07	.20E-04	.784E-04	.860E-04	30.884

PROGRAM LISTING: INTER.FOR

```
C     ********************************************************
C
C     THIS IS AN INTERACTIVE PROGRAM DEVELOPED TO ASSIST
C     THE USER IN INPUTING THE REQUISITE DATA TO SELEC.FOR
C
C     ********************************************************
      DIMENSION AM(10)


      WRITE*,'THIS IS AN INTERACTIVE PROGRAM '
      WRITE*
      WRITE*,'PLEASE ENTER THE DATA ASKED FOR IN FREE FORMAT'
      WRITE*,'_____________________________________________'

      WRITE*,'REACTION TEMPERATURE (deg.K) =? '
      READ*,T
      WRITE(12,100)T
      WRITE*,'REACTION PRESSURE (atm) =?'
      READ*,P
      WRITE(12,100)P
      WRITE*,'REACTOR LENGTH (cm)=?'
      READ*,AL
      WRITE(12,100)AL
      WRITE*,'REACTOR DIAMETER (cm)=?'
      READ*,DIAM
      WRITE(12,100)DIAM
      WRITE*,'INLET GAS VELOCITY (cm/sec)=?'
      READ*,UGO
      WRITE(12,100)UGO
      WRITE*,'WT. OF CATALYST (gm)=?'
      READ*,AMCAT
      WRITE(12,100)AMCAT
      WRITE*,'WT. OF SUSPENSION (gm)=?'
      READ*,AMSUS
      WRITE(12,100)AMSUS
      WRITE*,'SOLB. COEFF. FOR H2O=?'
      READ*,AM(8)
      WRITE(12,100)AM(8)
      WRITE*,'SOLB.COEFF.FOR H2=?'
      READ*,AM(9)
      WRITE(12,100)AM(9)
      WRITE*,'SOLB.COEFF. FOR CO=?'
      READ*,AM(10)
      WRITE(12,100)AM(10)
      WRITE*,'SOLB. COEFF. FOR HYDROCARBON=?'
      READ*,AMN
      WRITE(12,100)AMN
      WRITE*,'DENSITY OF CATALYST (gm/c.c) =?'
      READ*,DENCAT
      WRITE(12,100)DENCAT
      WRITE*,'DENSITY OF LIQ. (gm/c.c) =?'
      READ*,DENL
      WRITE(12,100)DENL
      WRITE*,'INLET PARTIAL PRESSURE OF H2 (atm) =?'
      READ*,PH2
      WRITE(12,100)PH2
      WRITE*,'INLET PARTIAL PRESSURE OF CO (atm) =?'
      READ*,PCO
      WRITE(12,100)PCO
      WRITE*,'-----------------------------------------
```

```
      WRITE*
      WRITE*,'ALL THE REQUIRED DATA HAS BEEN PROVIDED'
      WRITE*
      WRITE*,'PROCEED TO ALPHA.FOR TO ENTER THE KINETIC PARAM.'

100   FORMAT(F15.5)

      STOP
      END
C     ------------------------------------------------------------
```

PROGRAM LISTING: ALPHA.FOR

```
C     ************************************************************
C
C     THIS IS AN INTERACTIVE PROGRAM TO BE USED TO INPUT
C     THE DATA FOR THE KINETIC PARAM. FOR C1 TO C4 HYDROCARBONS
C
C     ************************************************************

      DIMENSION H(4),E(4),A(4),B(4)

      WRITE*,'INPUT ALL THE VALUES IN FREE FORMAT'
      WRITE*
      DO 10 I=1,4
      WRITE*,'-----------------------------------------------'
      WRITE*,'INPUT THE DATA FOR C',I,' HYDROCARBON'
      WRITE*,'-----------------------------------------------'
      WRITE*
      WRITE*,'PRE-EXPONENTIAL FACTOR (An)'
      READ*,H(I)
      WRITE(11,100)H(I)
      WRITE*,'ACTIVATION ENERGY (En) '
      READ*,E(I)
      WRITE(11,100)E(I)
      WRITE*,'EXPONENT FOR HYDROGEN (an)'
      READ*,A(I)
      WRITE(11,100)A(I)
      WRITE*,'EXPONENT FOR CARBON MONOXIDE (bn)'
      READ*,B(I)
      WRITE(11,100)B(I)
      WRITE*
10    CONTINUE


      WRITE*,'*****************************************'
      WRITE*
      WRITE*
      WRITE*,'ALL THE DATA HAS BEEN OBTAINED'
      WRITE*,'PROCEED TO THE MAIN SIMULATOR'

100   FORMAT(F15.5)

      STOP
      END
```

PROGRAM LISTING: EC2.FOR

```
C       ************************************************************

C       THIS PROGRAM IS DEVELOPED TO SOLVE THE AXIAL DISP. MODEL
C       DESCRIBING THE ASPECT OF SELECTIVITY IN BCSR.
C
C       ************************************************************

C       FOLLOWING IS A LIST OF THE INPUT VARIABLES USED:

C       T         :OPERATING TEMPERATURE (K)
C       P         :OPERATING PRESSURE (ATM)
C       AL        :COLUMN HEIGHT (CM)
C       D         :COLUMN DIAMETER (CM)
C       UGO       :INLET GAS VELOCITY (CM/SEC)
C       AMCAT     :WT. OF CATALYST (GM)
C       AMSUS     :WT. OF SUSPENSION (GM)
C       AM        :SOLUBILITY COEFFIECIENT
C       DENCAT    :DENSITY OF CATALYST (GM/CC)
C       DENL      :DENSITY OF LIQUID (GM/CC)
C       H(I)      :PRE-EXPONENTIAL FACTOR FOR CARBON NO. I
C       E(I)      :ACTIVATION ENERGY FOR CARBON NO. I (KCAL/MOL)
C       A(I)      :INDEX OF H2 CONC. FOR CARBON NO. I
C       B(I)      :INDEX OF CO CONC. FOR CARBON NO. I
C       PH2       :INLET PARTIAL PRESSURE OF H2 (ATM)
C       PCO       :INLET PARTIAL PRESSURE OF CO (ATM)
C
C       ------------------------------------------------------

C       THIS IS THE MAIN PROGRAM

        IMPLICIT REAL *8(A-H,O-Z)

        COMMON/PAR1/ALPHA
        COMMON/PAR2/D,AL,UGO
        COMMON/PAR3/CCAT,CGHO,CGCO,P,T
        COMMON/PAR4/AM,AKN
        COMMON/PAR5/DA,A,B
        COMMON/PAR6/PEG,PEL,EL,EG
        COMMON/PAR8/DERU,AN,UGB

        DIMENSION AN(9),AKLA(9),AM(9),AKN(4),A(4),B(4),DA(4),IPAR(11),
     *  ZETA(36),LTOL(18),TOL(18),Z(36),FSPACE(25000),ISPACE(500),M(18),
     *  RATE(6)

        EXTERNAL FSUB,DFSUB,GSUB,DGSUB,SOLUTN,RHOH,RHON,RHOC,DHC33,
     *  DHC35

        OPEN (UNIT=10,FILE='CONV.DAT')
        OPEN (UNIT=13,FILE='SUP.DAT' )
        OPEN (UNIT=21,FILE='LCON.DAT')

        NUMB=1

        WRITE(10,*)' ************************************************'
        WRITE(10,*)'     FISCHER TROPSCH SYNTHESIS IN SLURRY BUBBLE   '
        WRITE(10,*)'                    COLUMN REACTOR               '
        WRITE(10,*)' ************************************************'

        CALL INPUT(T,P,AL,D,UGO,AMCAT,AMSUS,AM,A,B,PH2,PCO,AKN,
```

```
*   CGHO,CGCO,DENCAT,DENL)

    CT=P/(82.05*T)
    CT=CT/CGHO

    GOD=CGHO+CGCO

    AREA=(22.0/(7.0*4.0))*(D**2.0)
    DEN1=PH2*2.0/(82.05*T)
    DEN2=PCO*28.0/(82.05*T)
    DENMIX=DEN1+DEN2
    VFR=UGO*AREA
    CATWT=41.3
    WHSV=VFR*DENMIX*3600.0/CATWT



    CALL VALUE(T,ALPHA)

    CALL CATCON(AMCAT,AMSUS,DENCAT,DENL,CCAT)


    RAT=CGCO/CGHO

    WRITE(10,*)
    WRITE(10,*)
    WRITE(10,*)' DESIGN PARAMETERS :'
    WRITE(10,*)' -------------------'
    WRITE(10,*)
    WRITE(10,230)' REACTOR DIAMETER         :',D,'  cm'
    WRITE(10,230)' REACTOR HEIGHT           :',AL,' cm'
    WRITE(10,*)
    WRITE(10,*)' OPERATING PARAMETERS :'
    WRITE(10,*)' ----------------------'
    WRITE(10,*)
    WRITE(10,230)' REACTOR TEMPERATURE      :',T,' Deg.K'
    WRITE(10,230)' REACTOR PRESSURE         :',P,' Atm.'
    WRITE(10,*)
    WRITE(10,*)' FEED CONDITIONS :'
    WRITE(10,*)' -----------------'
    WRITE(10,*)
    WRITE(10,230)' INLET GAS VELOCITY       :',UGO,'  cm/sec'
    WRITE(10,230)' INLET P.P OF H2          :',PH2,'  atm.'
    WRITE(10,230)' INLET P.P OF CO          :',PCO,' atm.'
    WRITE(10,*)
    WRITE(10,*)' KINETIC PARAMETERS :'
    WRITE(10,*)' --------------------'
    WRITE(10,*)
    WRITE(10,*)' A POWER LAW RATE EXP : An=(PH2**an)*PCO**bn)
*   IS USED'
    WRITE(10,*)
    WRITE(10,230)' CHAIN GROWTH PROB. FACTOR :',ALPHA
    WRITE(10,*)
    WRITE(10,*)
    WRITE(10,*)' OUTPUT FILE 1   GAS PHASE COMPOSITIONS :-'
    WRITE(10,*)
    WRITE(10,110)
    WRITE(10,120)'X','C1','C2','C3','C4','C5','C6','H2O',
*   'H2','CO',' % CONV.'
```

```
      WRITE(10,110)


      WRITE(13,*)' OUTPUT FILE 2  VARIATION OF SUP. GAS VELOCITY :'
      WRITE(13,*)
      WRITE(13,*)
      WRITE(13,121)
      WRITE(13,125)'X','GAS VEL.'
      WRITE(13,121)


      WRITE(21,*)' OUTPUT FILE 4  LIQUID PHASE COMPOSITIONS :'
      WRITE(21,*)
      WRITE(21,*)
      WRITE(21,*)
      WRITE(21,110)
      WRITE(21,122)'X','C1','C2','C3','C4','C5','C6','H2O',
     *  'H2','CO'
      WRITE(21,110)



C     INPUT TO COLSYS

      NCOMP=18

      DO 10 J=1,18
      M(J)=2
 10   CONTINUE

      ALEFT=0.DO
      ARIGHT=1.DO

      DO 20 J=1,18
      ZETA(J)=0.DO
 20   CONTINUE

      DO 30 J=19,36
      ZETA(J)=1.DO
 30   CONTINUE

      DO 40 J=1,11
      IPAR(J)=0
 40   CONTINUE

      IPAR(1)=1
      IPAR(2)=2
      IPAR(4)=18
      IPAR(5)=25000
      IPAR(6)=500
      IPAR(8)=1
      IPAR(7)=1

      DO 50 J=1,18
      LTOL(J)=2*J-1
      TOL(J)=1.D-3
 50   CONTINUE

 52   CALL HOLDUP(UGO,EG)
      CALL GASDIF(D,UGO,DG)
```

```
      CALL LIQDIF(D,UGO,DL)

      PEG=UGO*AL/DG
      PEL=UGO*AL/DL
      EL=1.-EG


57    CALL COLSYS(NCOMP,M,ALEFT,ARIGHT,ZETA,IPAR,LTOL,TOL,
     *  FIXPNT,ISPACE,FSPACE,IFLAG,FSUB,DFSUB,GSUB,DGSUB,SOLUTN)

      X=0.DO

      WRITE(10,*)' IFLAG=',IFLAG

      DO 60 J=1,11
      CALL APPSLN(X,Z,FSPACE,ISPACE)

      CALL SIGMA(AM,Z,RSUM)
      CALL SUPER(X,UGO,RSUM,UGB)
      UG=UGB*UGO
      USE=(1.0-(Z(15)*UGB))/(RAT-(Z(17)*UGB))

      BALU=(Z(15)+Z(17))*CGMO

      CONSYM=(UGO*GOD-UG*BALU)/(UGO*GOD)

      GARY=(UGO*GOD-UG*BALU)*AREA
      STY=GARY/CATWT


      WRITE(10,100)X,Z(1)*CGMO,Z(3)*CGMO,Z(5)*CGMO,Z(7)*CGMO,Z(9)*CGMO,
     *  Z(11)*CGMO,Z(13)*CGMO,Z(15)*CGMO,Z(17)*CGMO,CONSYM*100.0

      WRITE(21,101)X,Z(19)*CGMO/AM(1),Z(21)*CGMO/AM(2),Z(23)*CGMO/
     *  AM(3),Z(25)*CGMO/AM(4),Z(27)*CGMO/AM(5),Z(29)*CGMO/AM(6),
     *  Z(31)*CGMO/AM(7),Z(33)*CGMO/AM(8),Z(35)*CGMO/AM(9)

      WRITE(6,*)Z(15)*CGMO,Z(17)*CGMO,Z(33)*CGMO/AM(8),Z(35)*CGMO/AM(9)

      WRITE(13,220)X,UG


      X=X+0.1
60    CONTINUE
      GOTO 70


100   FORMAT(2X,F8.2,2X,9(E8.3,2X),F8.2)
101   FORMAT(2X,F8.2,2X,9(E8.3,2X))
110   FORMAT(100('-'))
115   FORMAT(70('-'))
120   FORMAT(3X,11(A,7X))
122   FORMAT(3X,10(A,7X))
210   FORMAT(4X,7(A,7X))
220   FORMAT(4X,2(F7.4,3X))
230   FORMAT(X,A,F7.3,A)
121   FORMAT(23('-'))
125   FORMAT(5X,3(A,4X))
300   FORMAT(X,F8.2,2X,8(E8.3,2X))
```

```
 350    FORMAT(X,7(E8.3,3X))

 70     WRITE(10,110)
        WRITE(10,*)' H2/CO USAGE RATIO =',USE
        WRITE(10,*)
        WRITE(10,*)' WHSV=',WHSV,'STY=',STY,'UGO=',UGO
        WRITE(13,115)
        WRITE(21,110)

C       IF(NUMB.EQ.6) GOTO 82

        UGO=UGO-1.0
        IPAR(9)=3
        IPAR(3)=ISPACE(1)
        NUMB=NUMB+1
        GOTO 57



 82     STOP
        END
C       ------------------------------------------------------------

        SUBROUTINE FSUB(X,Z,F)

C       THIS SUBROUTINE DEFINES THE DIFFERENTIAL EQNS.

        IMPLICIT REAL *8(A-H,O-Z)

        COMMON/PAR2/D,AL,UGO
        COMMON/PAR3/CCAT,CGHO,CGCO,P,T
        COMMON/PAR4/AM,AKN
        COMMON/PAR5/DA,A,B
        COMMON/PAR6/PEG,PEL,EL,EG
        COMMON/PAR8/DERU,AN,UGB

        DIMENSION F(18),Z(36),AKLA(9),AN(9),AM(9),AKN(4),A(4),
     *  B(4),DA(4)

        EXTERNAL RHOH,RHON,RHOC

        CT=P/(82.05*T)
        CT=CT/CGHO


        DO 10 J=9,1,-1
        NN=J
        CALL MASTRN(UGO,NN,AKLA)
        AN(J)=(AKLA(J)*AL)/(AM(J)*UGO)
 10     CONTINUE

        DO 20 J=1,4
        DAC=CCAT*AL*(1.-EG)*AKN(J)*(CGHO**(A(J)+B(J)-1.))
        DAD=UGO*(AM(8)**A(J))*(AM(8)**B(J))
        DA(J)=DAC*((82.05*T)**(A(J)+B(J)))/DAD
 20     CONTINUE

        CALL SIGMA(AN,Z,RSUM)
        CALL SUPER(X,UGO,RSUM,UGB)
        DERU=-RSUM/CT
```

```
      F(1)=(UGB*Z(2)+Z(1)*DERU+AN(1)*(Z(1)-Z(19)))*(PEG/EG)
      F(2)=(UGB*Z(4)+Z(3)*DERU+AN(2)*(Z(3)-Z(21)))*(PEG/EG)
      F(3)=(UGB*Z(6)+Z(5)*DERU+AN(3)*(Z(5)-Z(23)))*(PEG/EG)
      F(4)=(UGB*Z(8)+Z(7)*DERU+AN(4)*(Z(7)-Z(25)))*(PEG/EG)
      F(5)=(UGB*Z(10)+Z(9)*DERU+AN(5)*(Z(9)-Z(27)))*(PEG/EG)
      F(6)=(UGB*Z(12)+Z(11)*DERU+AN(6)*(Z(11)-Z(29)))*(PEG/EG)
      F(7)=(UGB*Z(14)+Z(13)*DERU+AN(7)*(Z(13)-Z(31)))*(PEG/EG)
      F(8)=(UGB*Z(16)+Z(15)*DERU+AN(8)*(Z(15)-Z(33)))*(PEG/EG)
      F(9)=(UGB*Z(18)+Z(17)*DERU+AN(9)*(Z(17)-Z(35)))*(PEG/EG)

      F(10)=(-AN(1)*(Z(1)-Z(19))-RHON(DA,A,B,Z,1))*(PEL*AM(1)/EL)
      F(11)=(-AN(2)*(Z(3)-Z(21))-RHON(DA,A,B,Z,2))*(PEL*AM(2)/EL)
      F(12)=(-AN(3)*(Z(5)-Z(23))-RHON(DA,A,B,Z,3))*(PEL*AM(3)/EL)
      F(13)=(-AN(4)*(Z(7)-Z(25))-RHON(DA,A,B,Z,4))*(PEL*AM(4)/EL)
      F(14)=(-AN(5)*(Z(9)-Z(27))-RHON(DA,A,B,Z,5))*(PEL*AM(5)/EL)
      F(15)=(-AN(6)*(Z(11)-Z(29))-RHON(DA,A,B,Z,6))*(PEL*AM(6)/EL)
      F(16)=(-AN(7)*(Z(13)-Z(31))+RHOC(DA,A,B,Z))*(PEL*AM(7)/EL)
      F(17)=(-AN(8)*(Z(15)-Z(33))-RHOH(DA,A,B,Z))*(PEL*AM(8)/EL)
      F(18)=(-AN(9)*(Z(17)-Z(35))-RHOC(DA,A,B,Z))*(PEL*AM(9)/EL)


      RETURN
      END

C     ------------------------------------------------------------

      SUBROUTINE DFSUB(X,Z,DF)

C     THIS IS A SUPPORTING SUBROUTINE AS PER COLSYS

      IMPLICIT REAL *8(A-H,O-Z)

      COMMON/PAR4/AM,AKN
      COMMON/PAR3/PEG,PEL,EL,EG
      COMMON/PAR3/DERU,AN,UGB

      EXTERNAL DHC33,DHC35

      DIMENSION DF(18,38),Z(38),AM(9),AN(9),AKN(4)

      DO 10 J=1,38
      DO 20 I=1,18
      DF(I,J)=0.D0
 20   CONTINUE
 10   CONTINUE

      DF(1,1)=(DERU+AN(1))*(PEG/EG)
      DF(2,3)=(DERU+AN(2))*(PEG/EG)
      DF(3,5)=(DERU+AN(3))*(PEG/EG)
      DF(4,7)=(DERU+AN(4))*(PEG/EG)
      DF(5,9)=(DERU+AN(5))*(PEG/EG)
      DF(6,11)=(DERU+AN(6))*(PEG/EG)
      DF(7,13)=(DERU+AN(7))*(PEG/EG)
      DF(8,15)=(DERU+AN(8))*(PEG/EG)
      DF(9,17)=(DERU+AN(9))*(PEG/EG)

      DF(1,2)=UGB*PEG/EG
      DF(2,4)=UGB*PEG/EG
      DF(3,6)=UGB*PEG/EG
      DF(4,8)=UGB*PEG/EG
```

```
DF(5,10)=UGB*PEG/EG
DF(6,12)=UGB*PEG/EG
DF(7,14)=UGB*PEG/EG
DF(8,16)=UGB*PEG/EG
DF(9,18)=UGB*PEG/EG

DF(1,19)=-AN(1)*PEG/EG
DF(2,21)=-AN(2)*PEG/EG
DF(3,23)=-AN(3)*PEG/EG
DF(4,25)=-AN(4)*PEG/EG
DF(5,27)=-AN(5)*PEG/EG
DF(6,29)=-AN(6)*PEG/EG
DF(7,31)=-AN(7)*PEG/EG
DF(8,33)=-AN(8)*PEG/EG
DF(9,35)=-AN(9)*PEG/EG

DF(10,1)=-AN(1)*(PEL*AM(1)/EL)
DF(11,3)=-AN(2)*(PEL*AM(2)/EL)
DF(12,5)=-AN(3)*(PEL*AM(3)/EL)
DF(13,7)=-AN(4)*(PEL*AM(4)/EL)
DF(14,9)=-AN(5)*(PEL*AM(5)/EL)
DF(15,11)=-AN(6)*(PEL*AM(6)/EL)
DF(16,13)=-AN(7)*(PEL*AM(7)/EL)
DF(17,15)=-AN(8)*(PEL*AM(8)/EL)
DF(18,17)=-AN(9)*(PEL*AM(9)/EL)

DF(10,19)=AN(1)*(PEL*AM(1)/EL)
DF(11,21)=AN(2)*(PEL*AM(2)/EL)
DF(12,23)=AN(3)*(PEL*AM(3)/EL)
DF(13,25)=AN(4)*(PEL*AM(4)/EL)
DF(14,27)=AN(5)*(PEL*AM(5)/EL)
DF(15,29)=AN(6)*(PEL*AM(6)/EL)
DF(16,31)=AN(7)*(PEL*AM(7)/EL)

DF(10,33)=-DHC33(Z,1)*(PEL*AM(1)/EL)
DF(11,33)=-DHC33(Z,2)*(PEL*AM(2)/EL)
DF(12,33)=-DHC33(Z,3)*(PEL*AM(3)/EL)
DF(13,33)=-DHC33(Z,4)*(PEL*AM(4)/EL)
DF(14,33)=-DHC33(Z,5)*(PEL*AM(5)/EL)
DF(15,33)=-DHC33(Z,6)*(PEL*AM(6)/EL)

CALL D33(Z,DHZ33,DCZ33)

DF(16,33)=DCZ33*(PEL*AM(7)/EL)
DF(17,33)=(-DHZ33+AN(8))*(PEL*AM(8)/EL)
DF(18,33)=-DCZ33*(PEL*AM(9)/EL)

DF(10,35)=-DHC35(Z,1)*(PEL*AM(1)/EL)
DF(11,35)=-DHC35(Z,2)*(PEL*AM(2)/EL)
DF(12,35)=-DHC35(Z,3)*(PEL*AM(3)/EL)
DF(13,35)=-DHC35(Z,4)*(PEL*AM(4)/EL)
DF(14,35)=-DHC35(Z,5)*(PEL*AM(5)/EL)
DF(15,35)=-DHC35(Z,6)*(PEL*AM(6)/EL)

CALL D35(Z,DHZ35,DCZ35)

DF(16,35)=DCZ35*(PEL*AM(7)/EL)
DF(17,35)=-DHZ35*(PEL*AM(8)/EL)
DF(18,35)=(-DCZ35+AN(9))*(PEL*AM(9)/EL)
```

```
      RETURN
      END


C     ------------------------------------------------
      SUBROUTINE GSUB(I,Z,G)

C     THIS SUBROUTINE DEFINES THE BOUNDARY CONDITIONS

      IMPLICIT REAL *8(A-H,O-Z)

      COMMON/PAR3/CCAT,CGHO,CGCO,P,T
      COMMON/PAR3/PEG,PEL,EL,EG

      DIMENSION Z(38)


      GOTO (1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,
     * 21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36),I

 1    G=Z(1)-(EG/PEG)*Z(2)-0.D0
      RETURN
 2    G=Z(3)-(EG/PEG)*Z(4)-0.D0
      RETURN
 3    G=Z(5)-(EG/PEG)*Z(6)-0.D0
      RETURN
 4    G=Z(7)-(EG/PEG)*Z(8)-0.D0
      RETURN
 5    G=Z(9)-(EG/PEG)*Z(10)-0.D0
      RETURN
 6    G=Z(11)-(EG/PEG)*Z(12)-0.D0
      RETURN
 7    G=Z(13)-(EG/PEG)*Z(14)-0.D0
      RETURN
 8    G=Z(15)-(EG/PEG)*Z(16)-1.D0
      RETURN
 9    G=Z(17)-(EG/PEG)*Z(18)-(CGCO/CGHO)
      RETURN
 10   G=Z(20)-0.D0
      RETURN
 11   G=Z(22)-0.D0
      RETURN
 12   G=Z(24)-0.D0
      RETURN
 13   G=Z(26)-0.D0
      RETURN
 14   G=Z(28)-0.D0
      RETURN
 15   G=Z(30)-0.D0
      RETURN
 16   G=Z(32)-0.D0
      RETURN
 17   G=Z(34)-0.0D0
      RETURN
 18   G=Z(36)-0.0D0
      RETURN
 19   G=Z(2)-0.D0
      RETURN
 20   G=Z(4)-0.D0
```

```
      RETURN
21    G=Z(6)-0.D0
      RETURN
22    G=Z(8)-0.D0
      RETURN
23    G=Z(10)-0.D0
      RETURN
24    G=Z(12)-0.D0
      RETURN
25    G=Z(14)-0.D0
      RETURN
26    G=Z(16)-0.D0
      RETURN
27    G=Z(18)-0.D0
      RETURN
28    G=Z(20)-0.D0
      RETURN
29    G=Z(22)-0.D0
      RETURN
30    G=Z(24)-0.D0
      RETURN
31    G=Z(26)-0.D0
      RETURN
32    G=Z(28)-0.D0
      RETURN
33    G=Z(30)-0.D0
      RETURN
34    G=Z(32)-0.D0
      RETURN
35    G=Z(34)-0.D0
      RETURN
36    G=Z(36)-0.D0

      RETURN
      END
C     ------------------------------------------------------
      SUBROUTINE DGSUB(I,Z,DG)

C     THIS IS A SUPPORTING SUBROUTINE

      IMPLICIT REAL *8(A-H,O-Z)

      COMMON/PAR8/PEG,PEL,EL,EG

      DIMENSION Z(36),DG(36)

      DO 50 J=1,36
      DG(J)=0.D0
50    CONTINUE

      GOTO(1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,
     * 21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36),I

1     DG(1)=1.D0
      DG(2)=-EG/PEG
      RETURN
2     DG(3)=1.D0
      DG(4)=-EG/PEG
      RETURN
3     DG(5)=1.D0
```

```
      DG(6)=-EG/PEG
      RETURN
4     DG(7)=1.D0
      DG(8)=-EG/PEG
      RETURN
5     DG(9)=1.D0
      DG(10)=-EG/PEG
      RETURN
6     DG(11)=1.D0
      DG(12)=-EG/PEG
      RETURN
7     DG(13)=1.D0
      DG(14)=-EG/PEG
      RETURN
8     DG(15)=1.D0
      DG(16)=-EG/PEG
      RETURN
9     DG(17)=1.D0
      DG(18)=-EG/PEG
      RETURN
10    DG(20)=1.D0
      RETURN
11    DG(22)=1.D0
      RETURN
12    DG(24)=1.D0
      RETURN
13    DG(26)=1.D0
      RETURN
14    DG(28)=1.D0
      RETURN
15    DG(30)=1.D0
      RETURN
16    DG(32)=1.D0
      RETURN
17    DG(34)=1.D0
      RETURN
18    DG(36)=1.D0
      RETURN
19    DG(2)=1.D0
      RETURN
20    DG(4)=1.D0
      RETURN
21    DG(6)=1.D0
      RETURN
22    DG(8)=1.D0
      RETURN
23    DG(10)=1.D0
      RETURN
24    DG(12)=1.D0
      RETURN
25    DG(14)=1.D0
      RETURN
26    DG(16)=1.D0
      RETURN
27    DG(18)=1.D0
      RETURN
28    DG(20)=1.D0
      RETURN
29    DG(22)=1.D0
      RETURN
```

```
 30     DG(24)=1.DO
        RETURN
 31     DG(26)=1.DO
        RETURN
 32     DG(28)=1.DO
        RETURN
 33     DG(30)=1.DO
        RETURN
 34     DG(32)=1.DO
        RETURN
 35     DG(34)=1.DO
        RETURN
 36     DG(36)=1.DO

        RETURN
        END
C       ------------------------------------------------------

        SUBROUTINE SOLUTN

C       THIS SUBROUTINE PROVIDES AN INITIAL GUESS TO THE SOLN.

        IMPLICIT REAL *8(A-H,O-Z)
        DIMENSION Z(36),DMVAL(18)

        Z(1)=0.674-0.6743*EXP(-0.1418*X)
        Z(2)=0.0956*EXP(-0.1418*X)
        Z(3)=0.532-5.32*EXP(-0.0038*X)
        Z(4)=0.0202*EXP(-0.0038*X)
        Z(5)=0.775-0.0775*EXP(-0.0038*X)
        Z(6)=0.00726*EXP(-0.0038*X)
        Z(7)=0.0193-0.0194*EXP(-0.1025*X)
        Z(8)=0.00198*EXP(-0.1025*X)
        Z(9)=-0.3708+0.37088*EXP(0.0032*X)
        Z(10)=0.001188*EXP(0.0032*X)
        Z(11)=0.364-0.364*EXP(-0.00205*X)
        Z(12)=0.000748*EXP(-0.00205*X)
        Z(13)=0.261-2.61*EXP(-0.0672*X)
        Z(14)=0.1753*EXP(-0.0672*X)
        Z(15)=-3.28+4.29*EXP(-0.0703*X)
        Z(16)=-0.3015*EXP(-0.0703*X)
        Z(17)=1.DO
        Z(18)=0.DO
        Z(19)=Z(1)
        Z(20)=Z(2)
        Z(21)=Z(3)
        Z(22)=Z(4)
        Z(23)=Z(5)
        Z(24)=Z(6)
        Z(25)=Z(7)
        Z(26)=Z(8)
        Z(27)=Z(9)
        Z(28)=Z(10)
        Z(29)=Z(11)
        Z(30)=Z(12)
        Z(31)=Z(13)
        Z(32)=Z(14)
        Z(33)=Z(15)
        Z(34)=Z(16)
        Z(35)=Z(17)
```

```
      Z(33)=Z(18)

      DMVAL(1)=-0.0133*EXP(-0.1418*X)
      DMVAL(2)=-0.0C0073*EXP(-0.0038*X)
      DMVAL(3)=-0.0C033*EXP(-0.0939*X)
      DMVAL(4)=-0.0C0302*EXP(-0.1023*X)
      DMVAL(5)=0.0C0C037*EXP(0.0032*X)
      DMVAL(6)=0.0C0C0152*EXP(-0.0020B*X)
      DMVAL(7)=-0.01178*EXP(-0.0872*X)
      DMVAL(8)=0.02119*EXP(-0.0703*X)
      DMVAL(9)=0.D0
      DMVAL(10)=DMVAL(1)
      DMVAL(11)=DMVAL(2)
      DMVAL(12)=DMVAL(3)
      DMVAL(13)=DMVAL(4)
      DMVAL(14)=DMVAL(5)
      DMVAL(15)=DMVAL(6)
      DMVAL(16)=DMVAL(7)
      DMVAL(17)=DMVAL(8)
      DMVAL(18)=DMVAL(9)

      RETURN
      END
C     ------------------------------------------------------

      SUBROUTINE SIGMA(AN,Z,RSUM)

C     EVALUATES THE NET KINETIC CONTRIBUTION

      IMPLICIT REAL *8(A-H,O-Z)
      DIMENSION Z(33),AN(9)

      SUM1=0.D0

      DO 10 J=1,9
      SUM1=SUM1+AN(J)*(Z(2*J-1)-Z(2*J+17))
 10   CONTINUE

      RSUM=SUM1

      RETURN
      END

C     ------------------------------------------------------

      FUNCTION RMCH(DA,A,B,Z)

      IMPLICIT REAL *8(A-H,O-Z)
      COMMON/PAR1/ALPHA
      DIMENSION DA(4),Z(33),A(4),B(4)

      SUM=0.D0
      DO 10 I=4,8
 10   SUM=SUM+((2.D0*FLOAT(I)+1.D0)*(ALPHA**(FLOAT(I)-4.D0)))


      HVAL1=Z(33)**A(1)
      HVAL2=Z(33)**A(2)
      HVAL3=Z(33)**A(3)
      HVAL4=Z(33)**A(4)
```

```
      IF(Z(35).EQ.0.0) GOTO 15

      HTAL1=Z(35)**B(1)
      HTAL2=Z(35)**B(2)
      HTAL3=Z(35)**B(3)
      HTAL4=Z(35)**B(4)
      GOTO 17

15    HTAL1=1.0
      HTAL2=1.0
      HTAL3=1.0
      HTAL4=1.0


17    RHOH=-(3.D0*DA(1)*HVAL1*HTAL1+
     *  5.D0*DA(2)*HVAL2*HTAL2+
     *  7.D0*DA(3)*HVAL3*HTAL3+
     *  DA(4)*HVAL4*HTAL4*SUM)

      RETURN
      END

C     ------------------------------------------------------

      FUNCTION RHOC(DA,A,B,Z)

      IMPLICIT REAL *8(A-H,O-Z)
      COMMON/PAR1/ALPHA
      DIMENSION DA(4),Z(36),A(4),B(4)

      SUM=0.D0
      DO 10 I=4,6
10    SUM=SUM+(FLOAT(I)*(ALPHA**(FLOAT(I)-4.D0)))

      CVAL1=Z(33)**A(1)
      CVAL2=Z(33)**A(2)
      CVAL3=Z(33)**A(3)
      CVAL4=Z(33)**A(4)

      IF(Z(35).EQ.0.0) GOTO 15

      CTAL1=Z(35)**B(1)
      CTAL2=Z(35)**B(2)
      CTAL3=Z(35)**B(3)
      CTAL4=Z(35)**B(4)
      GOTO 17


15    CTAL1=1.0
      CTAL2=1.0
      CTAL3=1.0
      CTAL4=1.0


17    RHOC=-(DA(1)*CVAL1*CTAL1+
     *  2.D0*DA(2)*CVAL2*CTAL2+
     *  3.D0*DA(3)*CVAL3*CTAL3+
     *  DA(4)*CVAL4*CTAL4*SUM)
```

```
      RETURN
      END
C     ------------------------------------------------------------

      FUNCTION RHON(DA,A,B,Z,NN)

      IMPLICIT REAL *8(A-H,O-Z)
      COMMON/PAR1/ALPHA
      DIMENSION DA(4),Z(33),A(4),B(4)

      IF (Z(33).EQ.0.0) GOTO 3

      YCAL=Z(33)**A(NN)
      YCAL4=Z(33)**A(4)
      GOTO 4

 3    YCAL=1.00
      YCAL4=1.00


 4    IF (Z(33).EQ.0.0) GOTO 5

      YTAL=Z(33)**B(NN)
      YTAL4=Z(33)**B(4)
      GOTO 7

 5    YTAL=1.0
      YTAL4=1.0

 7    IF(NN.GE.4) GOTO 10

      RHON=DA(NN)*YCAL*YTAL
      GOTO 20

 10   RHON=DA(4)*YCAL4*YTAL4*(ALPHA**(FLOAT(NN)-4.D0))

 20   RETURN
      END

C     ------------------------------------------------------------

      SUBROUTINE D33(Z,GHZ33,DCZ33)

      IMPLICIT REAL *8(A-H,O-Z)
      COMMON/PAR1/ALPHA
      COMMON/PAR3/DA,A,B
      DIMENSION DA(4),A(4),B(4),Z(33)

      SUM1=0.D0
      SUM2=0.D0
      DO 5 I=4,6
      SUM1=SUM1+((2.D0*FLOAT(I)+1.D0)*(ALPHA**(FLOAT(I)-4.D0)))
      SUM2=SUM2+(FLOAT(I)*(ALPHA**(FLOAT(I)-4.D0)))
 5    CONTINUE


      IF (Z(33).EQ.0.0) GOTO 15
      V331=Z(33)**(A(1)-1.D0)
      V332=Z(33)**(A(2)-1.D0)
      V333=Z(33)**(A(3)-1.D0)
```

```
      V334=Z(33)**(A(4)-1.DO)
      GOTO 20

15    V331=1.00
      V332=1.00
      V333=1.00
      V334=1.00

20    IF(Z(35).EQ.0.0) GOTO 25
      T331=Z(35)**B(1)
      T332=Z(35)**B(2)
      T333=Z(35)**B(3)
      T334=Z(35)**B(4)
      GOTO 30

25    T331=1.00
      T332=1.00
      T333=1.00
      T334=1.00

30    DHZ33=-(3.DO*A(1)*DA(1)*V331*T331+
     *  5.DO*A(2)*DA(2)*V332*T332+
     *  7.DO*A(3)*DA(3)*V333*T333+
     *  A(4)*DA(4)*V334*T334*SUM1)

      DCZ33=-(DA(1)*A(1)*V331*T331+
     *  2.DO*DA(2)*A(2)*V332*T332+
     *  3.DO*DA(3)*A(3)*V333*T333+
     *  DA(4)*A(4)*V334*T334*SUM2)

      RETURN
      END
C     ------------------------------------------------------
      SUBROUTINE D35(Z,DHZ35,DCZ35)

      IMPLICIT REAL *8(A-H,O-Z)
      COMMON/PAR1/ALPHA
      COMMON/PAR5/DA,A,B
      DIMENSION DA(4),A(4),B(4),Z(36)

      SUM1=0.DO
      SUM2=0.DO
      DO 10 I=4,6
      SUM1=SUM1+((2.DO*FLOAT(I)+1.DO)*(ALPHA**(FLOAT(I)-4.DO)))
      SUM2=SUM2+(FLOAT(I)*(ALPHA**(FLOAT(I)-4.DO)))
10    CONTINUE

      IF(Z(33).EQ.0.00) GOTO 15

      C331=Z(33)**A(1)
      C332=Z(33)**A(2)
      C333=Z(33)**A(3)
      C334=Z(33)**A(4)
      GOTO 16

15    C331=1.0
      C332=1.0
      C333=1.0
      C334=1.0
```

```
 12     IF(Z(33).EQ.0.0) GOTO 20

        E331=Z(33)**(B(1)-1.D0)
        E332=Z(33)**(B(2)-1.D0)
        E333=Z(33)**(B(3)-1.D0)
        E334=Z(33)**(B(4)-1.D0)

        GOTO 30
 20     E331=1.00
        E332=1.00
        E333=1.00
        E334=1.00

 30     DHZ33=-(3.0*B(1)*DA(1)*C331*E331+
     *  5.0*B(2)*DA(2)*C332*E332+
     *  7.D0*B(3)*DA(3)*C333*E333+
     *  DA(4)*B(4)*C334*E334*SUM1)

        DCZ33=-(DA(1)*B(1)*C331*E331+
     *  2.0*DA(2)*B(2)*C332*E332+
     *  3.0*DA(3)*B(3)*C333*E333+
     *  DA(4)*B(4)*C334*E334*SUM2)

        RETURN
        END

C       ------------------------------------------------------

        FUNCTION DHC33(Z,NN)

        IMPLICIT REAL *8(A-H,O-Z)
        COMMON/PAR1/ALPHA
        COMMON/PAR3/DA,A,B
        DIMENSION DA(4),A(4),B(4),Z(33)

        IF(Z(33).EQ.0.0) GOTO 10
        P33=Z(33)**(A(NN)-1.D0)
        P334=Z(33)**(A(4)-1.D0)
        GOTO 20

 10     P33=1.00
        P334=1.00

 20     IF(Z(33).EQ.0.0) GOTO 30
        S33=Z(33)**B(NN)
        S334=Z(33)**B(4)
        GOTO 40

 30     S33=1.00
        S334=1.00

 40     IF(NN.GE.4) GOTO 50
        DHC33=DA(NN)*A(NN)*P33*S33
        GOTO 60

 50     DHC33=DA(4)*A(4)*P334*S334*(ALPHA**(FLOAT(NN)-4.D0))

 60     RETURN
        END
C       ------------------------------------------------------
```

```
      FUNCTION DHC35(Z,NN)

      IMPLICIT REAL *8(A-H,O-Z)
      COMMON/PAR1/ALPHA
      COMMON/PAR5/DA,A,B
      DIMENSION DA(4),A(4),B(4),Z(38)

      IF(Z(33).EQ.0.0) GOTO 5

      Q33=Z(33)**A(NN)
      Q334=Z(33)**A(4)
      GOTO 8

 5    Q33=1.0
      Q334=1.0

 8    IF (Z(35).EQ.0.0) GOTO 10
      R33=Z(35)**(B(NN)-1.D0)
      R334=Z(35)**(B(4)-1.D0)
      GOTO 20

 10   R33=1.0
      R334=1.0

 20   IF(NN.GE.4) GOTO 30

      DHC35=DA(NN)*B(NN)*Q33*R33
      GOTO 40
 30   DHC35=DA(4)*B(4)*Q334*R334*(ALPHA**(FLOAT(NN)-4.D0))

 40   RETURN
      END

C     ------------------------------------------------------
      SUBROUTINE INPUT(T,P,AL,D,UGO,AMCAT,AMSUS,AM,A,B,PH2,
     *  PCO,AKN,CGHO,CGCO,DENCAT,DENL)

C     RETRIEVES THE INPUT DATA FROM FOR12.DAT

      IMPLICIT REAL *8(A-H,O-Z)
      DIMENSION AM(9),H(4),E(4),A(4),B(4),AKN(4)

      READ(12,100)T
      READ(12,100)P
      READ(12,100)AL
      READ(12,100)D
      READ(12,100)UGO
      READ(12,100)AMCAT
      READ(12,100)AMSUS
      READ(12,100)AM(7)
      READ(12,100)AM(8)
      READ(12,100)AM(9)
      READ(12,100)AMN
      READ(12,100)DENCAT
      READ(12,100)DENL

      DO 10 I=1,6
 10   AM(I)=AMN

      DO 20 I=1,4
```

```
      READ(11,150)H(I)
      READ(11,150)E(I)
      READ(11,150)A(I)
      READ(11,150)B(I)
      AKH(I)=H(I)*EXP(-E(I)*1000.D0/(1.98D0*T))
 20   CONTINUE

      READ(12,100)PH2
      READ(12,100)PCO
      CGH0=PH2/(82.05D0*T)
      CGC0=PCO/(82.05D0*T)


 100  FORMAT(F15.5)
 150  FORMAT(F15.5)

      RETURN
      END
C     ------------------------------------------------------

      SUBROUTINE CATCON(AMCAT,AMSUS,DENCAT,DENL,CCAT)

C     THIS SUBROUTINE CALCULATES THE AVG. CATALYST CONC.

      IMPLICIT REAL *8(A-H,O-Z)

      WCAT=AMCAT/AMSUS

      CALL VOLFRA(AMCAT,AMSUS,DENL,DENCAT,WCAT,VCAT)
      CALL SLUDEN(VCAT,DENCAT,DENL,DENSL)

      CCAT=WCAT*DENSL

      RETURN
      END
C     ------------------------------------------------

      SUBROUTINE HOLDUP(UG,EG)

C     THIS ROUTINE CALC.THE GAS PHASE HOLDUP

      IMPLICIT REAL *8(A-H,O-Z)

      EG=0.033D0*(UG**1.1D0)

      RETURN
      END

C     ------------------------------------------------------

      SUBROUTINE MASTRN(UGO,NN,AKLA)

C     THIS ROUTINE CALC. THE MASS TRNF. COEFF.

      IMPLICIT REAL *8(A-H,O-Z)
      DIMENSION AKLA(9)

      IF(NN.NE.9) GOTO 10
      AKLA(9)=0.1*UGO
      GOTO 40
```

```
 10     IF(NN.NE.8) GOTO 20
        AKLA(8)=AKLA(9)
        GOTO 40
 20     IF(NN.NE.7) GOTO 30
        AKLA(7)=AKLA(9)*2.4467
        GOTO 40
 30     AKLA(NN)=AKLA(9)*8.198

 40     RETURN
        END
C       ------------------------------------------------

        SUBROUTINE SLUDEN(VCAT,DENCAT,DENL,DENSL)

C       THIS ROUTINE CALC. THE DENSITY OF THE SLURRY

        IMPLICIT REAL *8(A-H,O-Z)

        DENSL=VCAT*DENCAT+(1.DO-VCAT)*DENL

        RETURN
        END
C       ------------------------------------------------------

        SUBROUTINE VOLFRA(AMCAT,AMSUS,DENL,DENCAT,WCAT,VCAT)

C       THIS ROUTINE CALC. THE VOLUME FRACTION OF THE SOLIDS

        IMPLICIT REAL *8(A-H,O-Z)

        VCAT=(DENL*WCAT)/(DENCAT-WCAT*(DENCAT-DENL))

        RETURN
        END
C       ------------------------------------------------

        SUBROUTINE VALUE(T,ALPHA)

C       THIS ROUTINE CALC. ALPHA AS A FUNCTION OF TEMP.

        IMPLICIT REAL *8(A-H,O-Z)

        VAL1=(-0.2855DO/T)-0.511DO
        VAL2=EXP(VAL1)+1.DO
        ALPHA=1.DO/VAL2

        RETURN
        END

C       ------------------------------------------------

        SUBROUTINE GASDIF(D,UG,DG)

C       EVALUATES THE GAS PHASE DISPERSION COEFF.

        IMPLICIT REAL *8(A-H,O-Z)

        DG=0.2*(D*D)*UG

        RETURN
```

```
      END
C     ------------------------------------------------
      SUBROUTINE LIQDIF(D,UG,DL)

C     EVALUATES THE LIQUID PHASE DISPERSION

      IMPLICIT REAL *8(A-H,O-Z)

      DL=2.7*(D**1.4)*(UG**0.3)

      RETURN
      END
C     ------------------------------------------------
      SUBROUTINE SUPER(X,UGO,RSUM,UGB)

C     DETERMINES THE VARIATION OF UG ALONG AXIS

      IMPLICIT REAL *8(A-H,O-Z)

      COMMON/PAR3/CCAT,CGHO,CGCO,P,T

      CT=P/(82.05*T)
      CT=CT/CGHO

      UGB=(-RSUM/CT)*X+1.DO


      RETURN
      END
C     ------------------------------------------------

C     PROGRAM ENDS HERE !!
```

FBR MODEL 1

The main computer program developed to solve the mass balance equations is entitled FBH2.FOR. As is the case with all the programs developed and described so far, the program is made modular, with subroutines incorporating the various correlations and expressions used for property and parameter estimation. The various subroutines used in the simulator are as given below:

SUBROUTINE	PURPOSE
INPUT	Retrieves the user supplied data.
VELO	Evaluates the various phase velocities.
TCOF	Evaluates the transfer coefficients.

Besides these, subroutines entitled FSUB, DFSUB, GSUB, DGSUB, and DUMMY are used to describe the boundary value problem as per the algorithm, COLSYS.

The data required for the simulator is supplied by the user via an interactive program FBIN.FOR, and is stored in a data file. Following variables have to be supplied by the user prior to the execution of FBH2.FOR.

Reactor Temperature (K)

Reactor Pressure (Atm)

Reactor Height (cm)

Reactor Diameter (cm)

Inlet concentration of H_2 (gmole/cc)

CO/H_2 usage ratio

Inlet CO/H_2 molar ratio

Gas phase diffusivity of $H_2(cm^2/sec)$

Voidage at minimum fluidization

Velocity and minimum fluidization (cm/sec)

Inlet superficial fluidizing velocity (cm/sec)

Activation Energy (kcal/mol)

Frequency Factor (per sec.)

On execution, the simulator FBH2.FOR, generates an output files, CONC.DAT and PVEL.DAT, which store all the input parameters supplied by the user along with the concentration of H_2 in the various phases, the variation of superficial gas velocity along the reactor axis and the syngas conversion obtained along the reactor.

Case Study

As indicated earlier, nitrided iron catalysts do not produce significant amounts of wax which permits their operation in fluidized bed reactors at temperatures below those usually maintained with reduced iron catalysts. Synthesis gas containing $1H_2$+1CO has generally be used with nitrides, and the usage ratio can be readily adjusted to equal the feed ratio by changing the recycle ratio.

The program was used to predict the performance of fluidized bed reactor. The design parameters used were similar to the Sasol Pilot plant reactor, viz., diameter of 5 cm and reactor height of 200 cm. The input parameters were provided via FBIN.FOR, an interactive program. A typical input sample is as shown. The output files include the variation of H_2 concentration in the bubble, the cloud-wake and the particulate phases, the variation of phase velocities and the variation of syn-gas conversion along the reactor axis. These results are as illustrated in Fig. A-B-8 to A-B-10 The output files, viz. CONC.DAT and PVEL.DAT are also shown herewith. The kinetic parameters used suggest that the rate of reaction is very slow in comparison to the transfer across the phases as seen in Fig. A-B-8 where the concentration in the three phases differ marginally.

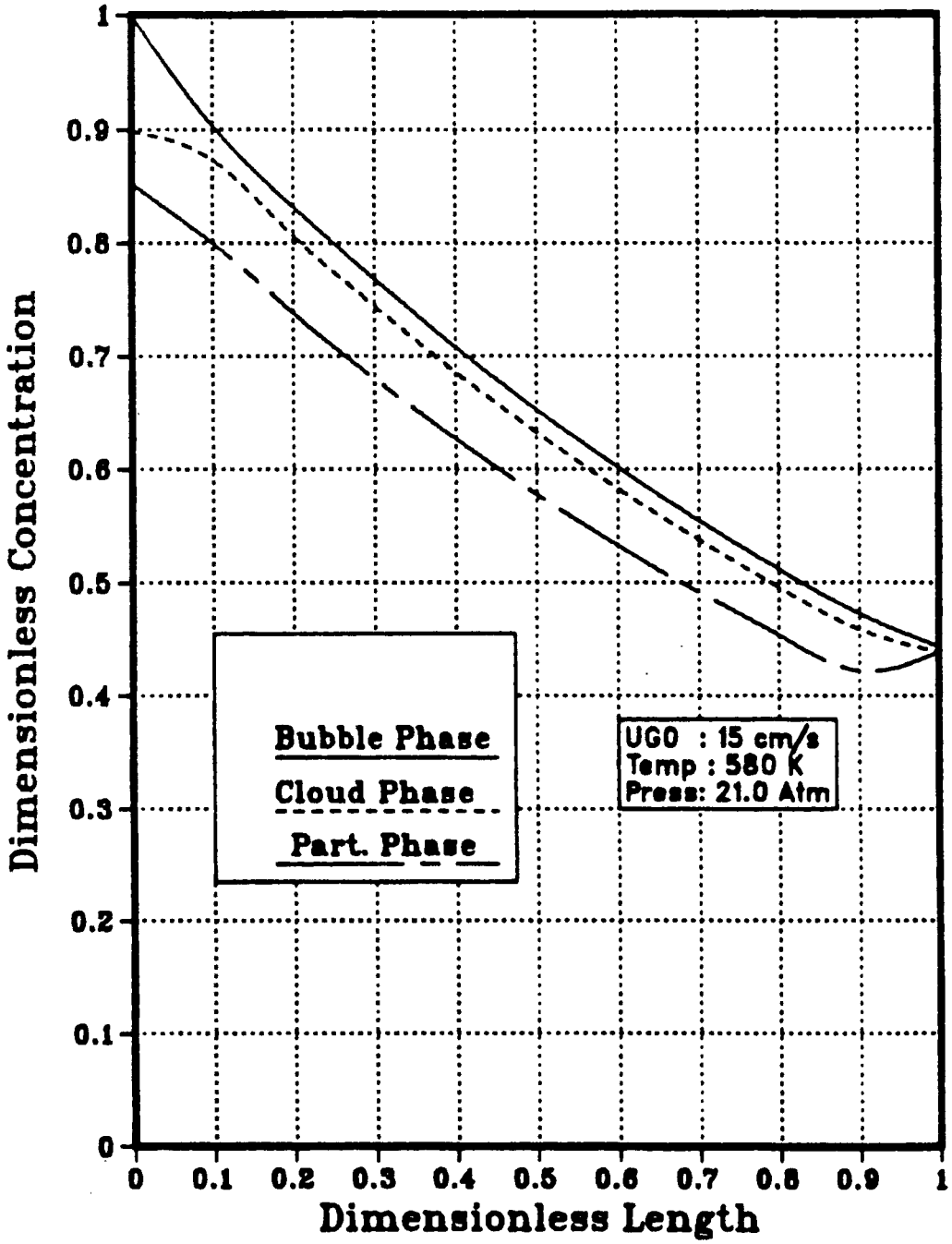

Figure A-B-8: Variation of H_2 Concentration in the Three Pases (FBR)

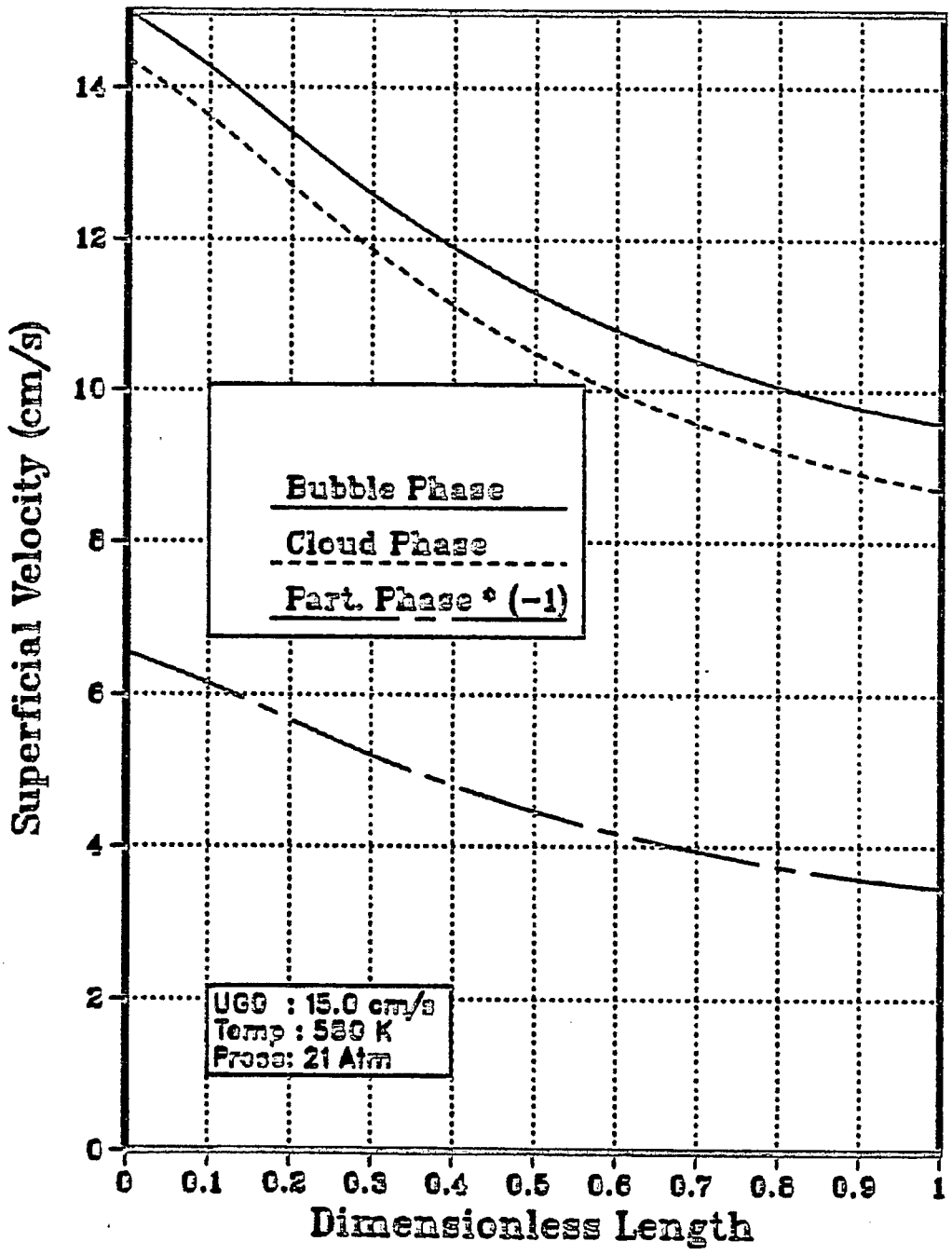

Figure A-B-9: Variation of Phase Velocities Along Length

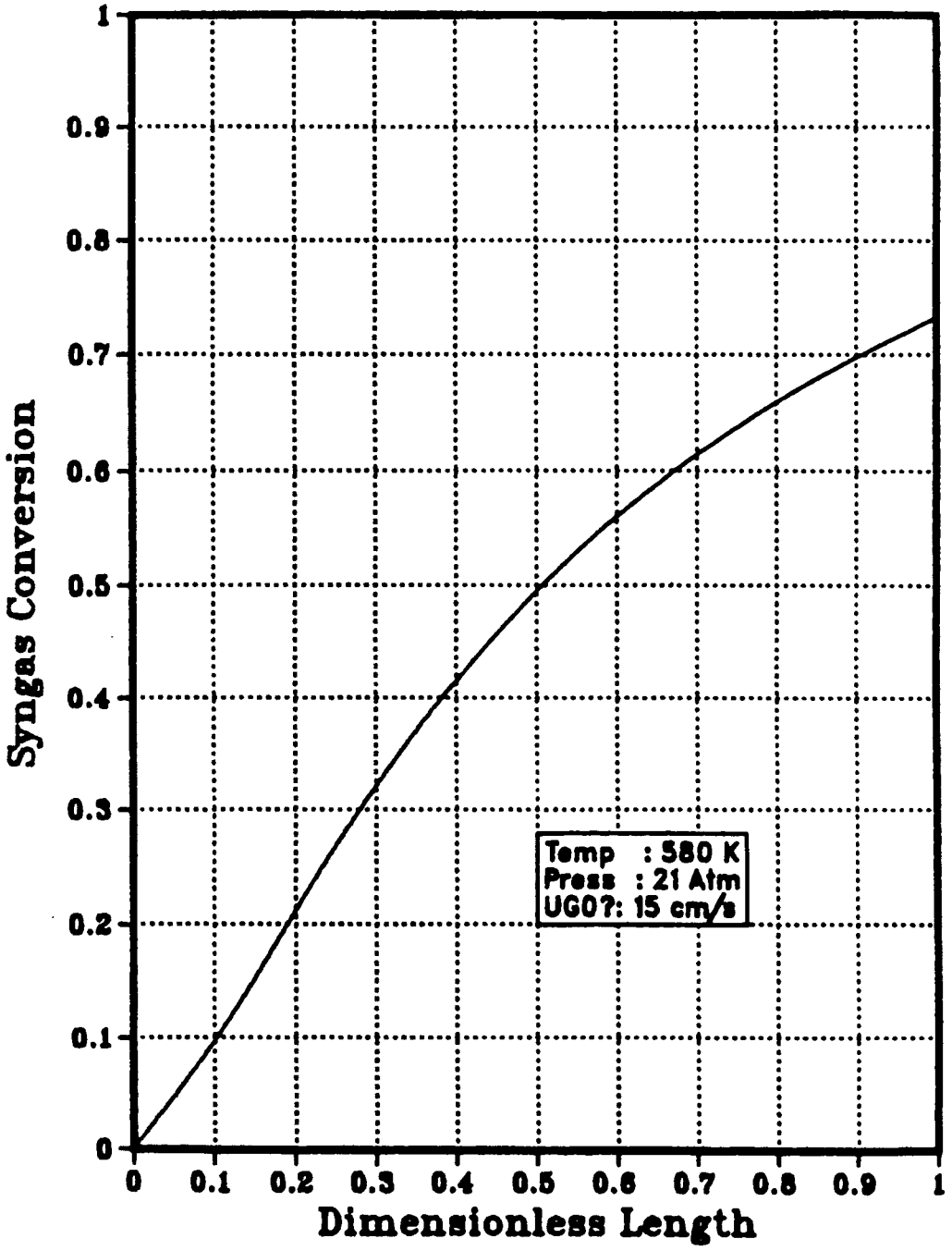

Figure A-B-10. Variation of Syngas Conversion Along Length (FBR)

TYPICAL INPUT SAMPLE: FBIN.FOR

```
 INPUT THE DATA ASKED FOR IN A FREE FORMAT


 FOLLOWING IS A LIST OF OPERATING CONDITIONS:
 ---------------------------------------------


 REACTOR TEMPERATURE (Deg.K) =?
>580.0
 REACTOR PRESSURE (Atm.) =?
>21.0
 REACTOR HEIGHT (cm.) =?
>200.0
 REACTOR DIAMETER (cm.) =?
>5.0


 FOLLOWING IS A SET OF INLET CONDITIONS :
 ----------------------------------------


  CO/H2 INLET RATIO =?
>0.833
  CO/H2 USAGE RATIO =?
>0.833


  GAS DIFFUSIVITY OF H2 (cm**2/sec) =?
>0.2


 FOLLOWING IS A LIST OF DESIGN PARARMETERS :
 -------------------------------------------


 VOIDAGE AT MINIMUM FLUIDISATION =?
>0.5
 VELOCITY AT MINIMUM FLUIDISATION (cm/sec) =?
>1.4
 DENSITY OF CATALYST (gm/cc) =?
>5.0
 INLET SUPERFICIAL GAS VELOCITY (cm/sec) =?
>15


 FOLLOWING IS A LIST OF KINETIC PARAMETERS :
 -------------------------------------------


  ACTIVATION ENERGY FOR FT SYNTHESIS Rn. (Kcal/mol)
>20.31
  FREQUENCY FACTOR FOR FT SYNTHESIS Rn. (per hr)
>5.807E8
  BUBBLE DIAMETER =?
>3.00


 ALL THE DATA HAS BEEN ENTERED. PROCEED TO FBR.FOR
```

OUTPUT FILES: CONC.DAT

PVEL.DAT

F-T SYNTHESIS IN FLUIDIZED BED REACTOR
-: COUNTERCURRENT BACKMIXING MODEL :-

DESIGN PARAMETERS :

REACTOR DIAMETER	:	5.00	cm.
REACTOR HEIGHT	:	200.00	cm.
VELOCITY @ MINIMUM FLUIDIZATION	:	1.40	cm/sec
VOIDAGE AT MINIMUM FLUIDIZATION	:	0.50	

OPERATING CONDITIONS :

OPERATING TEMPERATURE	:	580.00	Deg. K
OPERATING PRESSURE	:	21.00	Atm.
INLET CONC. OF H2	:	.241E-03	mol/cc
INLET CO/H2 MOLE RATIO	:	0.83	
INLET SUP GAS VELOCITY	:	15.00	cm/sec

KINETIC PARAMETER :

A FIRST ORDER DEPENDENCE ON H2 CONC. IS ASSUMED

RATE CONSTANT (K) :.404E-01 per sec.

X	BUBBLE PHASE	CLOUD PHASE	PART. PHASE	SYNGAS CONV.
.000E+00	.100E+01	.898E+00	.853E+00	0.00
.100E+00	.904E+00	.874E+00	.800E+00	9.63
.200E+00	.833E+00	.807E+00	.738E+00	21.07
.300E+00	.768E+00	.744E+00	.680E+00	31.99
.400E+00	.708E+00	.686E+00	.627E+00	41.51
.500E+00	.653E+00	.633E+00	.578E+00	49.46
.600E+00	.602E+00	.583E+00	.533E+00	56.01
.700E+00	.555E+00	.538E+00	.492E+00	61.43
.800E+00	.512E+00	.496E+00	.454E+00	65.95
.900E+00	.473E+00	.459E+00	.422E+00	69.74
.100E+01	.444E+00	.439E+00	.439E+00	73.23

VARIATION OF PHASE VELOCITY ALONG REACTOR

X	SUP.VEL.	BUBBLE PHASE	CLOUD PHASE	PART.PHASE
0.00	15.00	14.37	7.19	-6.56
0.10	14.28	13.62	6.81	-6.15
0.20	13.42	12.72	6.36	-5.67
0.30	12.60	11.87	5.93	-5.20
0.40	11.89	11.12	5.56	-4.80
0.50	11.29	10.50	5.25	-4.46
0.60	10.80	9.98	4.99	-4.17
0.70	10.39	9.56	4.78	-3.94
0.80	10.05	9.20	4.60	-3.74
0.90	9.77	8.90	4.45	-3.58
1.00	9.56	8.68	4.34	-3.46

PROGRAM LISTING: FBIN.FOR

```
C       ------------------------------------------------
C       THIS PROGRAM IS DEVELOPED TO INPUT THE REQUISITE
C       DATA TO THE FLUIDISED BED REACTOR MODEL :
C                       FBH2.FOR
C       ------------------------------------------------

        IMPLICIT REAL *8(A-H,O-Z)

        WRITE*,'INPUT THE DATA ASKED FOR IN A FREE FORMAT'
        WRITE*
        WRITE*
        WRITE*,'FOLLOWING IS A LIST OF OPERATING CONDITIONS:'
        WRITE*,'-------------------------------------------'
        WRITE*
        WRITE*
        WRITE*,'REACTOR TEMPERATURE (Deg.K) =?'
        READ*,T
        WRITE(22,*)T
        WRITE*,'REACTOR PRESSURE (Atm.) =?'
        READ*,P
        WRITE(22,*)P
        WRITE*,'REACTOR HEIGHT (cm.) =?'
        READ*,H
        WRITE(22,*)H
        WRITE*,'REACTOR DIAMETER (cm.) =?'
        READ*,D
        WRITE(22,*)D
        WRITE*
        WRITE*
        WRITE*,'FOLLOWING IS A SET OF INLET CONDITIONS :'
        WRITE*,'---------------------------------------'
        WRITE*
        WRITE*
        WRITE*,' CO/H2 INLET RATIO =?'
        READ*,RAT
        WRITE(22,*)RAT
        WRITE*,' CO/H2 USAGE RATIO =?'
        READ*,USE
        WRITE(22,*)USE
        WRITE*
        WRITE*
        WRITE*,' GAS DIFFUSIVITY OF H2 (cm**2/sec) =?'
        READ*,DC
        WRITE(22,*)DC
        WRITE*
        WRITE*
        WRITE*,'FOLLOWING IS A LIST OF DESIGN PARARMETERS :'
        WRITE*,'-------------------------------------------'
        WRITE*
        WRITE*
        WRITE*,' VOIDAGE AT MINIMUM FLUIDISATION =? '
        READ*,EMF
        WRITE(22,*)EMF
        WRITE*,'VELOCITY AT MINIMUM FLUIDISATION (cm/sec) =?'
        READ*,UMF
        WRITE(22,*)UMF
        WRITE*,' DENSITY OF CATALYST (gm/cc) =?'
        READ*,RHOCAT
        WRITE(22,*)RHOCAT
        WRITE*,'INLET SUPERFICIAL GAS VELOCITY (cm/sec) =?'
```

```
      READ*,UGO
      WRITE(22,*)UGO
      WRITE*
      WRITE*
      WRITE*,'FOLLOWING IS A LIST OF KINETIC PARAMETERS :'
      WRITE*,'-----------------------------------------'
      WRITE*
      WRITE*
      WRITE*,' ACTIVATION ENERGY FOR FT SYNTHESIS Rn. (Kcal/mol)'
      READ*,EA
      WRITE(22,*)EA
      WRITE*,' FREQUENCY FACTOR FOR FT SYNTHESIS Rn. (per hr) '
      READ*,FF
      WRITE(22,*)FF
      WRITE*,' BUBBLE DIAMETER =?'
      READ*,DE
      WRITE(22,*)DE
      WRITE*
      WRITE*
      WRITE*
      WRITE*,'ALL THE DATA HAS BEEN ENTERED. PROCEED TO FBR.FOR'

100   FORMAT(F8.3)

      STOP
      END
C     ------------------------------------------------------
```

PROGRAM LISTING: FBH2.FOR

```
C       ------------------------------------------------
C       THIS IS THE MAIN PROGRAM,DEVELOPED TO SOLVE
C       THE MODEL EQUATIONS DESCRIBING FT SYNTHESIS IN
C                 FLUIDISED BED REACTOR.
C       ------------------------------------------------

C       FOLLOWING IS LIST OF VARIABLES USED IN THE PROGRAM :

C       T               :OPERATING TEMPERATURE (K)
C       P               :OPERATING PRESSURE (ATM)
C       D               :REACTOR DIAMETER (CM)
C       H               :REACTOR HEIGHT (CM)
C       RAT             :INLET CO/H2 RATIO
C       CGHO            :INLET CONC OF H2 (GMOLES/CC)
C       DC              :GAS PHASE DIFFUSIVITY (GM/CM**2)
C       EMF             :VOIDAGE AT MINIMUM FLUIDIZATION
C       UMF             :VELOCITY AT MINIMUM FLUIDIZATION  (CM/S)
C       RHOCAT          :DENSITY OF CATALYST (GM/CC)
C       UGO             :INLET SUPERFICIAL GAS VELOCITY (CM/S)
C       EA              :ACTIVATION ENERGY (KCAL/MOL)
C       FF              :FREQUENCY FACTOR (PER Hr)
C       AK              :KINETIC RATE CONST. (PER SEC)
C       DE              :BUBBLE EQUV.DIAMETER (CM)
C       EPSB            :VOID FRACTION
C       UA              :BUUBLE RISE VELOCITY (CM/S)
C       UGC             :VELOCITY OF CLOUD WAKE-PHASE (CM/S)
C       UGB             :VELOCITY OF BUBBLE PHASE (CM/S)
C       UGP             :VELOCITY OF PARTICULATE PHASE (CM/S)
C       AKBC            :BUBBULE TO CLOUD TRANSFER COEFF.
C       AKCP            :CLOUD TO PARTICULATE TRANSFER COEFF.
C       ------------------------------------------------------------

C       THIS IS THE MAIN PROGRAM

        IMPLICIT REAL *8(A-H,O-Z)

        COMMON/PAR1/AKBC,AKCP
        COMMON/PAR2/U,UGB,UGC,UGP,UMF
        COMMON/PAR3/EMF,EPSB,FW,RHOCAT
        COMMON/PAR4/CGHO,UGO,UGBO
        COMMON/PAR5/AK,USE,RAT
        COMMON/PAR6/H,T,D,DE,P
        COMMON/PAR7/DC

        DIMENSION FSPACE(9000),ISPACE(600),ZETA(3),TOL(3),
     *  LTOL(3),Z(3),M(3),IPAR(11)

        EXTERNAL FSUB,DFSUB,DGSUB,GSUB,DUMMY

        OPEN (UNIT=23,FILE='CONV.DAT')
        OPEN (UNIT=24,FILE='VEL.DAT')


        CALL INPUT


        U=UGO
        FW=1.DO
```

```
      WRITE(23,*)' ------------------------------------------------'
      WRITE(23,*)'       F-T SYNTHESIS IN FLUIDIZED BED REACTOR  '
      WRITE(23,*)'        -: COUNTERCURRENT BACKMIXING MODEL :-   '
      WRITE(23,*)' ------------------------------------------------'
      WRITE(23,*)
      WRITE(23,*)
      WRITE(23,*)
      WRITE(23,*)' DESIGN PARAMETERS :'
      WRITE(23,*)' -------------------'
      WRITE(23,*)
      WRITE(23,200)' REACTOR DIAMETER                 :',D,'  cm.'
      WRITE(23,200)' REACTOR HEIGHT                   :',H,'  cm.'
      WRITE(23,200)' VELOCITY  MINIMUM FLUIDIZATION :',UMF,'  cm/sec'
      WRITE(23,200)' VOIDAGE AT MINIMUM FLUIDIZATION :',EMF
      WRITE(23,*)
      WRITE(23,*)
      WRITE(23,*)' OPERATING CONDITIONS :'
      WRITE(23,*)' ----------------------'
      WRITE(23,*)
      WRITE(23,200)' OPERATING TEMPERATURE            :',T,'  Deg. K'
      WRITE(23,200)' OPERATING PRESSURE               :',P,'  Atm.'
      WRITE(23,250)' INLET CONC. OF H2                :',CGHO,' mol/cc'
      WRITE(23,200)' INLET CO/H2 MOLE RATIO           :',RAT
      WRITE(23,200)' INLET SUP. GAS VELOCITY          :',UGO,'  cm/sec'
      WRITE(23,*)
      WRITE(23,*)
      WRITE(23,*)' KINETIC PARAMETER :'
      WRITE(23,*)' --------------------'
      WRITE(23,*)
      WRITE(23,*)' A FIRST ORDER DEPENDENCE ON H2 CONC. IS ASSUMED'
      WRITE(23,*)
      WRITE(23,250)' RATE CONSTANT  (K) :',AK,' per sec.'
      WRITE(23,*)
      WRITE(23,*)
      WRITE(23,*)
      WRITE(23,150)
      WRITE(23,160)'X','BUBBLE PHASE','CLOUD PHASE','PART. PHASE',
     *  'SYNGAS CONV.'
      WRITE(23,150)

      WRITE(24,*)' VARIATION OF PHASE VELOCITY ALONG REACTOR '
      WRITE(24,*)
      WRITE(24,*)
      WRITE(24,*)
      WRITE(24,*)
      WRITE(24,150)
      WRITE(24,160)'X','SUP.VEL.','BUBBLE PHASE','CLOUD PHASE',
     *  'PART.PHASE'
      WRITE(24,150)

      CALL VELO(U,UMF,EMF,DE,UA,EPSB,FW,UGC,UGB,UGP)
      CALL TCOF(DC,UMF,DE,EMF,UA,AKBC,AKCP)
      UGBO=UGB


C     INPUT TO COLSYS

      NCOMP=3
```

```
      DO 10 I=1,NCOMP
      M(I)=1
10    CONTINUE

      ALEFT=0.DO
      ARIGHT=1.DO

      ZETA(1)=0.DO
      ZETA(2)=0.DO
      ZETA(3)=1.DO


      DO 40 I=1,11
      IPAR(I)=0
40    CONTINUE

C     IPAR(1)=1
      IPAR(4)=3
      IPAR(5)=9000
      IPAR(6)=600
      IPAR(7)=1

      DO 50 I=1,3
      LTOL(I)=I
      TOL(I)=8.D-3
50    CONTINUE

      CALL COLSYS(NCOMP,M,ALEFT,ARIGHT,ZETA,IPAR,LTOL,TOL,
     * FIXPNT,ISPACE,FSPACE,IFLAG,FSUB,DFSUB,GSUB,DGSUB,DUMMY)

      X=0.0D0
      U=UG0
      CONSYN=0.0
      UGB=UGB0

      DO 60 I=1,11
      CALL APPSLN(X,Z,FSPACE,ISPACE)


      CONVH=(UGB0-UGB*Z(1))/UGB0
      CONC0=CONVH*USE/RAT
      CONSYN=(1.0+USE)*CONVH/(1.0+RAT)

      U=UG0*(1.0-0.5*CONSYN)

      CALL VELO(U,UMF,EMF,DE,UA,EPSB,FW,UGC,UGB,UGP)
      CALL TCOF(DC,UMF,DE,EMF,UA,AKBC,AKCP)


      WRITE(24,110)X,U,UGB,UGC,UGP

      IF(I.EQ.11) GOTO 65
      WRITE(23,100)X,Z(1),Z(2),Z(3),CONC0*100.0
      WRITE(30,*)CONVH*100.0,CONC0*100.0,CONSYN*100.0

      X=X+0.1
60    CONTINUE


65    CH=(UGB*Z(1)+(U-UGB)*Z(2))/U
```

```
      CONVH=(UGBO-UGB*CH)/UGBO
      CONCO=USE*CONVH/RAT
      CONSYN=(1.0+USE)*CONVH/(1.0+RAT)

      WRITE(23,100)X,Z(1),Z(2),Z(3),CONCO*100.0
      WRITE(30,*)CONVH*100.0,CONCO*100.0,CONSYN*100.0
      WRITE(23,150)
      WRITE(24,150)

  100 FORMAT(2X,4(E9.3,5X),3X,F6.2)
  110 FORMAT(3X,5(F6.2,6X))
  150 FORMAT(70('-'))
  160 FORMAT(7X,5(A,4X))
  200 FORMAT(X,A,F8.2,A)
  250 FORMAT(X,A,E8.3,A)
  300 FORMAT(3X,A,E8.3,3X,A,E8.3)
      CLOSE (UNIT=23)
      CLOSE (UNIT=24)

      STOP
      END
C     ------------------------------------------------
      SUBROUTINE FSUB(X,Z,F)

C     THIS SUBROUTINE DEFINES THE BOUNDRY VALUE PROBLEM
C     AS PER COLSYS


      IMPLICIT REAL *8(A-H,O-Z)

      COMMON/PAR1/AKBC,AKCP
      COMMON/PAR2/U,UGB,UGC,UGP,UMF
      COMMON/PAR3/EMF,EPSB,FW,RHOCAT
      COMMON/PAR4/CGHO,UGO,UGBO
      COMMON/PAR5/AK,USE,RAT
      COMMON/PAR6/H,T,D,DE,P
      COMMON/PAR7/DC

      DIMENSION Z(3),F(3)

      R=82.05

      CONVH=(UGBO-UGB*Z(1))/UGBO
      CONSYN=(1.0+USE)*CONVH/(1.0+RAT)

      U=UGO*(1.0-0.5*CONSYN)

      CALL VELO(U,UMF,EMF,DE,UA,EPSB,FW,UGC,UGB,UGP)
      CALL TCOF(DC,UMF,DE,EMF,UA,AKBC,AKCP)



      A1=-AKBC*H*EPSB/UGB
      A2=-A1
      A3=AKBC*H*EPSB/UGC
      A4=-H*EPSB*(AKBC+AKCP+(AK*FW))/UGC
      A5=AKCP*H*EPSB/UGC
      A6=AKCP*H*EPSB/UGP
      A7=-(AKCP*H*EPSB+(AK*H)*(1.0-EPSB*(1.0+FW)))/UGP
```

```
      F(1)=A1*Z(1)+A2*Z(2)
      F(2)=A3*Z(1)+A4*Z(2)+A5*Z(3)
      F(3)=A6*Z(2)+A7*Z(3)

      RETURN
      END
C     ------------------------------------------------------

      SUBROUTINE DFSUB(X,Z,DF)


C     THIS IS A SUPPORTING SUBROUTINE TO COLSYS

      IMPLICIT REAL *8(A-H,O-Z)
      DIMENSION DF(3,3),WORK1(3),WORK2(3),Z(3)

      EPS=1.E-7
      DO 10 J=1,3
      Z(J)=Z(J)+EPS
      CALL FSUB(X,Z,WORK1)
      Z(J)=Z(J)-2.0*EPS
      CALL FSUB(X,Z,WORK2)
      Z(J)=Z(J)+EPS

      DO 10 I=1,3
 10   DF(I,J)=(WORK1(I)-WORK2(I))*0.5/EPS

      RETURN
      END
C     ------------------------------------------------------
      SUBROUTINE GSUB(I,Z,G)

C     THIS IS A SUPPORTING SUBROUTINE TO COLSYS  IT DEFINES
C     THE BOUNDARY CONDITIONS FOR THE BVP

      IMPLICIT REAL *8(A-H,O-Z)

      COMMON/PAR2/U,UGB,UGC,UGP,UMF

      DIMENSION Z(3)

      B1=(U-UGB)/UGC
      B2=1.0-B1

      GOTO (1,2,3),I

 1    G=Z(1)-1.0
      RETURN
 2    G=Z(2)-B1-(B2*Z(3))
      RETURN
 3    G=Z(2)-Z(3)
      RETURN
      END
C     ------------------------------------------------------------
      SUBROUTINE DGSUB(I,Z,DG)


C     THIS IS A SUPPORTING SUBROUTINE FOR COLSYS

      IMPLICIT REAL *8(A-H,O-Z)
```

```
      COMMON/PAR2/U,UGB,UGC,UGP,UMF

      DIMENSION Z(3),DG(3)

      DO 50 J=1,3
50    DG(J)=0.DO

      B1=(U-UGB)/UGC
      B2=1.0-B1

      GOTO(1,2,3),I

1     DG(1)=1.DO
      RETURN
2     DG(2)=1.DO
      DG(3)=-B2
      RETURN
3     DG(2)=1.DO
      DG(3)=-1.DO
      RETURN
      END
C     ------------------------------------------------------
      SUBROUTINE  DUMMY

C     THIS IS A SUPPORTING SUBROUTINE FOR COLSYS

      RETURN
      END
C     ------------------------------------------------------
      SUBROUTINE INPUT

C     THIS SUBROUTINE RETRIEVES THE REQUISITE DATA FROM THE DATA
C     FILE

      IMPLICIT REAL *8(A-H,O-Z)

      COMMON/PAR2/U,UGB,UGC,UGP,UMF
      COMMON/PAR3/EMF,EPSB,FW,RHOCAT
      COMMON/PAR4/CGHO,UGO,UGBO
      COMMON/PAR5/AK,USE,RAT
      COMMON/PAR6/H,T,D,DE,P
      COMMON/PAR7/DC


      READ(22,*)T
      READ(22,*)P
      READ(22,*)H
      READ(22,*)D
      READ(22,*)RAT

      READ(22,*)USE

      CGHO=P=(1.0/(1.0+RAT))/(82.05*T)

      READ(22,*)DC

      READ(22,*)EMF
      READ(22,*)UMF
      READ(22,*)RHOCAT
      READ(22,*)UGO
```

```
      READ(22,*)EA
      READ(22,*)FF

      AK=FF*EXP(-EA*1000.0/(1.98*T))/3600.0
      AK=AK/USE

      READ(22,*)DE

      RETURN
      END


C     ------------------------------------------------------
      SUBROUTINE VELO(U,UMF,EMF,DE,UA,EPSB,FW,UGC,UGB,UGP)

C     THIS SUBROUITNE EVALUATES THE PHASE VELOCITIES

      IMPLICIT REAL *8(A-H,O-Z)

      IDUM=0

 5    UA=U-UMF+(0.711*((981.0*DE)**0.5))

      UGB=(U-UMF)/(1.0-((UMF/UA)*(1.0+FW)))
      EPSB=UGB/UA
      IF(IDUM.EQ.1) GOTO 10
      IF(EPSB.LT.0.333) GOTO 10
      FW=(1.0-EPSB)/(2.0*EPSB)
      IDUM=1
      GOTO 5

 10   UGC=FW*EMF*UGB
      UGP=(UMF*(1.0-EPSB*(1.0+FW))*(1.0+EMF*FW))-(U*FW*EMF)


      RETURN
      END
C     ------------------------------------------------------
      SUBROUTINE TCOF(DC,UMF,DE,EMF,UA,AKBC,AKCP)

C     THIS SUBROUTINE EVALUATES THE TRANSFER COEFF.

      IMPLICIT REAL *8(A-H,O-Z)

      AKBC=(4.5*(UMF/DE))+5.85*(((981.0**0.25)*(DC**0.5))/
     *  (DE**1.25))

      AKCP=6.78*(((EMF*DC*UA)/(DE**3.0))**(0.5))


      RETURN
      END
C     ------------------------------------------------------------
```

FBR MODEL 2

Input data in the form of design and operating conditions along with the kinetic parameters has to be supplied by the user. This is done using an interactive program RUIN.FOR. The data file created on the execution of FBSEL.FOR is retrieved by the main simulator. The following variables have to be provided by the user:

Reactor Temperature (K)

Reactor Pressure (atm)

Reactor Height (cm)

Reactor Diameter (cm)

Inlet partial pressure of CO (atm)

Inlet partial pressure of H_2 (atm)

Density of catalyst (gm/cc)

Gas phase diffusion coefficient (cm^2/sec)

Voidage at minimum fluidization

Velocity at minimum fluidization (cm/sec)

Inlet fluidizing velocity (cm/sec)

Besides, kinetic parameters in the form of activation energies and pre-exponential factors along with the power-law indices as indicated in Table I-B-3 have to be provided. Except for the subroutines used to evaluate the system properties and parameters, the rest of the subroutines describe the boundary value problem as required by the algorithm COLSYS. Because of the non-linear nature of the differential equations and due to the number exceeding the normal limits which COLSYS can handle, the boundary value problem comprising of 30 differential equations failed to converge.

FIXED BED REACTOR

The main computer program developed to solve the mass balance, the heat balance, and the pressure balance equations is entitled SFIX.FOR. The physico-chemical properties and the design parameters pertinent to a pseudo-homogeneous plug flow model of a fixed bed are incorporated into the main program in the form of subroutines which can be changed by the user, as and when required.

Following is a list of the various subroutines used in the simulator along with their purpose:

SUBROUTINE	PURPOSE
INPUT	Retrieves the requisite data from the input file
MIXDEN	Calculates the density of the fluid mixture
MASVEL	Calculates the mass velocity of the fluid
SPHTM	Calculates the specific heat of the fluid mixture
RATCON	Evaluates the kinetic constants as a function of temperature
MUMIX	Calculates the viscosity of the mixture
HTCOF	Calculates the wall heat transfer coefficient
HEAT	Evaluates the heat of reaction
FRICF	Calculates the friction factor along the bed

Besides these subroutines, subroutine entitled FNC1 is used in the program which defines the initial value problem as per DVERK.

The data required for the simulator is supplied by the user, via an interactive program SFIXIN.FOR. Following is a list of variables that are to be provided by the user, prior to execution of the main program.

Inlet fluid temperature (Deg C)

Inlet fluid pressure (Atm)

Inlet partial pressure of CO (Atm)

Inlet partial pressure of H_2 (Atm)

Tube diameter (cm)

Tube height (cm)

Diameter of particle (cm)

Bed voidage

Inlet superficial gas velocity (cm/sec)

Wall cooling temperature (Deg C)

Bulk density of catalyst (gm/cc)

Chain growth probability factor

Kinetic parameters in the form of pre-exponential factors, activation energies and power law indices pertinent to F-T synthesis over $Ru-Al_2O_3$ catalyst as given in Table I-B-3 have to be provided to the simulator. Once the data file is created, the main program can be executed. The output from SFIX.FOR is stored in two files viz.

COMP.DAT — stores the component concentration along the reactor and the syngas conversion obtainable.

VARI.DAT — stores the variation of superficial gas velocity, the fluid temperature and the fluid pressure along the reactor axis.

Case Study

The program, SFIX.FOR was used to predict the performance of a reactor with dimensions of the tube, 4.6cm in diameter and 3 meter in height. All the input parameters required for the program were provided via SFIXIN.FOR. A typical input sample is as shown. The main program SFIX.FOR was then executed in a batch mode with a core requirement of 60K. The execution statement to be used is EX.SFIX.FOR, PRG:IMSL/LIB. The output files include, COMP.DAT and VARI.DAT which are also shown herewith. The variation of the H_2 and CO concentration along the reactor is as shown in Fig. A-B-11. The variation of syngas conversion is indicated in Fig. A-B-12. In this run, the reactor was assumed to operate isothermally. As seen from the output files, COMP.DAT, the amount of CH_4 formed during the reaction is significant in comparison to the other hydrocarbon species excepting water.

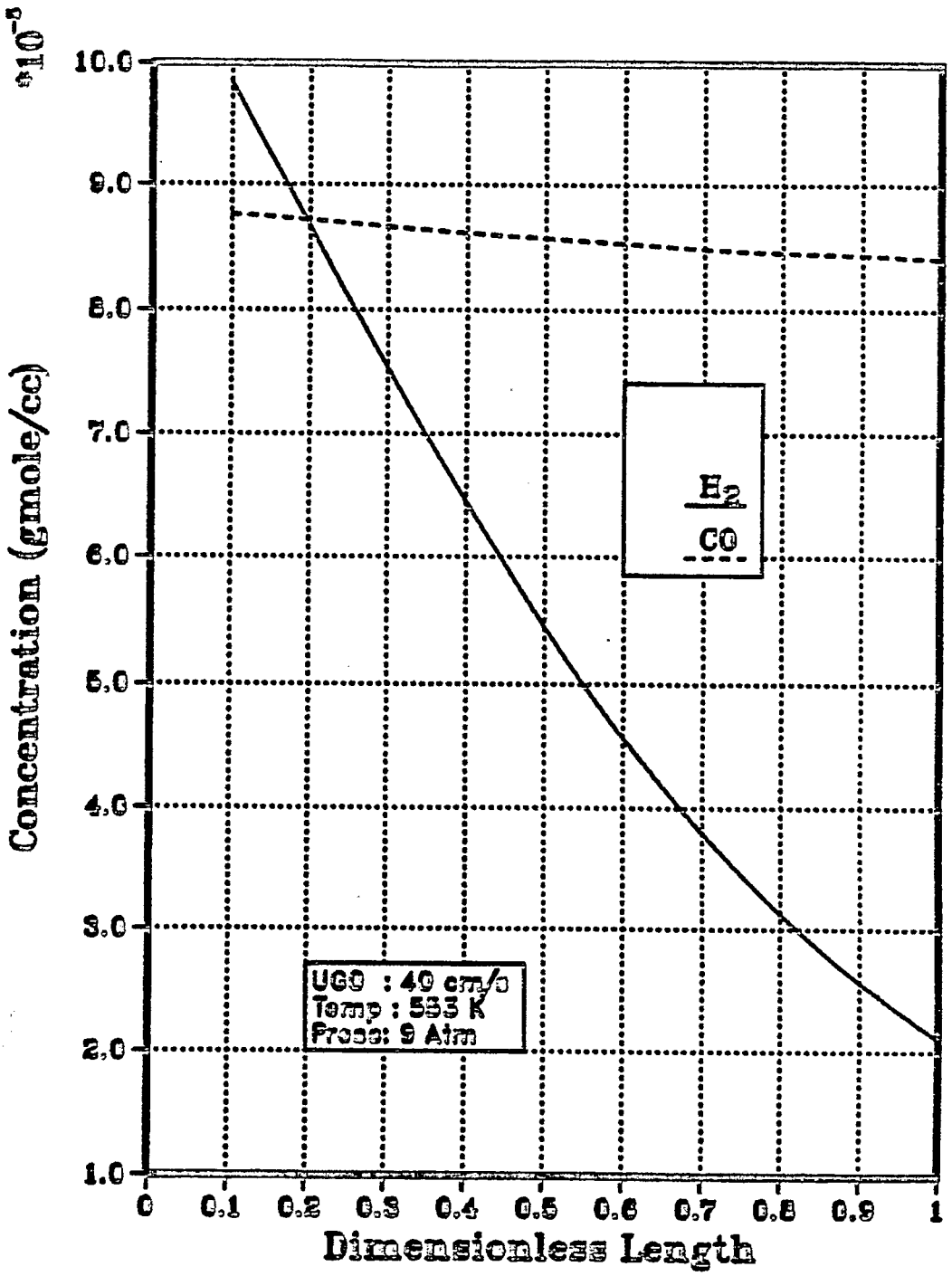

Figure A-B-11: Variation of H_2 and CO concentration along length

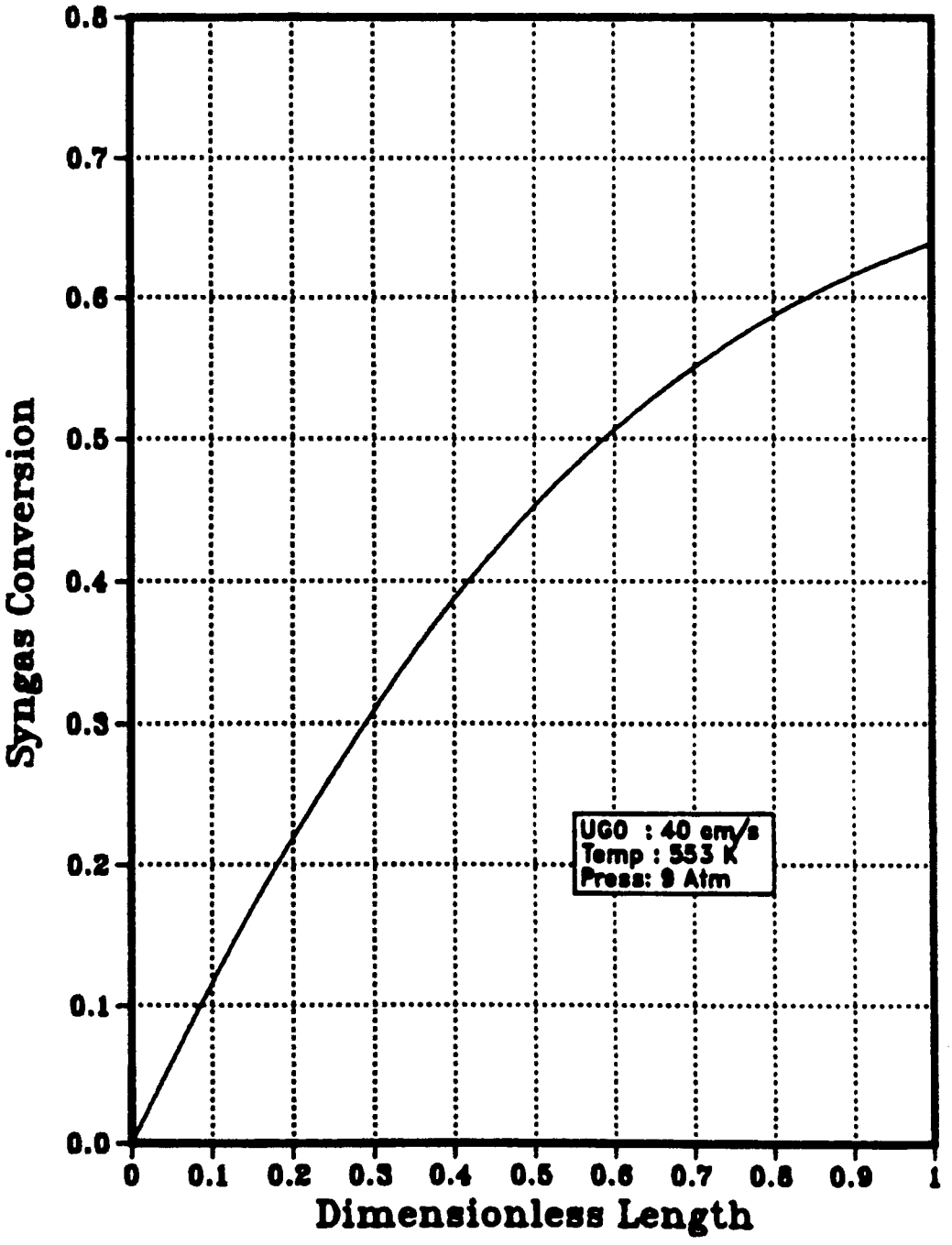

Figure A-B-12: Variation of Syngas Conversion along length

TYPICAL INPUT SAMPLE: FIXIN.FOR

```
  ENTER ALL THE DATA IN A FREE FORMAT


  INLET TEMPERATURE (deg. C)=?
>280.0
  INLET PRESSURE (atm.)=?
>9.00
  INLET P.P OF CO (atm.) =?
>4.00
  INLET P.P. OF H2 (atm.) =?
>5.00
  TUBE DIAMETER (cm.) =?
>5.00
  LENGTH OF TUBE (cm.) =?
>300.0
  DIAMETER OF CATALYST PARTICLE (cm.)=?
>0.25
  BED POROSITY =?
>0.4
  INLET SUPERFICIAL GAS VELOCITY (cm.)=?
>40.0
  CATALYST BULK DENSITY (gm/cc) =?
>2.5
  IS THE REACTOR OPERATED ISOTHERMALLY ?
  IF YES..... TYPE 0.0
  IF NO ..... TYPE 1.0
>0.0


  EXPONENT OF H2 (an) FOR C1=?
>1.37
  EXPONENT OF CO (bn) FOR C1=?
>-0.84
  FREQUENCY FACTOR FOR C1=?
>92000.0
  ACTIVATION ENERGY FOR C1=?
>28.0
  ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
  EXPONENT OF H2 (an) FOR C2=?
>0.66
  EXPONENT OF CO (bn) FOR C2=?
>-0.73
  FREQUENCY FACTOR FOR C2=?
>6700.0
  ACTIVATION ENERGY FOR C2=?
>27.0
  ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
  EXPONENT OF H2 (an) FOR C3=?
>1.04
  EXPONENT OF CO (bn) FOR C3=?
>-0.35
  FREQUENCY FACTOR FOR C3=?
>2300.0
  ACTIVATION ENERGY FOR C3=?
>27.0
  ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
  EXPONENT OF H2 (an) FOR C4=?
>1.11
  EXPONENT OF CO (bn) FOR C4=?
>-5.00E-2
```

```
  FREQUENCY FACTOR FOR C4=?
>0.97
  ACTIVATION ENERGY FOR C4=?
>20.0
  ------------------------------------
  CHAIN GROWTH PROBABILITY FACTOR =
>0.823


 ALL THE DATA HAS BEEN ENTERED

  PROCEED TO SFIX.FOR
```

OUTPUT FILES: COMP.DAT

VARL.DAT

PERFORMANCE OF FIXED BED REACTOR FOR FT SYNTHESIS
PRODUCT DISTRIBUTION

DESIGN PARAMETERS :

TUBE DIAMETER :4.600000 cm.
TUBE HEIGHT :300.0000 cm.
PARTICLE DIAMETER :0.2500000 cm.
BED VOIDAGE :0.4000000

OPERATING CONDITIONS :

INLET TEMPERATURE :280.0000 Deg.C
INLET PRESSURE :9.000000 Atm
INLET P.P. OF H2 :5.000000 Atm
INLET P.P. OF CO :4.000000 Atm
INLET GAS VELOCITY :40.00000 cm/sec

ISOTHERMAL OPERATION

KINETIC PARAMETERS :

A POWER LAW RATE EXPRESSION : An*(PH2**an)*(PCO**bn) IS USED.

VALUE OF ALPHA :0.6250000

L	C1	C2	C3	C4	C5	C6	C7	H2O	H2	CO	% CONV
30.00	.383E-05	.267E-06	.280E-06	.119E-06	.746E-07	.466E-07	.291E-07	.653E-05	.996E-04	.874E-04	10.78
60.00	.760E-05	.549E-06	.565E-06	.239E-06	.149E-06	.934E-07	.584E-07	.131E-04	.891E-04	.866E-04	20.44
90.00	.112E-04	.842E-06	.847E-06	.357E-06	.223E-06	.140E-06	.872E-07	.195E-04	.789E-04	.858E-04	28.98
120.00	.147E-04	.114E-05	.112E-05	.471E-06	.294E-06	.184E-06	.115E-06	.256E-04	.691E-04	.850E-04	36.42
150.00	.178E-04	.144E-05	.138E-05	.578E-06	.361E-06	.226E-06	.141E-06	.313E-04	.600E-04	.843E-04	42.80
180.00	.207E-04	.173E-05	.163E-05	.677E-06	.423E-06	.264E-06	.165E-06	.366E-04	.516E-04	.837E-04	48.23
210.00	.232E-04	.200E-05	.185E-05	.767E-06	.479E-06	.299E-06	.187E-06	.413E-04	.441E-04	.831E-04	52.79
240.00	.254E-04	.227E-05	.205E-05	.846E-06	.529E-06	.331E-06	.207E-06	.455E-04	.375E-04	.826E-04	56.60
270.00	.272E-04	.251E-05	.223E-05	.916E-06	.573E-06	.358E-06	.224E-06	.492E-04	.317E-04	.821E-04	59.77
300.00	.288E-04	.274E-05	.238E-05	.977E-06	.610E-06	.381E-06	.238E-06	.523E-04	.267E-04	.817E-04	62.39

H2/CO USAGE RATIO = 2.873972

L (cm)	UG (cm/s)	T (deg C)	P (atm)
30.00	37.84	280.00	8.992
60.00	35.91	280.00	8.984
90.00	34.20	280.00	8.977
120.00	32.72	280.00	8.970
150.00	31.44	280.00	8.964
180.00	30.35	280.00	8.957
210.00	29.44	280.00	8.951
240.00	28.68	280.00	8.945
270.00	28.05	280.00	8.940
300.00	27.52	280.00	8.934

PROGRAM LISTING: FIXIN.FOR

```
C       ------------------------------------------
C       THIS IS AN INTERACTIVE PROG. DEVELOPED TO
C             INPUT THE DATA TO :SFIX.FOR
C       ------------------------------------------

        DIMENSION A(4),B(4),AN(4),EN(4)

        WRITE*,' ENTER ALL THE DATA IN A FREE FORMAT'
        WRITE*
        WRITE*
        WRITE*,' INLET TEMPERATURE (deg. C)=?'
        READ*,TO
        WRITE(26,*)TO
        WRITE*,'INLET PRESSURE (atm.)=?'
        READ*,PO
        WRITE(26,*)PO
        WRITE*,' INLET P.P OF CO (atm.) =?'
        READ*,PCO
        WRITE(26,*)PCO
        WRITE*,' INLET P.P. OF H2 (atm.) =?'
        READ*,PH2
        WRITE(26,*)PH2
        WRITE*,' TUBE DIAMETER (cm.) =?'
        READ*,DT
        WRITE(26,*)DT
        WRITE*,' LENGTH OF TUBE (cm.) =?'
        READ*,AL
        WRITE(26,*)AL
        WRITE*,' DIAMETER OF CATALYST PARTICLE (cm.)=?'
        READ*,DP
        WRITE(26,*)DP
        WRITE*,' BED POROSITY =?'
        READ*,EPS
        WRITE(26,*)EPS
        WRITE*,' INLET SUPERFICIAL GAS VELOCITY (cm.)=?'
        READ*,UGO
        WRITE(26,*)UGO
        WRITE*,' CATALYST DENSITY (gm/cc) =?'
        READ*,RCAT
        WRITE(26,*)RCAT
        WRITE*,' IS THE REACTOR OPERATED ISOTHERMALLY ?'
        WRITE*,' IF YES..... TYPE 0.0'
        WRITE*,' IF NO ..... TYPE 1.0'
        READ*,VT
        WRITE(26,*)VT
        IF(VT.EQ.0.0) GOTO 5
        WRITE*,' WALL TEMPERATURE (Deg.C)=?'
        READ*,TW
        WRITE(26,*)TW

5       DO 10 I=1,4
        WRITE*,' EXPONENT OF H2 (an) FOR C',I,'=?'
        READ*,A(I)
        WRITE(26,*)A(I)
        WRITE*,' EXPONENT OF CO (bn) FOR C',I,'=?'
        READ*,B(I)
        WRITE(26,*)B(I)
        WRITE*,' FREQUENCY FACTOR FOR C',I,'=?'
        READ*,AN(I)
        WRITE(26,*)AN(I)
```

```
      WRITE*,' ACTIVATION ENERGY FOR C',I,'=?'
      READ*,EN(I)
      WRITE(26,*)EN(I)
      WRITE*,' ------------------------------------'
10    CONTINUE
      WRITE*,' CHAIN GROWTH PROBABILITY FACTOR ='
      READ*,ALPHA
      WRITE(26,*)ALPHA
      WRITE*
      WRITE*
      WRITE*
      WRITE*,'ALL THE DATA HAS BEEN ENTERED '
      WRITE*
      WRITE*,' PROCEED TO SFIX.FOR '

      STOP
      END
C     ----------------------------------------
```

PROGRAM LISTING: SFIX.FOR

```
C       ------------------------------------------------
C        THIS PROG. IS DEVELOPED TO SOLVE THE MODEL EQNS.
C       DESCRIBING SELECTIVITY IN A FIXED BED REACTOR
C       USE IS MADE OF ONE DIMENSIONAL PSEUDO HOMOGENEOUS
C              MODEL WITH PLUG FLOW ASSUMPTION
C       ------------------------------------------------

C       FOLLOWING IS A LIST OF THE VARIABLES USED IN THE PROGRAM:

C       TO              :INLET TEMPERATURE (DEG C)
C       PO              :INLET PRESSURE (ATM)
C       PCO             :INLET P.P. OF CO (ATM)
C       PH2             :INLET P.P. OF H2 (ATM)
C       DT              :DIAMETER OF TUBE (CM)
C       AL              :HEIGHT OF TUBE (CM)
C       DP              :DIAMETER OF CATALYST (CM)
C       EPS             :BED VOIDAGE
C       UGO             :INLET GAS VELOCITY (CM/SEC)
C       TW              :WALL TEMPERATURE (DEG C)
C       RCAT            :CATALYST BULK DENSITY (GM/CC)
C       A(I)            :INDEX OF H2 FOR CARBON I
C       B(I)            :INDEX OF CO FOR CARBON I
C       AN(I)           :FREQUENCY FACTOR FOR CARBON I
C       EN(I)           :ACTIVATION ENERGY FOR CARBON I
C       ALPHA           :CHAIN GROWTH PROBABILITY FACTOR

C       ------------------------------------------------

C       THIS IS THE MAIN PROGRAM



        COMMON/PAR1/TO,PO,TW,PH2,PCO
        COMMON/PAR2/DT,AL,NT
        COMMON/PAR3/DP,EPS,RCAT
        COMMON/PAR4/A,B,AN,EN,ALPHA
        COMMON/PAR5/UGO,VT
        COMMON/PAR6/G,CPM,AMU
        COMMON/PAR7/SUM1,SUM2
        COMMON/PAR8/AM1,AM2,AM3,AM4,AM5,AM6,AM7,AM8,AM9,AM10
        COMMON/PAR9/UG,CONIN
        COMMON/PAR10/PPH2,PPCO

        EXTERNAL FCN1

        DIMENSION Y(12),C(24),W(12,9),A(4),B(4),AN(4),EN(4)

        R=82.05

        CALL INPUT

        CGHO=PH2/(82.05*(TO+273.0))
        CGCO=PCO/(82.05*(TO+273.0))

        CALL MIXDEN(PCO,PH2,TO,DENM)
        CALL MASVEL(DENM,UGO,G)
        CALL SPHTM(PO,PH2,PCO,CPM)
        CALL MUMIX(PO,PH2,PCO,AMU)
```

```
      WRITE(28,*)' ------------------------------------------------'
      WRITE(28,*)' PERFORMANCE OF FIXED BED REACTOR FOR FT SYNTHESIS'
      WRITE(28,*)'              PRODUCT DISTRIBUTION '
      WRITE(28,*)' ------------------------------------------------'
      WRITE(28,*)
      WRITE(28,*)
      WRITE(28,*)' DESIGN PARAMETERS :'
      WRITE(28,*)' -------------------'
      WRITE(28,*)
      WRITE(28,*)' TUBE DIAMETER        :',DT,'   cm.'
      WRITE(28,*)' TUBE HEIGHT          :',AL,'   cm.'
      WRITE(28,*)' PARTICLE DIAMETER    :',DP,'   cm.'
      WRITE(28,*)' BED VOIDAGE          :',EPS
      WRITE(28,*)
      WRITE(28,*)' OPERATING CONDITIONS :'
      WRITE(28,*)' ----------------------'
      WRITE(28,*)
      WRITE(28,*)' INLET TEMPERATURE    :',TO,'  Deg.C'
      WRITE(28,*)' INLET PRESSURE       :',PO,'  Atm'
      WRITE(28,*)' INLET P.P. OF H2     :',PH2,' Atm'
      WRITE(28,*)' INLET P.P. OF CO     :',PCO,' Atm'
      WRITE(28,*)' INLET GAS VELOCITY   :',UGO,' cm/sec'
      IF(VT.EQ.0.0) GOTO 2
      WRITE(28,*)' NON-ISOTHERMAL OPERATION '
      WRITE(28,*)
      WRITE(28,*)' WALL TEMPERATURE     :',TW,' Deg.C'
      WRITE(28,*)
2     RWITE(28,*)
      WRITE(28,*)' ISOTHERMAL OPERATION '
      WRITE(28,*)
      WRITE(28,*)
      WRITE(28,*)' KINETIC PARAMETERS :'
      WRITE(28,*)' --------------------'
      WRITE(28,*)
      WRITE(28,*)' A POWER LAW RATE EXPRESSION : An*(PH2**an)*(PCO**bn)
     *  IS USED.'
      WRITE(28,*)
      WRITE(28,*)' VALUE OF ALPHA       :',ALPHA
      WRITE(28,*)
      WRITE(28,*)

      WRITE(28,200)
      WRITE(28,250)'L','C1','C2','C3','C4','C5','C8','C7','H20',
     *  'H2','CO','% CONV.'
      WRITE(28,200)

      WRITE(27,270)
      WRITE(27,280)'L (cm)','UG (cm/s)','T (deg C)','P (atm) '
      WRITE(27,270)

      R1=PH2/PO
      R2=PCO/PO
      R3=(R1*2.0)/(R2*28.0)
      R4=1.0/(1.0+R3)
      R5=1.0-R4


      X=0.0
      NW=12
      N=12
```

```
      TOL=0.001
      IND=1

      DO 5 I=1,8
      Y(I)=0.0
5     CONTINUE

      Y(9)=R3
      Y(10)=R4
      Y(11)=TO
      Y(12)=PO

      CALL RATCON(AN,EN,Y,AK1,AK2,AK3,AK4)


      SUM1=0.0
      SUM2=0.0

      CONIN=(PH2/(R*(TO+273.0)))+(PCO/(R*(TO+273.0)))

      DO 10 I=4,7
      SUM1=SUM1+((2.0*FLOAT(I)+1.0)*(ALPHA**(FLOAT(I)-4.0)))
      SUM2=SUM2+(FLOAT(I)*(ALPHA**(FLOAT(I)-4.0)))
10    CONTINUE

      UG=UGO

      DO 50 K=1,10

      XEND=AL*FLOAT(K)/10.0

      CALL DVERK(N,FCN1,X,Y,XEND,TOL,IND,C,NW,W,IER)


      DD=(Y(1)/AM1)+(Y(2)/AM2)+(Y(3)/AM3)+(Y(4)/AM4)+(Y(5)/AM5)+
     *(Y(6)/AM6)+(Y(7)/AM7)+(Y(8)/AM8)+(Y(9)/AM9)+(Y(10)/AM10)

      Q1=1.0/DD

      UGCON=82.05*(Y(11)+273.0)

      BPH2=Y(9)*(Q1/AM9)*Y(12)/UGCON
      BPCO=Y(10)*(Q1/AM10)*Y(12)/UGCON
      BP1=Y(1)*(Q1/AM1)*Y(12)/UGCON
      BP2=Y(2)*(Q1/AM2)*Y(12)/UGCON
      BP3=Y(3)*(Q1/AM3)*Y(12)/UGCON
      BP4=Y(4)*(Q1/AM4)*Y(12)/UGCON
      BP5=Y(5)*(Q1/AM5)*Y(12)/UGCON
      BP6=Y(6)*(Q1/AM6)*Y(12)/UGCON
      BP7=Y(7)*(Q1/AM7)*Y(12)/UGCON
      BPH2O=Y(8)*(Q1/AM8)*Y(12)/UGCON

      CONX=BPH2+BPCO
      CONSYN=(UGO*CONIN-UG*CONX)/(UGO*CONIN)
      UG=UGO*(1.0-0.5*CONSYN)

      USE=(UGO*CGHO-UG*BPH2)/(UGO*CGCO-UG*BPCO)


      WRITE(28,100)X,BP1,BP2,BP3,BP4,BP5,BP6,BP7,BPH2O,BPH2,BPCO,
```

```
     *   CONSYN*100.0

         WRITE(29,*)X,BP1,BP2,BP3,BP4,BP5,BP6,BP7,BPH2O,BPH2,BPCO

         WRITE(27,280)X,UG,Y(11),Y(12)

         BH2=BPH2*82.05*(Y(11)+273.0)
         BCO=BPCO*82.05*(Y(11)+273.0)


         RATE1=AK1*(BH2**A(1))*(BCO**B(1))
         RATE2=AK2*(BH2**A(2))*(BCO**B(2))/RATE1
         RATE3=AK3*(BH2**A(3))*(BCO**B(3))/RATE1
         RATE4=AK4*(BH2**A(4))*(BCO**B(4))/RATE1
         RATE5=RATE4*ALPHA
         RATE6=RATE4*(ALPHA**2.0)
         RATE7=RATE4*(ALPHA**3.0)
         RATE1=1.00

C        WRITE(35,350)X,RATE1,RATE2,RATE3,RATE4,RATE5,RATE6,RATE7


 50      CONTINUE

         WRITE(28,*)' H2/CO USAGE RATIO = ',USE
         WRITE(27,270)
         WRITE(28,290)'1'
         WRITE(27,290)'1'

 100     FORMAT(2X,F8.2,2X,10(E9.3,2X),F8.2,2X,F8.2)
 150     FORMAT(2X,3(A,3X),3X,A)
 200     FORMAT(1X,130('-'))
 250     FORMAT(6X,12(A,9X))
 260     FORMAT(4X,4(A,5X))
 270     FORMAT(1X,80('-'))
 280     FORMAT(3X,3(F8.2,4X),F8.3)
 290     FORMAT(A)
 300     FORMAT(X,A,F6.4,2X,A,E8.3)
 350     FORMAT(X,F8.2,2X,7(E8.3,2X))

         STOP
         END

C        ------------------------------------------------------------

         SUBROUTINE FCN1(N,X,Y,YPRIME)

C        THIS SUBROUTINE DEFINE THE DIFFERENTIAL EQNS. AS PER
C        DVERK

         COMMON/PAR1/TO,PO,TW,PH2,PCO
         COMMON/PAR2/DT,AL,NT
         COMMON/PAR3/DP,EPS,RCAT
         COMMON/PAR4/A,B,AN,EN,ALPHA
         COMMON/PAR5/UGO,VT
         COMMON/PAR6/G,CPM,AMU
         COMMON/PAR7/SUM1,SUM2
         COMMON/PAR8/AM1,AM2,AM3,AM4,AM5,AM6,AM7,AM8,AM9,AM10
         COMMON/PAR9/UG,CONIN
         COMMON/PAR10/PPH2,PPCO
```

```
      DIMENSION Y(12),YPRIME(12),A(4),B(4),AN(4),EN(4)


      GC=980.665
      R=82.05

      AM1=16.0
      AM2=30.0
      AM3=44.0
      AM4=58.0
      AM5=72.0
      AM6=86.0
      AM7=100.0
      AM8=18.0
      AM9=2.0
      AM10=28.0

      DD=(Y(1)/AM1)+(Y(2)/AM2)+(Y(3)/AM3)+(Y(4)/AM4)+(Y(5)/AM5)+
     *  (Y(6)/AM6)+(Y(7)/AM7)+(Y(8)/AM8)+(Y(9)/AM9)+(Y(10)/AM10)

      VV=(Y(1)/DD)+(Y(2)/DD)+(Y(3)/DD)+(Y(4)/DD)+(Y(5)/DD)+
     *  (Y(6)/DD)+(Y(7)/DD)+(Y(8)/DD)+(Y(9)/DD)+(Y(10)/DD)

      ROM=Y(12)*VV/(R*(Y(11)+273.0))


      CALL RATCON(AN,EN,Y,AK1,AK2,AK3,AK4)
      RAT=PCO/PH2
      CALL HTCOF(RAT,DT,DP,G,AMU,HTW)
      CALL HEAT(DELH)
      CALL FRICF(EPS,DP,G,AMU,FF)


      PROD=AM1*AM2*AM3*AM4*AM5*AM6*AM7*AM8*AM9*AM10
      S=DD*PROD
      Q1=PROD/S

      GASCON=R*(Y(11)+273.0)


      PPH2=Y(9)*(Q1/AM9)*Y(12)
      PPCO=Y(10)*(Q1/AM10)*Y(12)
      PP1=Y(1)*(Q1/AM1)*Y(12)
      PP2=Y(2)*(Q1/AM2)*Y(12)
      PP3=Y(3)*(Q1/AM3)*Y(12)
      PP4=Y(4)*(Q1/AM4)*Y(12)
      PP5=Y(5)*(Q1/AM5)*Y(12)
      PP6=Y(6)*(Q1/AM6)*Y(12)
      PP7=Y(7)*(Q1/AM7)*Y(12)
      PPH2O=Y(8)*(Q1/AM8)*Y(12)


      S1=PP1/GASCON
      S2=PP2/GASCON
      S3=PP3/GASCON
      S4=PP4/GASCON
      S5=PP5/GASCON
      S6=PP6/GASCON
      S7=PP7/GASCON
      S8=PPH2O/GASCON
```

```
      S9=PPH2/GASCON
      S10=PPCO/GASCON

      CONX=S9+S10
      CONSYN=(UGO*CONIN-UG*CONX)/(UGO*CONIN)
      UG=UGO*(1.0-0.5*CONSYN)


      B91=PPH2**A(1)
      B92=PPH2**A(2)
      B93=PPH2**A(3)
      B94=PPH2**A(4)

      C11=PPCO**B(1)
      C12=PPCO**B(2)
      C13=PPCO**B(3)
      C14=PPCO**B(4)

      YPRIME(1)=(AK1*RCAT/G)*AM1*B91*C11
      YPRIME(2)=(AK2*RCAT/G)*AM2*B92*C12
      YPRIME(3)=(AK3*RCAT/G)*AM3*B93*C13
      YPRIME(4)=(AK4*RCAT/G)*AM4*B94*C14
      YPRIME(5)=(AK4*RCAT/G)*AM5*B94*C14*ALPHA
      YPRIME(6)=(AK4*RCAT/G)*AM6*B94*C14*(ALPHA**2.0)
      YPRIME(7)=(AK4*RCAT/G)*AM7*B94*C14*(ALPHA**3.0)

      SUMH=(3.0*AK1*B91*C11)+(5.0*AK2*B92*C12)+
     *  (7.0*AK3*B93*C13)+(AK4*B94*C14*SUM1)

      SUMC=(AK1*B91*C11)+(2.0*AK2*B92*C12)+
     *  (3.0*AK3*B93*C13)+(AK4*B94*C14*SUM2)

      YPRIME(8)=(RCAT/G)*AM8*SUMC
      YPRIME(9)=-(RCAT/G)*AM9*SUMH
      YPRIME(10)=-(RCAT/G)*AM10*SUMC

      YPRIME(11)=(VT/(CPM*G))*((-4.0*HTW*(Y(11)-TW)/DT)+
     *  SUMH*RCAT*DELH)


      YPRIME(12)=-(FF*G*G/(ROM*DP*GC))/1033.0

      RETURN
      END

C     ------------------------------------------------------------

      SUBROUTINE INPUT


C     THIS SUBROUTINE RETRIEVES THE REQUISITE DATA FORM THE
C     DATA FILE

      COMMON/PAR1/TO,PO,TW,PH2,PCO
      COMMON/PAR2/DT,AL,NT
      COMMON/PAR3/DP,EPS,RCAT
      COMMON/PAR4/A,B,AN,EN,ALPHA
      COMMON/PAR5/UGO,VT

      DIMENSION A(4),B(4),AN(4),EN(4)
```

```
      READ(26,*)TO
      READ(26,*)PO
      READ(26,*)PCO
      READ(26,*)PH2
      READ(26,*)DT
      READ(26,*)AL
      READ(26,*)DP
      READ(26,*)EPS
      READ(26,*)UGO
      READ(26,*)RCAT
      READ(26,*)VT
      IF(VT.EQ.0.0) GOTO 5
      READ(26,*)TW

5     DO 10 I=1,4
      READ(26,*)A(I)
      READ(26,*)B(I)
      READ(26,*)AN(I)
      READ(26,*)EN(I)
10    CONTINUE

      READ(26,*)ALPHA

      RETURN
      END
C     ------------------------------------------------------------

      SUBROUTINE MIXDEN(PCO,PH2,TO,DENM)

C     THIS SUBROUTINE EVALUATES THE INLET DENSITY OF THE GAS

      R=82.05
      AMWH=2.0
      AMWCO=28.0


      DENH=PH2*AMWH/(R*(TO+273.0))
      DENCO=PCO*AMWCO/(R*(TO+273.0))

      DENM=DENH+DENCO

      RETURN
      END
C     ------------------------------------------------

      SUBROUTINE MASVEL(DENM,UGO,G)

C     THIS SUBROUTINE EVALUATES THE MASS VEL. OFTHE GAS

      G=UGO*DENM

      RETURN
      END
C     ------------------------------------------------------

      SUBROUTINE SPHTM(PO,PH2,PCO,CPM)

C     THIS SUBROUTINE CALCULATES THE SP.HEAT OF THE MIX.

      CPM=3.5
```

```
      CPCO=0.27

      AMFH=PH2/PO
      AMFCO=PCO/PO

      CPM=(AMFCO*CPCO+AMFH*CPH)

      RETURN
      END
C     ------------------------------------------------

      SUBROUTINE RATCON(AN,EN,Y,AK1,AK2,AK3,AK4)

C     THIS SUBROUTINE CALCULATES THE RATE CONSTANTS (K)

      DIMENSION Y(12),AN(4),EN(4)


      GR=1.98
      AK1=AN(1)*EXP(-EN(1)*1000.0/(GR*(Y(11)+273.0)))
      AK2=AN(2)*EXP(-EN(2)*1000.0/(GR*(Y(11)+273.0)))
      AK3=AN(3)*EXP(-EN(3)*1000.0/(GR*(Y(11)+273.0)))
      AK4=AN(4)*EXP(-EN(4)*1000.0/(GR*(Y(11)+273.0)))

      RETURN
      END
C     ------------------------------------------------

      SUBROUTINE MUMIX(PO,PH2,PCO,AMU)

C     THIS SUBROUTINE CALC. THE VISCOSITY OF THE MIX.

      AMWH=2.0
      AMWCO=28.0

      AMUH=0.018*0.01
      AMUCO=0.034*0.01

      Z1=PH2/PO
      Z2=PCO/PO

      AMU=Z2*AMUCO*(AMWCO**0.5)+Z1*AMUH*(AMWH**0.5)
      DENOM=Z2*(AMWCO**0.5)+Z1*(AMWH**0.5)
      AMU=AMU/DENOM

      RETURN
      END
C     ------------------------------------------------

      SUBROUTINE HTCOF(RAT,DT,DP,G,AMU,HTW)

C     THIS SUBROUTINE CALC. THE HEAT TRNSF. COEFF.


      AMWH=2.0
      AMWCO=28.0

      HLAMB=6.825E-4
      CLAMB=9.679E-5
```

```
      RE=DP*G/AMU
      R1=EXP(-4.6*DP/DT)

      R2=RAT*CLAMB*(AMWCO**0.333)+HLAMB*(AMWH**0.333)
      R3=RAT*(AMWCO**0.333)+(AMWH**0.333)
      GLAMB=R2/R3

      HTW=3.5*(RE**0.7)*R1*GLAMB/DT

      RETURN
      END
C     ------------------------------------------------

      SUBROUTINE HEAT(DELH)

C     THIS SUBROUTINE CALC. THE HEAT OF REACTION

      DELH=20.0

      RETURN
      END
C     ------------------------------------------------

      SUBROUTINE FRICF(EPS,DP,G,AMU,FF)

C     THIS SUBROUTINE CALC. THE FRICTION FACTOR

      RE=DP*G/AMU
      R2=(1.0-EPS)/(EPS**3.0)

      FF=R2*(1.75+(1.50*(1.0-EPS)/RE))

      RETURN
      END
C     ------------------------------------------------
```