APPENDIX I-C

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I-C-1 User Manual for Methanol Synthesis Reactor Simulators

.This manual describes the use of computer programs that predict the performance of methanol synthesis reactors under a set of operating conditions. Instructions for their use, sample executions showing the input data and the resulting outputs in a tabular form and source code of the programs are presented.

C-I Use of Simulator

Fixed Bed Reactor Model

To use the simulator, the user must provide the following information:

- Feed characteristics

  Temperature (Deg K)

  Pressure (atm)

  Gas composition (mole fractions)

  Volumetric gas veocity (Nm^3/sec)

- Reactor characteristics

  Length (m)

  Diameter (m)

  Bed void fraction (-)

  Bed number (to indicate which bed is to be designed for a multibed reactor)

- Catalyst characteristics

  Diameter (m)

  Density (kg/m^3)

  Porosity (-)

  Tortousity (-)

  Thermal conductivity (kJ/m-s-K)

The above input data are entered via an interactive program FIXED.DAT. A file called INPUT.DAT is created by this program. Then the main program FIXED.BED can be executed in a batch mode. Since the software package COLSYS.FOR (Ascher et al., 1981) which is used currently in the Mathematical Library at the University of Pittsburgh is used, the program is executed by invoking the following command;

EX FIXED.BED, MTH: COLSYS.REL

The output from FIXED.BED is stored in different data files. The following is the list of output files created by FIXED.BED and the information they provide:

File Name	Content
OUTPUT.SUM	All data supplied by the user, output gas composition temperature and gas velocity conversions, space time yield
CONV.PRO	Conversion profiles for methanol formation and shift reactions.
COMP.PRO	Gas composition profiles in mole fractions.
TEMP.PRO	Temperature profile

GAS.PRO	Gas flow rate profile
EFF.PRO	Effectiveness factors profiles for methanol and shift reactions
ERATE.PRO	Effective reaction rate profiles for the reactions.

The main program for fixed bed reactor model consists of several subroutines. The name and the purpose of each are indicated in the following list:

Subroutine Name	Purpose
INPUT	Retrieves input data
DMIX	Calculate the mixture diffusion coefficients.
DCOEF	Evaluates the binary diffusion coefficients.
AMASS	Evaluates the mass transfer coefficients.
AHEAT	Evaluates the heat transfer coefficient.

CPGAS	Provides heat capacity data.
VISMIX	Evaluates the viscosity of the gas mixture.
VISGAS	Evaluates the viscosity of gas species.
CONMIX	Evaluates the thermal conductivity of gas mixture.
CONDUC	Provides the thermal conductivity of methanol synthesis gas mixture.
FUGA	Calculates the fugacities.
FUCOEF	Calculates the fugacity coefficients.
REAC1	Calculates the reaction rates.
DEN	Evaluates the gas density.
AHEAT	Provides heat of reaction data.
INTER	Evaluates the solid phase temperature and concentrations for a given surface and point conversion.

INTER2	Evaluates the concentrations, temperature and gas velocity for a given set of conversions.
FSUB	Evaluates the differential equations.
DFSUB	Evaluates the Jacobian of the differential equations.
GSUB	Evaluates the boundary conditions.
DGSUB	Evaluates the partials of the boundary conditions.
SOLUTN	Provides an initial solution to the differential equation.

The program can also be used for a multi-bed reactor where intercooling or quench type cooling is used. For the latter case the feed conditoins to the next bed can be calculated by an interactive package named INTBED.FOR. This program uses the output conditions of prior bed and the quench conditions (temperature, gas composition and flow rate) and evaluates the feed conditions to the next bed. The program FIXED.DAT then has to be executed to provide the data for the next execution of FIXED.BED.

A typical run showing both input and output is given in the following pages. Also presented is the execution of INTBED.FOR for a further simulation.

Bubble Column Slurry Reactor Model

The following information is needed for the simulator to be executed:

- Reactor characteristics

  Diameter (m)

  Length (m)

- Operating conditions

  Feed temperature (K)

  Inlet gas flow rate (Nm^3/sec)

  Slurry flow rate (m^3/sec)

  Inlet gas composition (mole fractions)

  Inlet liquid composition (mole fractions)

  Catalyst loading (% weight)

- Catalyst properties

  Density

  Diameter

  Thermal conductivity

All the input data are entered via an interactive program SLURRY.DAT. The execution of this program creates a dat file named INPUT1.DAT. Once the data is supplied the main program SLURRY.BED can be executed in a batch mode. The program is executed by involving the command,

EX SLURRY.BED, MTH; COLSYS.REL

The output from the SLURRY.BED is stored in different data files. The name and the content of these files are indicated in the following list.

File Name	Content
OUTPUT.SUM	All data supplied by the User, outlet temperature coversions, space time yield.
CONV.PRO	Conversion profiles for methanol and shift reactions.
CONC.GAS	Gas phase concentration profiles (mole fraction).
CONC.LIQ	Liquid phase concentration profiles (in $kmol/m^3$).
DIMCON.PRO	Liquid phase dimensionless concentration profiles.
TEMP.PRO	Temperature profile.
CAT.PRO	Catalyst concentration profile.

The main program for slurry reactor consists of several subroutines. The following list gives the name and the purpose of each.

Subroutine Name	Purpose
INPUT1	Retrieves the input data.
LIQ.PRO	Provides liquid phase physical properties.
DIFCF	Evaluates diffusion coefficients.
SOLUB	Supplies solubility data of the gases.
CPGAS	Provides heat capacity data.
RHEAT	Provides heat of reaction data.
HOLDUP	Evaluates gas holdup.
MASSTR	Evaluates volumetric mass transfer coefficients.
SLUPRO	Evaluates slurry physical properties.
LIQ.DIF	Computes the dispersion coefficients in the liquid phase.
SOLDIF	Computes solid phase diffusion coefficient.

HEATDF	Computes heat dispersion coefficient.
REAC1	Evaluates the reaction rates.
CATCON	Evaluates the dimensionless catalyst concentration at any axial position.
CALPRO	Used to give an initial solution (analytical solution of differential equations in the absence of reaction).
INTER	Evaluates the actual liquid concentrations with dimensionless ones.
FSUB	Evaluates the differential equations.
DFSUB	Evaluates the Jacobian of the differential equations.
GSUB	Evaluates the boundary conditions.
DGSUB	Evaluates the partials of the boundary condition.
SOLUTN	Provides an initial solution to the differential equations.

A typical run showing both input and output is given in the following pages.

I-C-2 Program Listing - FIXED DAT

```
C
C
C       THIS IS AN INTERACTIVE PROGRAM THAT RECEIVES THE INPUT
C       DATA FOR THE SIMULATION OF FIXED-BED METHANOL SYNTHESIS
C       REACTOR.THE DATA ARE THEN STORED IN A FILE NAMED
C       INPUT.DAT  AND USED IN THE SIMULATOR.
C
C       THE USER CAN GET A COMPLETE LIST OF INPUT DATA
C       FROM THE FILE NAMED  CHECK.DAT
C
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DIMENSION YF(7)
C
        OPEN (UNIT=8,FILE='INPUT.DAT')
        OPEN (UNIT=9,FILE='CHECK.DAT')
C
        WRITE(06,10)
10      FORMAT(///,5X,'*****************************************************'
     * //,9X,'SIMULATION OF A FIXED-BED ADIABATIC REACTOR',/,5X,
     * '                    FOR',/,5X,
     * '              METHANOL  SYNTHESIS',//,5X,
     * '*****************************************************',//)
C
C
        WRITE(06,20)
20      FORMAT(5X,'INSTRUCTIONS',///,5X,
     * 'THIS PROGRAM SIMULATES  ICI "S QUENCH TYPE LOW-PRESSURE',/,5X,
     * 'FIXED-BED METHANOL SYNTHESIS REACTOR.',/,5X,
     * 'ONE-DIMENSIONAL PLUG FLOW MODEL IS USED TO BE A GOOD',/,5X,
     * 'REPRESENTATIVE PICTURE OF THE REACTOR BEHAVIOUR.',/,5X,
     * 'INPUT VARIABLES INCLUDING FEED,REACTOR AND CATALYST',/,5X,
     * 'CHARACTERISTICS ARE PROVIDED BY THE USER VIA THIS',/,5X,
     * 'INTERACTIVE PACKAGE.THE SIMULATOR THEN EVALUATES ',/,5X,
     * 'TEMPERATURE AND CONCENTRATION PROFILES TOGETHER WITH',/,5X,
     * 'CONVERSIONS,EFFECTIVENESS FACTORS AND THE REACTION',/,5X,
     * 'RATES FOR EACH CATALYST BED.',///,5X,
     * 'TO RUN THE SIMULATOR ,PLEASE ENTER THE FOLLOWING DATA',/,5X,
     * 'IN FREE FORMAT',//)
C
        WRITE(06,30)
        WRITE(09,30)
30      FORMAT(/,5X,'************** FEED CHARACTERISTICS *************',
     * //,5X,'INLET TEMPERATURE (K) = ? ')
        READ(05,*) TF
        WRITE(08,*) TF
        WRITE(09,*) TF
C
        WRITE(06,40)
        WRITE(09,40)
40      FORMAT(/,5X,'PRESSURE (ATM) = ?')
        READ(05,*) P
        WRITE(08,*) P
        WRITE(09,*) P
C
        WRITE(06,50)
        WRITE(09,50)
50      FORMAT(/,5X,'GAS COMPOSITION',/,5X,
     * 'ENTER THE MOL FRACTIONS. THE SQUENCE IS :',/,5X,
```

```
     * '1:CO  2:CO2  3:H2  4:CH3OH  5:H2O  6:N2  7:CH4')
       READ(05,*) (YF(I),I=1,7)
       WRITE(08,*) (YF(I),I=1,7)
       WRITE(09,*) (YF(I),I=1,7)
C
       WRITE(06,60)
       WRITE(09,60)
60     FORMAT(/,5X,'VOLUMETRIC GAS VELOCITY (Nm**3/sec) = ?')
       READ(05,*) Q
       WRITE(08,*) Q
       WRITE(09,*) Q
C
       WRITE(06,65)
       WRITE(09,65)
65     FORMAT(/,5X,'DO YOU WANT TO GET SOLID PHASE CONCENTRATION',/,5X,
     * 'AND TEMPERATURE PROFILES AT EACH POINT ? ',/,5X,
     * 'YES = 1, NO = 0')
       READ(05,*) NN
       WRITE(08,*) NN
       WRITE(09,*) NN
C
C
       WRITE(06,70)
       WRITE(09,70)
70     FORMAT(//,5X,'******** REACTOR CHARACTERISTICS ********',//,5X,
     * 'DIAMETER (M) = ?')
       READ(05,*) D
       WRITE(08,*) D
       WRITE(09,*) D
C
       WRITE(06,80)
       WRITE(09,80)
80     FORMAT(5X,'LENGHT (M) = ?')
       READ(05,*) AL
       WRITE(08,*) AL
       WRITE(09,*) AL
C
       WRITE(06,90)
       WRITE(09,90)
90     FORMAT(5X,'BED VOID FRACTION = ?')
       READ(05,*) EB
       WRITE(08,*) EB
       WRITE(09,*) EB
C
       WRITE(06,100)
       WRITE(09,100)
100    FORMAT(5X,'NUMBER OF CATALYST BEDS = ?',/,5X,
     *  'IF THIS NOT THE FIRST BED  GIVE A NUMBER',/,5X,
     *  'TO IDENTIFY THE BED')
       READ(05,*) N
       WRITE(08,*) N
       WRITE(09,*) N
C
       WRITE(06,120)
       WRITE(09,120)
120    FORMAT(//,5X,'******** CATALYST CHARACTERISTICS *********',//,
     * 5X,'CATALYST DIAMETER (M) = ?',/,5X,'ASSUME SPHERICAL')
       READ(05,*) DP
       WRITE(08,*) DP
```

```
      WRITE(09,*) DP
C
      WRITE(06,130)
      WRITE(09,130)
130   FORMAT(10X,'DENSITY (KG/M**3) = ?')
      READ(05,*) DENCAT
      WRITE(08,*) DENCAT
      WRITE(09,*) DENCAT
C
      WRITE(06,140)
      WRITE(09,140)
140   FORMAT(10X,'POROSITY = ?')
      READ(05,*) EP
      WRITE(08,*) EP
      WRITE(09,*) EP
C
      WRITE(06,150)
      WRITE(09,150)
150   FORMAT(10X,'TORTOUSITY = ?')
      READ(05,*) TOR
      WRITE(08,*) TOR
      WRITE(09,*) TOR
C
      WRITE(06,160)
      WRITE(09,160)
160   FORMAT(10X,'THERMAL CONDUCTIVITY (KJ/M-S-K) = ?',/,
     * 10X,'IF NOT AVAILABLE ENTER  0.0 ')
      READ(05,*) CONS
      WRITE(08,*) CONS
      WRITE(09,*) CONS
C
      WRITE(06,170)
170   FORMAT(//,5X,'END OF DATA INPUT....',//,5X,
     * 'INPUT DATA ARE STORED IN THE FILE NAMED  INPUT.DAT',/,5X,
     * 'PLEASE CHECK YOUR DATA FROM THE FILE NAMED  CHECK.DAT'//,5X,
     *  'THE SIMULATOR  FIXED.BED  CAN NOW BE EXECUTED',/,5X,
     *  'IF YOU HAVE ANOTHER BED , PLEASE REMEMBER TO USE ',/,5X,
     *  'INTERACTIVE PROGRAM  INTBED.FOR  WITH THE OUTPUT',/,5X,
     *  'OF THIS RUN TO CALCULATE THE FEED CONDITIONS TO NEXT',/,5X,
     *  'BED. THEN YOU CAN PREPARE INPUT DATA BY USING THIS',/,5X,
     *  'PROGRAM AFTERWARDS')
C
      STOP
      END
```

I-C-3 Sample Run Showing Interactive Input

```
**************************************************

    SIMULATION OF A FIXED-BED ADIABATIC REACTOR
                    FOR
            METHANOL  SYNTHESIS

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


INSTRUCTIONS


THIS PROGRAM SIMULATES  ICI "S QUENCH TYPE LOW-PRESSURE
FIXED-BED METHANOL SYNTHESIS REACTOR.
ONE-DIMENSIONAL PLUG FLOW MODEL IS USED TO BE A GOOD
REPRESENTATIVE PICTURE OF THE REACTOR BEHAVIOUR.
INPUT VARIABLES INCLUDING FEED,REACTOR AND CATALYST
CHARACTERISTICS ARE PROVIDED BY THE USER VIA THIS
INTERACTIVE PACKAGE.THE SIMULATOR THEN EVALUATES
TEMPERATURE AND CONCENTRATION PROFILES TOGETHER WITH
CONVERSIONS,EFFECTIVENESS FACTORS AND THE REACTION
RATES FOR EACH CATALYST BED.


TO RUN THE SIMULATOR ,PLEASE ENTER THE FOLLOWING DATA
IN FREE FORMAT



********** FEED CHARACTERISTICS **********

INLET TEMPERATURE (K) = ?
>470.

PRESSURE (ATM) = ?
>80.

GAS COMPOSITION
ENTER THE MOL FRACTIONS. THE SQUENCE IS :
1:CO  2:CO2  3:H2  4:CH3OH  5:H2O  6:N2  7:CH4
>0.25 0.1 0.5 0.0 0.0 0.01 0.14

VOLUMETRIC GAS VELOCITY (Nm**3/sec) = ?
>58.437

DO YOU WANT TO GET SOLID PHASE CONCENTRATION
AND TEMPERATURE PROFILES AT EACH POINT ?
YES = 1, NO = 0
>1

******** REACTOR CHARACTERISTICS ********

DIAMETER (M) = ?
>2.0
LENGHT (M) = ?
>0.8
```

```
BED VOID FRACTION = ?
>0.4
NUMBER OF CATALYST BEDS = ?
IF THIS NOT THE FIRST BED  GIVE A NUMBER
TO IDENTIFY THE BED
>1


******** CATALYST CHARACTERISTICS *********

CATALYST DIAMETER (M) = ?
ASSUME SPHERICAL
>0.005
     DENSITY (KG/M**3) = ?
>1980.
     POROSITY = ?
>0.3
     TORTOUSITY = ?
>7.0
     THERMAL CONDUCTIVITY (KJ/M-S-K) = ?
     IF NOT AVAILABLE ENTER  0.0
>0.00418


END OF DATA INPUT....

INPUT DATA ARE STORED IN THE FILE NAMED  INPUT.DAT
PLEASE CHECK YOUR DATA FROM THE FILE NAMED  CHECK.DAT

THE SIMULATOR  FIXED.BED  CAN NOW BE EXECUTED .
IF YOU HAVE ANOTHER BED , PLEASE REMEMBER TO USE
INTERACTIVE PROGRAM  INTBED.FOR  WITH THE OUTPUT
OF THIS RUN TO CALCULATE THE FEED CONDITIONS TO NEXT
BED. THEN YOU CAN PREPARE INPUT DATA BY USING THIS
PROGRAM AFTERWARDS
```

I-C-4 Program Listing - FIXED BED

```
C
C
C     ************************************************************************
C
C     MAIN PROGRAM FOR THE SIMULATION OF FIXED-BED
C     METHANOL SYNTHESIS REACTOR.
C
C     THIS PROGRAM SIMULATES AN ADIABATIC FIXED BED REACTOR FOR
C     METHANOL SYNTHESIS.
C
C     CONVERSION, TEMPERATURE, CONCENTRATION, REACTION RATE
C     PROFILES ARE CALCULATED FOR A SET OF DESIGN AND OPERATING
C     CONDITIONS. ALTHOUGH THE PROGRAM IS WRITTEN FOR
C     LOW-PRESSURE SYNTHESIS AND NORMALLY EMPLOYS A KINETIC
C     RATE EXPRESSION OBTAINED FOR A Cu/Zn/Cr2O3 CATALYST
C     (United Catalyst T-2370) THE USER CAN ACCOMODATE HIS
C     OWN KINETIC DATA BY UPDATING THE SUBROUTINE REAC1.
C     THE SUBROUTINE FUGA  CAN BE USED TO CALCULATE THE FUGACITIES
C     WHEN NEEDED FOR THE RATE EXPRESSIONS.
C
C     ************************************************************************
C
C     VARIABLE LIST
C
C     AL   :REACTOR LENGTH (m)
C     ANU  :NUSSELT NUMBER (-)
C     CATDEN,DENCAT  :CATALYST DENSITY (kg/m**3)
C     CG   :GAS PHASE CONCENTRATION (kmol/m**3)
C     CF   :GAS PHASE FEED CONCENTRATION (kmol/m**3)
C     CONG  :GAS PHASE CONCENTRATION (kmol/m**3)
C     CONS,TCONS  :THERMAL CONDUCTIVITY OF THE PELLET (kJ/m-s-K)
C     CONV  :CONVERSIONS
C             1 :METHANOL REACTION
C             2 :SHIFT REACTION
C     DE   :EFFECTIVE DIFFUSIVITY (m**2/sec)
C     DR   :REACTOR DIAMETER (m)
C     DP,DPAR  :PELLET DIAMETER (m)
C     EB   :BED VOID FRACTION (-)
C     EP   :PELLET POROSITY (-)
C     FACEF  :OVERALL EFFECTIVENESS FACTOR
C             1 :METHANOL REACTION
C             2 :SHIFT REACTION
C     NAME  :NAME VECTOR FOR COMPONENTS
C     NB   :BED NUMBER
C     NE   :CONTROL VARIABLE
C             1 :SOLID PHASE PROFILES REQUIRED
C             0 :NOT REQUIRED
C     P,PT  :PRESSURE (atm)
C     Q,QFG  :GAS VOLUMETRIC FLOW RATE (Nm**3/sec)
C     REFF  :EFFECTIVE REACTION RATE
C             1 :METHANOL REACTION
C             2 :SHIFT REACTION
C     TG   :TEMPERATURE (K)
C     TF   :FEED TEMPERATURE (K)
C     TB   :DIMENSIONLESS TEMPERATURE (-)
C     TO   :OUTLET TEMPERATURE (K)
C     TOR :TORTUOSITY (-)
C     SH   :SHERWOOD NUMBER (-)
C     STY :SPACE TIME YIELD ( Nm**3 gas converted/kg Cat-hr)
C     UZ   :DIMENSIONLESS GAS VELOCITY (-)
```

```
C       UF   :SUPERFICIAL GAS VELOCITY (m/sec)
C       WHSV  :WEIGHT HOURLY SPACE VELOCITY (Nm**3/kg Cat-hr)
C       Y   :GAS PHASE CONCENTRATION (mole fraction)
C       YF   :FEED GAS MOLE FRACTIONS
C       YS1,YS2  :PELLET SURFACE CONCENTRATIONS FOR METHANOL AND CO2
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        COMMON/PAR1/TF,PT,YF(7),Q,NN
        COMMON/PAR2/DR,EB,NB,AL
        COMMON/PAR3/DPAR,CATDEN,EP,TOR,TCONS
        COMMON/PAR4/DP,CONS,SH(7),ANU,YS1,YS2,P,TG,CG(7),DE(7),DENCAT
        COMMON/PAR9/CF(7),X(11),UZ(11),TB(11),CONV(2,11)
        COMMON/PAR10/CONG(7,11),REFF(2,11),FACEF(2,11)
        DIMENSION NAME(7),Y(7)
C
        DATA NAME/' CO  ',' CO2 ',' H2  ','CH3OH',' H2O ',' N2  ',' CH4 '/
C
        OPEN (UNIT=8,FILE='INPUT.DAT')
        OPEN (UNIT=20,FILE='OUTPUT.SUM')
        OPEN (UNIT=21,FILE='CONV.PRO')
        OPEN (UNIT=22,FILE='COMP.PRO')
        OPEN (UNIT=23,FILE='TEMP.PRO')
        OPEN (UNIT=24,FILE='GAS.PRO')
        OPEN (UNIT=25,FILE='EFF.PRO')
        OPEN (UNIT=26,FILE='ERATE.PRO')
C
        CALL INPUT
C
        DP=DPAR
        P=PT
        DENCAT=CATDEN
        CONS=TCONS
        N=NB
        DF=EP/TOR
C
        S=3.1416/4.*DR**2.
C
        UF=Q*TF/P/273.2/S
C
        WRITE(20,10)
10      FORMAT(///,10X,'************************************************',
     * //,14X,'SIMULATION OF A FIXED-BED ADIABATIC REACTOR',//,10X,
     * '                    FOR',//,10X,
     * '             METHANOL  SYNTHESIS',//,10X,
     * '************************************************',//)
C
C
        WRITE(20,25)
25      FORMAT(/,5X,'SUMMARY OF THE INPUT DATA',///)
        WRITE(20,30) TF
30      FORMAT(5X,'************** FEED CHARACTERISTICS *************',
     * //,10X,'INLET TEMPERATURE = ',F10.5,' Deg. K')
        WRITE(20,40) PT
40      FORMAT(/,10X,'PRESSURE = ',F10.5,' atm')
        WRITE(20,50)
50      FORMAT(/,10X,'GAS COMPOSITION',/,10X,
     * 'Component',3X,'Mole fraction',/,10X,9('*'),3X,13('*'))
        WRITE(20,55) (NAME(I),YF(I),I=1,7)
55      FORMAT(12X,A5,7X,F10.5)
```

```
      WRITE(20,60) Q
60    FORMAT(/,10X,'VOLUMETRIC GAS VELOCITY = ',D12.5,
     *  ' N.m**3/Sec')
      WRITE(20,65) UF
65    FORMAT(/,10X,'SUPERFICIAL GAS VELOCITY = ',F10.5,' m/sec')
      WRITE(20,70) DR
70    FORMAT(//,5X,'******** REACTOR CHARACTERISTICS ********',//,10X,
     * 'DIAMETER = ',F10.5,' m')
      WRITE(20,80) AL
80    FORMAT(/,10X,'LENGTH = ',F10.5,' m')
      WRITE(20,90) EB
90    FORMAT(10X,'BED VOID FRACTION = ',F10.5)
      IF(NB.EQ.0) NB=1
      WRITE(20,100) NB
100   FORMAT(10X,'BED NUMBER = ',I2)
C
      WRITE(20,120) DPAR
120   FORMAT(//,5X,'******** CATALYST CHARACTERISTICS *********',//,
     * 10X,'CATALYST DIAMETER = ',F10.5,' m')
      WRITE(20,130) CATDEN
130   FORMAT(19X,'DENSITY = ',F10.5,'(Kg/m**3) ')
      WRITE(20,140) EP
140   FORMAT(19X,'POROSITY = ',F10.5)
      WRITE(20,150) TOR
150   FORMAT(19X,'TORTOUSITY = ',F10.5)
C
      IF(TCONS.EQ.0.) TCONS=4.18D-03
      WRITE(20,160) TCONS
160   FORMAT(10X,'THERMAL CONDUCTIVITY  = ',
     * F10.5,' KJ/m-sec-K')
C
      QFG=Q
C
C
      R=.082
      CO=P/R/TF
      DO 33 I=1,7
33    CF(I)=YF(I)*CO
      NBED=NB
      ALEN=AL
C
      CALL BEDCAL(NBED,TF,UF,NN,ALEN,EB,DF)
C
      AWCAT=S*ALEN*(1.-EB)*DENCAT
      WHSV=QFG=3600./AWCAT
      STY=QFG*YF(1)*CONV(1,11)*3600./AWCAT
C
      CTOT=0.
      DO 180 I=1,7
180   CTOT=CTOT+CONC(I,11)
C
      DO 190 I=1,7
190   Y(I)=CONC(I,11)/CTOT
C
      TO=TF*(1.+TB(11))
C
      WRITE(20,170) TO
170   FORMAT(//,5X,'SUMMARY OF THE OUTPUT DATA',///,10X,
     * 'OUTPUT TEMPERATURE = ',F10.5,' Deg. K')
C
```

```
      WRITE(20,40) P
      WRITE(20,50)
      WRITE(20,55) (NAME(I),Y(I),I=1,7)
C
      CONV1=CONV(1,11)-CONV(2,11)
      CONV2=CONV(2,11)
      CONV0=CONV(1,11)
      WRITE(20,200) CONV1,VONV2,CONV0
200   FORMAT(/,10X,'CONVERSION 1 = ',E10.5,/,10X,'CONVERSION 2 = ',
     * E10.5,/,10X,'OVERALL CONV. = ',E10.5)
C
      QFOUT=QFG*UZ(11)
      WRITE(20,60) QFOUT
C
      WRITE(20,300) WHSV,STY
300   FORMAT(///,5X,'SPACE VELOCITY = ',E12.5,' Nm**3/kg-hr',/,
     * 5X,'SPACE TIME YIELD = ',E12.5,' NM**3 Gas Converted/kg-hr')
C
      WRITE(21,400)
400   FORMAT(//,15X,'LENGTH',/,5X,'DIMENSIONLESS',3X,'ACTUAL (m) ',
     * 5X,'CONVERSION 1',3X,'CONVERSION 2',3X,'OVERALL CONV.',
     * /,5X,12('*'),3X,12('*'),2X,3(3X,12('*')))
C
      WRITE(22,410) (NAME(I),I=1,7)
410   FORMAT(//,15X,'LENGTH',35X,'GAS PHASE MOLE FRACTIONS',/,
     * 3X,'DIMENSIONLESS',2X,'ACTUAL (m) ',7(8X,A5),/,5X,
     * 10('*'),3X,10('*'),2X,7(3X,10('*')))
C
      WRITE(23,420)
420   FORMAT(//,15X,'LENGTH',24X,'TEMPERATURE',/,5X,'DIMENSIONLESS',
     * 3X,'ACTUAL (m) ',5X,'DIMENSIONLESS',3X,'ACTUAL (K) ',/,
     * 5X,12('*'),3X,12('*'),5X,12('*'),3X,12('*'))
C
      WRITE(24,430)
430   FORMAT(//,14X,'LENGTH',20X,'GAS FLOW RATE ',/,5X,'DIMENSIONLESS',
     * 3X,'ACTUAL (m) ',5X,'DIMENSIONLESS',3X,'ACTUAL (m/s)',/,
     * 5X,12('*'),3X,12('*'),5X,12('*'),3X,12('*'))
C
      WRITE(25,440)
440   FORMAT(//,14X,'LENGTH',/,5X,'DIMENSIONLESS',3X,'ACTUAL (m) ',
     * 5X,'EFF.FACTOR 1',3X,'EFF.FACTOR 2',/,5X,12('*'),3X,12('*'),
     * 2X,2(3X,12('*')))
C
      WRITE(26,450)
450   FORMAT(//,14X,'LENGTH',/,5X,'DIMENSIONLESS',3X,'ACTUAL (m) ',
     * 'EFF. RATE 1',3X,'EFF. RATE 2',/,5X,12('*'),3X,12('*'),2X,
     * 2(3X,12('*')))
C
C
      DO 460 I=1,11
      AX=X(I)*AL
C
      CONV1=CONV(1,I)-CONV(2,I)
      CONV2=CONV(2,I)
      CONV0=CONV(1,I)
      WRITE(21,500) X(I),AX,CONV1,CONV2,CONV0
500   FORMAT(5X,F12.5,3X,F12.5,5X,E12.5,3X,E12.5,3X,E12.5)
C
      CTOT=0.
      DO 510 J=1,7
```

```
510     CTOT=CTOT+CONC(J,I)
        DO 520 J=1,7
520     Y(J)=CONC(J,I)/CTOT
        WRITE(22,530) X(I),AX,(Y(J),J=1,7)
530     FORMAT(5X,F10.5,3X,F10.5,2X,7(3X,E10.5))
C
        TEMP=TF*(1.+TB(I))
        WRITE(23,540) X(I),AX,TB(I),TEMP
540     FORMAT(5X,F12.5,3X,F12.5,5X,E12.5,3X,E12.5)
C
        UGAS=UZ(I)*UF
        WRITE(24,550) X(I),AX,UZ(I),UGAS
550     FORMAT(5X,F12.5,3X,F12.5,5X,E12.5,3X,F12.5)
C
        IF(I.EQ.1) GO TO 460
C
        WRITE(25,560) X(I),AX,FACEF(1,I),FACEF(2,I)
560     FORMAT(5X,F12.5,3X,F12.5,5X,E12.5,3X,E12.5)
        WRITE(26,560) X(I),AX,REFF(1,I),REFF(2,I)
C
460     CONTINUE
        STOP
        END

C
C       ------------------------------------------------------
C
        SUBROUTINE INPUT
C
C
C       THIS SUBROUTINE PROVIDES THE INPUT DATA TO THE FIXED-BED
C       METHANOL SYNTHESIS REACTOR SIMULATOR.
C
        IMPLICIT REAL*8(A-H,O-Z)
        INTEGER NB,NN
C
        COMMON/PAR1/TF,PT,YF(7),Q,NN
        COMMON/PAR2/DR,EB,NB,AL
        COMMON/PAR3/DPAR,CATDEN,EP,TOR,TCONS
C
        OPEN (UNIT=8,FILE='INPUT.DAT')
C
        READ(08,*) TF
        READ(08,*) PT
        READ(08,*) (YF(I),I=1,7)
        READ(08,*) Q
        READ(08,*) NN
        READ(08,*) DR
        READ(08,*) AL
        READ(08,*) EB
        READ(08,*) NB
        READ(08,*) DPAR
        READ(08,*) CATDEN
        READ(08,*) EP
        READ(08,*) TOR
        READ(08,*) TCONS
        RETURN
        END
C
C
```

```
C     ------------------------------------------------------------------
C
      SUBROUTINE BEDCAL(NBED,TF,UF,NN,ALEN,EB,DF)
C
C
C     SUB PROGRAM FOR FIXED-BED METHANOL SYNTHESIS REACTOR
C     SIMULATION
C
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      COMMON/PAR4/DP,CONS,SH(7),ANU,YS1,YS2,P,TG,CG(7),DE(7),DENCAT
      COMMON/PAR5/FSPACE(5000),ZETA(4),TOL(4),Z(4)
      COMMON/PAR6/ISPACE(250),M(2),IPAR(11),LTOL(4)
      COMMON/PAR7/RATE(2),YG(7),C(7),Y(7),NAME(7),FLUX(7)
      COMMON/PAR8/EFFR(2),EFAC(2),CONT(2)
C
      COMMON/PAR9/CF(7),X(11),UZ(11),TB(11),CONV(2,11)
      COMMON/PAR10/CONG(7,11),REFF(2,11),FACEF(2,11)
      DIMENSION D(7),YF(7)
C
      DATA NAME/'  CO ','  CO2','  H2 ','CH3OH',' H2O ','  N2 ',' CH4 '/
C
      CO=0.
      DO 43 I=1,7
43    CO=CO+CF(I)
C
      DO 45 I=1,7
45    YF(I)=CF(I)/CO
C
      RA=DP/2.
      AL=ALEN
C
      M(1)=2
      M(2)=2
      ZETA(1)=0.
      ZETA(2)=0.
      ZETA(3)=1.
      ZETA(4)=1.
      DO 10 I=1,11
10    IPAR(I)=0
      IPAR(1)=1
      IPAR(4)=2
      IPAR(5)=5000
      IPAR(6)=250
      IPAR(7)=1
      IPAR(9)=1
C
      DO 30 I=1,2
      LTOL(I)=I*2
30    TOL(I)=1.E-04
C
C     INITIATION
C
      CONV(1,1)=0.
      CONV(2,1)=0.
      UZ(1)=1.
      TB(1)=0.
      X(1)=0.
      DO 35 I=1,7
```

```
35      CONG(I,1)=CF(I)
        JJ=0
C
C       CALCULATIONS
C
        N=11
        DELZ=1./(N-1.)
        DO 60 IJ=2,N
        J=0
        NN1=NN
        K=IJ-1
        X(IJ)=K*DELZ
        XA=CONV(1,K)
        XB=CONV(2,K)
        TEST=1.05*(TB(K)+1.)*TF
70      CONTINUE
        CALL INTER2(TF,UF,CF,TEST,XA,XB,TG,CG,U)
        J=J+1
        CTOT=0.
        DO 20 I=1,7
20      CTOT=CTOT+CG(I)
        DO 11 I=1,7
11      YG(I)=CG(I)/CTOT
        CALL DEN(P,TG,YG,DENG)
        G=U*DENG
        CALL CPGAS(0,YG,TG,HEATCP,CPMASS,CONT)
        CALL VISMIX(TG,YG,VISCO)
        CALL DMIX(1,TG,P,YG,FLUX,D)
        DO 50 I=1,7
50      DE(I)=DP*D(I)
        CALL CONDUC(YG,TG,CONGAS)
        CALL AHEAT(G,VISCO,DENG,CPMASS,CONGAS,DP,EB,COHEAT)
        ANU=COHEAT*RA/CONGAS
        CALL AMASS(7,G,D,EB,DP,VISCO,DENG,SH)
        DO 14 I=1,7
14      SH(I)=SH(I)*RA/DE(I)
        KK=1
        IF(JJ.EQ.0) KK=0
        CALL ERATE(KK,NN1)
        JJ=1
C
        AV=6.*(1.-EB)/DP
        AV=AV/3.1416/DP**2.
        GRAT1=AV*EFFR(1)
        GRAT2=AV*EFFR(2)
        IF(J.NE.1) GO TO 75
        REFF(1,IJ)=GRAT1
        REFF(2,IJ)=GRAT2
        FACEF(1,IJ)=EFAC(1)
        FACEF(2,IJ)=EFAC(2)
        NN1=0
75      GRAT1=GRAT1+AL*DELZ/UF/CF(1)
        GRAT2=GRAT2+AL*DELZ/UF/CF(1)
C
C
        GO TO (80,90,100,110),J
80      AKO=GRAT1
        AHO=GRAT2
        XA=CONV(1,K)+AKO/2.
        XB=CONV(2,K)+AHO/2.
```

```
      GO TO 70
90    AK1=GRAT1
      AM1=GRAT2
      XA=CONV(1,K)+AK1/2.
      XB=CONV(2,K)+AM1/2.
      GO TO 70
100   AK2=GRAT1
      AM2=GRAT2
      XA=CONV(1,K)+AK2
      XB=CONV(2,K)+AM2
      GO TO 70
110   AK3=GRAT1
      AM3=GRAT2
C
      CONV(1,IJ)=CONV(1,K)+(AK0+2.*AK1+2.*AK2+AK3)/6.
      CONV(2,IJ)=CONV(2,K)+(AM0+2.*AM1+2.*AM2+AM3)/6.
      XA=CONV(1,IJ)
      XB=CONV(2,IJ)
C
      CALL INTER2(TF,UF,CF,TEST,XA,XB,TG,CG,U)
C
      UZ(IJ)=U/UF
      TB(IJ)=(TG-TF)/TF
      DO 200 I=1,7
200   CONG(I,IJ)=CG(I)
80    CONTINUE
C
C
      RETURN
      END
C
C     ------------------------------------------------------------
C
      SUBROUTINE ERATE(KK,NN)
C
C     CALCULATES THE EFFECTIVE REACTION RATES BY THE SOLUTION
C     OF SOLID PHASE DIFFERENTIAL EQUATIONS.
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/PAR4/DP,CONS,SH(7),ANU,YS1,YS2,P,TG,CG(7),DE(7),DENCAT
      COMMON/PAR5/FSPACE(5000),ZETA(4),TOL(4),Z(4)
      COMMON/PAR6/ISPACE(250),M(2),IPAR(11),LTOL(4)
      COMMON/PAR7/RATE(2),YG(7),C(7),Y(7),NAME(7),FLUX(7)
      COMMON/PAR8/EFFR(2),EFAC(2),CONT(2)
      EXTERNAL FSUB,DFSUB,GSUB,DGSUB,SOLUTN
C
C
      R=.082
C
      RA=DP/2.
C
      IF(TG.GT.450.) GO TO 10
      NI=1
      GO TO 20
10    IF(KK.NE.0) GO TO 120
      NI=(TG-450.)/5.+1
      TG=450.
20    CONTINUE
C
C
```

```
C
      DO 777 IJK=1,NI
C
      IF(IJK.EQ.1) GO TO 701
      TG=TG+5.
C
120   CONTINUE
C
      IPAR(9)=3
      IPAR(3)=ISPACE(1)
701   CONTINUE
      CALL COLSYS(2,M,0.,1.,ZETA,IPAR,LTOL,TOL,
     * FIXPNT,ISPACE,FSPACE,IFLAG,FSUB,DFSUB,GSUB,DGSUB,
     * SOLUTN)
C
      IF(NN.EQ.0) GO TO 50
      WRITE(20,67)TG,P
67    FORMAT(//,5X,'TEMPERATURE = ',F10.4,/,5X,'PRESSURE = ',F10.4)
      WRITE(20,87)(NAME(I),I=1,5)
87    FORMAT(//,5X,'     X    ',5(7X,A5),2X,' SLOPE 1  ',2X,
     * 'SLOPE 2',5X,'TEMPERATURE(K)',/,5X,9(10('='),2X))
C
      X=0.
      DO 40 I=1,11
      CALL APPSLN(X,Z,FSPACE,ISPACE)
      Y1=Z(1)
      Y2=Z(3)
C
      CALL INTER(TG,CG,CONS,YS1,YS2,Y1,Y2,SH,ANU,DE,C,T)
C
      CO=0.
      DO 89 IH=1,7
89    CO=CO+C(IH)
C
      DO 99 IH=1,7
99    Y(IH)=C(IH)/CO
C
      WRITE(20,13)X,(Y(IJ),IJ=1,5),Z(2),Z(4),T
13    FORMAT(5X,9(E10.3,2X),/)
40    X=X+.1
C
50    CONTINUE
      CALL APPSLN(1.,Z,FSPACE,ISPACE)
      SLOPE1=Z(2)
      SLOPE2=Z(4)
C
      EFFR(1)=-4.*3.1416*DE(4)*CG(1)*SLOPE1*RA
      EFFR(2)=-4.*3.1416*DE(2)*CG(1)*SLOPE2*RA
C
      IF(EFFR(1).LT.0.) EFFR(1)=1.D-10
      IF(EFFR(2).LT.0.) EFFR(2)=1.D-10
C
      CALL REAC1(TG,CG,RATE)
C
      DO 30 I=1,2
30    RATE(I)=RATE(I)*DENCAT
C
C
      EFAC(1)=-3.*DE(4)*CG(1)*SLOPE1/RATE(1)/RA**2.
      EFAC(2)=-3.*DE(2)*CG(1)*SLOPE2/RATE(2)/RA**2.
```

```
C
      IF(NN.EQ.0) GO TO 777
      WRITE(20,33) EFFR(1),EFFR(2),EFAC(1),EFAC(2)
33    FORMAT(//,5X,'EFF RATE 1 = ',E10.4,/,5X,'EFF RATE 2 = ',
     * E10.4,/,5X,'EFF1 = ',E10.4,/,5X,'EFF2 = ',E10.4)
C
777   CONTINUE
      RETURN
      END
C
C
C     ------------------------------------------------------------
C
      SUBROUTINE FSUB(X,Z,F)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/PAR4/DP,CONS,SH(7),ANU,YS1,YS2,P,TG,CG(7),DE(7),DENCAT
      DIMENSION RATE(2)
      DIMENSION Z(4),C(7),F(2)
C
      Y1=Z(1)
      Y2=Z(3)
      RA=DP/2.
      IF(X.NE.1.) GO TO 10
      YS1=Y1
      YS2=Y2
10    CALL INTER(TG,CG,CONS,YS1,YS2,Y1,Y2,SH,ANU,DE,C,T)
C
      CALL REAC1(T,C,RATE)
C
      DO 20 I=1,2
20    RATE(I)=RATE(I)*DENCAT
C
      A=RA**2./CG(1)/DE(4)
      B=RA**2./DE(2)/CG(1)
      F(1)=-RATE(1)*A-2./X*Z(2)
      F(2)=-RATE(2)*B-2./X*Z(4)
      RETURN
      END
C
C     ------------------------------------------------------------
C
C
      SUBROUTINE DFSUB(X,Z,DF)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/PAR4/DP,CONS,SH(7),ANU,YS1,YS2,P,TG,CG(7),DE(7),DENCAT
      DIMENSION Z(4),DF(2,4),WORK1(2),WORK2(2)
C
      EPS=1.D-07
      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
      DF(I,J)=(WORK1(I)-WORK2(I))*.5/EPS
10    CONTINUE
      RETURN
      END
C
```

```
C       ------------------------------------------------------------
C
        SUBROUTINE GSUB(I,Z,G)
        IMPLICIT REAL*8(A-H,O-Z)
        COMMON/PAR4/DP,CONS,SH(7),ANU,YS1,YS2,P,TG,CG(7),DE(7),DENCAT
        DIMENSION Z(4)
        GO TO(1,2,3,4),I
1       G=Z(2)
        RETURN
2       G=Z(4)
        RETURN
3       G=Z(2)+SH(4)*Z(1)
        YS1=Z(1)
        RETURN
4       G=Z(4)+SH(2)*Z(3)
        YS2=Z(3)
        RETURN
        END
C
C       ------------------------------------------------------------
C
C
        SUBROUTINE DGSUB(I,Z,DG)
        IMPLICIT REAL*8(A-H,O-Z)
        COMMON/PAR4/DP,CONS,SH(7),ANU,YS1,YS2,P,TG,CG(7),DE(7),DENCAT
        DIMENSION Z(4),DG(4)
        DO 10 J=1,4
10      DG(J)=0.D00
        GO TO(1,2,3,4),I
1       DG(2)=1.D00
        RETURN
2       DG(4)=1.D00
        RETURN
3       DG(1)=SH(4)
        DG(2)=1.D00
        RETURN
4       DG(3)=SH(2)
        DG(4)=1.D00
        RETURN
        END
C
C       ------------------------------------------------------------
C
        SUBROUTINE SOLUTN(X,Z,DMVAL)
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION Z(4),DMVAL(2)
        DMVAL(1)=0.
        DMVAL(2)=1.
        Z(1)=0.D00
        Z(2)=0.D00
        Z(3)=0.D00
        Z(4)=0.D00
        RETURN
        END
C
C       ------------------------------------------------------
C
        SUBROUTINE REAC1(T,C,RATE)
C
C       CALCULATES THE REACTION RATES BY BERTY'S EQUATIONS
```

```
C
C       T   :TEMPERATURE (K)
C       C   :CONCENTRATION (kmol/m**3)
C                1 :CO   2 :CO2   3 :H2   4 :CH3OH   5 :H2O
C       RATE   :REACTION RATE   kmol/kg-SEC
C                1 :METHANOL REACTION
C                2 :SHIFT REACTION
C
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION C(7),RATE(2)
C
        R=.082
C
        AKK1=3.27D-11*EXP(11678./T)*(R*T)**2
        AKK2=1.17D+02*EXP(-4827./T)
        AK1=39.144*EXP(-7488.7/T)
        AK2=.01189*EXP(-5068.4/T)
C
C
        RATE(1)=AK1*(C(3)-C(4)/(AKK1*C(3)*C(1)))
        RATE(2)=AK2*(C(3)-C(1)*C(5)/(AKK2*C(2)))
C
        RETURN
        END
C
C       ----------------------------------------------------------------
C
        SUBROUTINE DMIX(KC,T,P,Y,FLUX,D)
C
C       MIXTURE DIFFUSION COEFFICIENTS FOR METHANOL SYNTHESIS
C
C       AM   :MOLECULAR WEIGHTS
C       D   :DIFFUSION COEFFICIENTS IN GAS MIXTURE (M**2/SEC)
C       DBIN   :BINARY DIFFUSION COEFFICIENTS (M**2/SEC)
C       FLUX   :FLUX OF THE SPECIES (KMOL/M**2-SEC)
C       P   :PRESSURE (ATM)
C       KC   :
C                1 :WILKE'S EQUATION
C                0 :STEFAN-MAXWELL'S EQUATION
C       T   :TEMPERATURE (K)
C       Y   :MOLE FRACTION (-)
C       V   :DIFFUSION VOLUMES (CM**3/MOL)
C
C       INDEX FOR THE COMPONENTS :
C       1:CO   2:CO2   3:H2   4:CH3OH   5:H2O   6:N2   7:CH4
C
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION Y(7),FLUX(7),DBIN(7,7),D(7),AM(7),V(7)
        DATA AM/28.,44.,2.,32.,18.,28.,16./
        DATA V/18.9,26.9,7.07,29.9,12.7,17.9,24.42/
        CALL DCOEF(7,AM,V,T,P,DBIN)
C
        IF(KC.NE.1) GO TO 20
        DO 30 I=1,7
        SUM=0.
        DO 31 J=1,7
        IF(I.EQ.J) GO TO 31
        SUM=SUM+Y(J)/DBIN(I,J)
31      CONTINUE
30      D(I)=(1.-Y(I))/SUM
```

```
      RETURN
20    CONTINUE
      DO 10 I=1,7
      SUM1=0.
      SUM2=0.
      DO 40 J=1,7
      SUM1=SUM1+(Y(J)*FLUX(I)-Y(I)*FLUX(J))/DBIN(I,J)
40    SUM2=SUM2+FLUX(J)
      A=SUM1/(FLUX(I)-Y(I)*SUM2)
10    D(I)=1./A
      RETURN
      END
C
C     ------------------------------------------------------------
C
      SUBROUTINE DCOEF(N,AM,V,T,P,DBIN)
C
C     BINARY DIFFUSION COEFFICIENTS
C     BY FULLER-SCHETTER-GIDDINS
C
C     N   :NO OF COMPONENTS
C     AM  :MOLECULAR WEIGHTS
C     V   :DIFFUSION VOLUMES (CM**3/MOL)
C     T   :TEMPERATURE (K)
C     P   :PRESSURE (ATM)
C     DBIN  :BINARY DIFFUSION COEFFICIENTS (M**2/SEC)
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION AM(N),V(N),DBIN(N,N)
      DO 10 I=1,N
      DO 10 J=1,N
10    DBIN(I,J)=1.E-07*T**(1.75)*SQRT((AM(I)+AM(J))/(AM(I)*AM(J)))/
     * (P*(V(I)**(.33)+V(J)**(.33))**2)
      RETURN
      END
C
C     ------------------------------------------------------------
C
      SUBROUTINE INTER(TG,CG,CONS,YS1,YS2,Y1,Y2,SH,ANU,D,C,T)
C
C     CALCULATES THE SOLID PHASE TEMPERATURE AND
C     CONCENTRATIONS FOR A GIVEN SURFACE AND POINT
C     CONVERSIONS.
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION CG(7),HEATR(2),SH(7),D(7),C(7)
C
      CALL RHEAT(TG,HEATR)
      DELTA1=HEATR(1)
      DELTA2=HEATR(2)
C
C
      A=D(4)*DELTA1*CG(1)/CONS
      B=D(2)*DELTA2*CG(1)/CONS
C
      A1=D(2)/D(1)
      A2=D(4)/D(1)
C
      C(1)=CG(1)*(1.-A1*(YS2*(1.-A1**(-.33))-Y2)+
```

```
     * A2*(YS1*(1.-A2**(-.33))-Y1))
C
        C(2)=CG(2)-CG(1)*Y2
C
        A1=D(4)/D(3)
        A2=D(2)/D(3)
C
        C(3)=CG(3)+CG(1)*(2.*A1*(YS1*(1.-A1**(-.33))-Y1)+
     * A2*(YS2*(1.-A2**(-.33))-Y2))
C
        C(4)=CG(4)+CG(1)*Y1
C
        A1=D(2)/D(5)
C
        C(5)=CG(5)-CG(1)*A1*(YS2*(1.-A1**(-.33))-Y2)
C
        C(6)=CG(6)
C
        C(7)=CG(7)
C
        T=TG+A*(YS1*(1.-SH(4)/ANU)-Y1)+
     * B*(YS2*(1.-SH(2)/ANU)-Y2)
C
        RETURN
        END
C
C       ------------------------------------------------------------
C
C
        SUBROUTINE AMASS(N,G,D,EB,DP,VIS,DEN,COEFMA)
C
C       MASS TRANSFER COEFFICIENTS FOR FIXED-BED
C
C       NO   :NO OF COMPONENTS
C       G    :SUPERFICIAL MASS VELOCITY (KG/M**2-SEC)
C       D    :DIFFUSION COEFFICIENTS (M**2/SEC)
C       EB   :VOID FRACTION OF THE BED (-)
C       DP   :PARTICLE DIAMETER (M)
C       VIS  :VISCOSITY OF THE GAS MIXTURE (KG/M-SEC)
C       DEN  :DENSITY OF THE GAS MIXTURE (KG/M**3)
C       COEFMA  :VOLUMETRIC MASS TRANSFER COEFFICIENTS (M/SEC)
C
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION COEFMA(N),D(N)
        RE=DP*G/VIS
        FAC=.458/EB*RE**(-0.407)
        DO 10 I=1,N
10      COEFMA(I)=FAC*G/DEN*(VIS/DEN/D(I))**(-2./3.)
        RETURN
        END
C
C       ------------------------------------------------------------
C
        SUBROUTINE AHEAT(G,VIS,DEN,CPMASS,COND,DP,EB,COHEAT)
C
C       HEAT TRANSFER COEFFICIENT FOR FIXED BED
C
C       G    :SUPERFICIAL MASS VELOCITY (KG/M**2-SEC)
C       VIS  :VISCOSITY OF THE GAS MIXTURE (KG/M-SEC)
C       DEN  :DENSITY OF THE GAS MIXTURE (KG/M**3)
```

```
C       CPMASS  :MASS HEAT CAPACITY OF THE GAS MIXTURE (KJ/KG-K)
C       COND  :THERMAL CONDUCTIVITY OF THE GAS MIXTURE (KJ/M**2-SEC-K)
C       DP  :PARTICLE DIAMETER (M)
C       EE  :VOID FRACTION OF THE BED (-)
C       COHEAT  :HEAT TRANSFER COEFFICIENT (KJ/M-SEC-K)
C
        IMPLICIT REAL*8(A-H,O-Z)
        RE=DP*G/VIS
        FAC=.458/EE*RE**(-.407)
        COHEAT=CPMASS*G*(CPMASS*VIS/COND)**(-2./3.)
        RETURN
        END
C
C       ------------------------------------------------------------
C
        SUBROUTINE CPGAS(N,Y,T,HEATCP,CPMASS,CONT)
C
C       THIS SUBROUTINE PROVIDES HEAT CAPACITY DATA
C       FOR METHANOL SYNTHESIS,
C       ALSO USED TO CALCULATE HEAT OF REACTION DATA
C
C       N  :CONTROL VARIABLE
C             0:ONLY HEAT CAPACITY IS TO BE CALCULATED
C             1:ONLY HEAT OF REACTION IS TO BE CALCULATED
C       Y  :MOLE FRACTIONS
C       T  :TEMPERATURE (K)
C       HEATCP  :MOLAL HEAT CAPACITY (KJ/KMOL-K)
C       CPMASS  :MASS HEAT CAPACITY (KJ/KG-K)
C       CONT  :CONTRIBUTION TO REACTION ENTHALPIES
C
C       CP(I,J) ARE THE CONSTANTS FOR HEAT CAPACITY EQUATION
C
C       CPGAS(I)=CP(I,1)+CP(I,2)*TC+CP(I,3)*TC**2+CP(I,4)*TC**3
C
C       UNITS ARE   CPGAS:KJ/KMOL-K,   T:K
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION CP(7,4),CONT(2),AM(7),SUM(7),Y(7)
C
        DATA AM/28.,44.,2.,32.,18.,28.,16./
C
C       CO
C
        CP(1,1)=28.86
        CP(1,2)=.411E-02
        CP(1,3)=.3548E-05
        CP(1,4)=-2.22E-09
C
C       CO2
C
        CP(2,1)=38.11
        CP(2,2)=4.233E-02
        CP(2,3)=-2.887E-05
        CP(2,4)=7.465E-09
C
C       H2
C
        CP(3,1)=28.84
        CP(3,2)=.00765E-02
        CP(3,3)=.3288E-05
        CP(3,4)=-.8698E-09
```

```
C
C       CH3OH
C
        CP(4,1)=42.93
        CP(4,2)=8.301E-02
        CP(4,3)=-1.89E-05
        CP(4,4)=-8.03E-09
C
C       H2O
C
        CP(5,1)=33.46
        CP(5,2)=.688E-02
        CP(5,3)=.7604E-05
        CP(5,4)=-3.593E-09
C
C       N2
C
        CP(6,1)=29.
        CP(6,2)=.2199E-02
        CP(6,3)=.5723E-05
        CP(6,4)=-2.871E-09
C
C       CH4
C
        CP(7,1)=34.33
        CP(7,2)=5.711E-02
        CP(7,3)=.3363E-05
        CP(7,4)=11.0092E-09
C
        TC=T-273.15
C
        IF(N.EQ.1) GO TO 40
        DO 20 I=1,7
        SUM(I)=0.
20      CONTINUE
        DO 10 I=1,7
        SUM(I)=SUM(I)+CP(I,1)+CP(I,2)*TC+CP(I,3)*TC**2.+CP(I,4)*TC**3.
10      CONTINUE
C
        HEATCP=0.
        CPMASS=0.
        DO 30 I=1,7
        CPMASS=CPMASS+SUM(I)*Y(I)/AM(I)
30      HEATCP=HEATCP+SUM(I)*Y(I)
C
        RETURN
C
40      A1=CP(4,1)-2.*CP(3,1)-CP(1,1)
        A2=CP(4,2)-2.*CP(3,2)-CP(1,2)
        A3=CP(4,3)-2.*CP(3,3)-CP(1,3)
        A4=CP(4,4)-2.*CP(3,4)-CP(1,4)
C
        B1=CP(5,1)+CP(1,1)-CP(3,1)-CP(2,1)
        B2=CP(5,2)+CP(1,2)-CP(3,2)-CP(2,2)
        B3=CP(5,3)+CP(1,3)-CP(3,3)-CP(2,3)
        B4=CP(5,4)+CP(1,4)-CP(3,4)-CP(2,4)
C
        CONT(1)=A1*(TC-25.)+A2*(TC**2.-25.**2.)*.5+
     * A3/3.*(TC**3.-25.**3.)+A4/4.*(TC**4.-25.**4.)
C
```

```
      CONT(2)=B1*(TC-25.)+B2*(TC**2.-25.**2.)*.5+
     * B3/3.*(TC**3.-25.**3.)+B4/4.*(TC**4.-25.**4.)
      RETURN
      END
C
C     ------------------------------------------------------------
C
      SUBROUTINE VISMIX(T,Y,VISCO)
C
C     VISCOSITY OF GAS MIXTURE FOR METHANOL SYNTHESIS
C     BY WILKE'S METHOD
C
C     T  :TEMPERATURE
C     Y  :MOLE FRACTIONS
C     TC  :CRITICAL TEMPERATURE (K)
C     PC  :CRITICAL PRESSURE (ATM)
C     ZC  :CRITICAL COMPRESSIBILITY FACTOR (-)
C     VISG  :VISCOSITY OF THE COMPONENTS (KG/M-SEC)
C     VISCO  :VISCOSITY OF THE MIXTURE (KG/M-SEC)
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Y(7),TC(7),PC(7),AM(7),ZC(7),VISG(7)
      DATA TC/132.9,304.2,33.2,512.6,647.3,126.2,190.6/
      DATA PC/34.5,72.8,12.8,79.9,217.6,33.5,45.4/
      DATA ZC/.295,.274,.305,.224,.229,.290,.228/
      DATA AM/28.,44.,2.,32.,18.,28.,16./
C
      CALL VISGAS(7,AM,TC,PC,ZC,T,VISG)
      VISCO=0.
      DO 10 I=1,7
      SUM=0.
      DO 20 J=1,7
      FAC=1./SQRT(8.)*(1.+AM(I)/AM(J))**(-.5)*(1.+DSQRT(
     * VISG(I)/VISG(J))*(AM(J)/AM(I))**(.25))**2.
20    SUM=SUM+FAC*Y(I)
10    VISCO=VISCO+Y(I)*VISG(I)/SUM
      RETURN
      END
C
C     ------------------------------------------------------------
C
      SUBROUTINE VISGAS(N,AM,TC,PC,ZC,T,VISG)
C
C     VISCOSITY OF THE GAS SPECIES
C
C     N  :NO OF COMPONENTS
C     AM  :MOLECULAR WEIGHTS
C     TC  :CRITICAL TEMPERATURE (K)
C     PC  :CRITICAL PRESSURE (ATM)
C     ZC  :CRITICAL COMPRESSIBILITY FACTOR (-)
C     T  :TEMPERATURE (K)
C     VISG  :VISCOSITY (KG/M-SEC
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION AM(N),TC(N),PC(N),ZC(N),VISG(N)
C
      DO 10 I=1,N
      TR=T/TC(I)
      EPS=TC(I)**(1./6.)/(AM(I)**(.5)*PC(I)**(2./3.))
      FAC=(1.9*TR-.29)*1.D-07/ZC(I)**(2./3.)
```

```
10      VISG(I)=FAC/EPS
        RETURN
        END
C
C       ------------------------------------------------------
C
        SUBROUTINE CONMIX(N,Y,CONG,VISG,AM,S,T,CONGAS)
C
C
C       THERMAL CONDUCTIVITY OF THE GAS MIXTURE
C       BY LINDSAY AND BROMLEY MODIFICATION
C
        IMPLICIT REAL*8(A-H,O-Z)
C
C       N   :NUMBER OF THE COMPONENTS
C       Y   :MOLE FRACTIONS
C       CONG   :THERMAL CONDUCTIVITY OF THE SPECIES (KJ/M-S-K)
C       VISG   :VISCOSITY OF THE SPECIES  (KG/M-S)
C       AM   :MOLECULAR WEIGHTS  (-)
C       S   :SUTHERLAND CONSTANTS (-)
C       T   :TEMPERATURE (K)
C       CONGAS   :MIXTURE THERMAL CONDUCTIVITY (KJ/M-S-K)
C
        DIMENSION Y(N),CONG(N),VISG(N),AM(N),S(N)
C
        SUM=0.
        DO 10 I=1,N
        SUM1=0.
        DO 20 J=1,N
        SIJ=DSQRT(S(I)*S(J))
        RU=.25*(1.+(VISG(I)/VISG(J)*(AM(J)/AM(I))**.75*(T+S(I))/
     * (T+S(J)))**.5)**2.*(T+SIJ)/(T+S(I))
20      SUM1=SUM1+Y(J)*RU
10      SUM=SUM+Y(I)*CONG(I)/SUM1
C
        CONGAS=SUM
        RETURN
        END
C
C       ------------------------------------------------------
C
        SUBROUTINE CONDUC(Y,T,CONGAS)
C
C       CALCULATES THE THERMAL CONDUCTIVITY OF METHANOL SYNTHESIS
C       MIXTURE
C
C       Y   :MOLE FRACTIONS
C       T   :TEMPERATURE (K)
C       CONMIX   :MIXTURE THERMAL CONDUCTIVITY (KJ/M-S-K)
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DIMENSION Y(7),CONG(7),VISG(7),AM(7),S(7)
C
        DATA CONG/3.799,4.242,1.326,.0855,.0995,3.988,.2496/
        DATA VISG/3.84,2.995,2.698,1.572,1.642,4.05,2.669/
        DATA AM/28.,44.,2.,32.,28.,16.,18./
        DATA S/122.6,292.1,30.6,506.7,116.1,167.6,559.8/
C
        DO 10 I=1,7
```

```
10      CONG(I)=4.188D-05*CONG(I)
C
        CALL CONMIX(7,Y,CONG,VISG,AM,S,T,CONGAS)
C
C.
        RETURN
        END
C
C       ------------------------------------------------------------
C
        SUBROUTINE FUGA(T,P,Y,FCOEF,FUGAG)
C
C       FUGACITIES FOR METHANOL SYNTHESIS MIXTURE
C
C       P   :PRESSURE (ATM)
C       T   :TEMPERATURE (K)
C       PC  :CRITICAL PRESSURE (ATM)
C       PR  :REDUCED PRESSURE (-)
C       TC  :CRITICAL TEMPERATURE (K)
C       TR  :REDUCED TEMPERATURE (-)
C       FUGAG  :FUGACITIES (ATM)
C       FCOEF  :FUGACITY COEFFICIENTS (-)
C       Y   :MOLE FRACTIONS (-)
C
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION PC(7),Y(I),TC(7),PR(7),TR(7),FCOEF(7),FUGAG(7)
        DATA PC/34.5,72.8,12.8,79.9,217.6,33.5,45.4/
        DATA TC/132.9,304.2,33.2,512.6,647.3,126.2,190.6/
        DO 10 I=1,7
        PR(I)=P/PC(I)
10      TR(I)=T/TC(I)
C
        CALL FUCOEF(7,PR,TR,FCOEF)
        DO 20 I=1,7
20      FUGAG(I)=Y(I)*P*FCOEF(I)
        RETURN
        END
C
C       ------------------------------------------------------------
C
        SUBROUTINE FUCOEF(N,PR,TR,FCOEF)
C
C       FUGACITY COEFFICIENTS
C
C       N   :NO OF COMPONENTS
C       PR  :REDUCED PRESSURE (-)
C       TR  :REDUCED TEMPERATURE (-)
C       FCOEF  :FUGACITY COEFFICIENTS (-)
C
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION PR(N),TR(N),FCOEF(N)
C
        DO 10 I=1,N
        A=(1.01981D-02/TR(I)-2.142D-02/TR(I)**2.-
     * 3.2548D-02/TR(I)**4.)*PR(I)
        B=(1.8498D-03/TR(I)**3.-2.1511D-03/TR(I)**5.+
     * .9144D-02/TR(I)**7.)*PR(I)**2.
        C=(-.4172D-04/TR(I)**3.+1.5469D-04/TR(I)**5.-
     * .5191D-04/TR(I)**7.)*PR(I)**3.
        D=(.42458D-05/TR(I)**3.-.28052D-05/TR(I)**5.+
```

```
     *  82075D-05/TR(I)**7.)*PR(I)**4.
        F=(A+B+C+D)/.08206
        WRITE(20,*) '---------',A,B,C,D,F
        WRITE(20,*)TR(I),PR(I)
        FCOEF(I)=DEXP(F)
10      CONTINUE
        RETURN
        END
C
C       ------------------------------------------------------------
C
        SUBROUTINE RHEAT(T,HEATR)
C
C       PROVIDES HEAT OF REACTION DATA FOR METHANOL
C       SYNTHESIS.
C
C       T   :TEMPERATURE , K
C       HEATR   :HEAT OF REACTION , KJ/KMOL
C                1:METHANOL FORMATION
C                2:CO2 REACTION
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DIMENSION HEATR(2),Y(7),CONT(2)
C
        CALL CPGAS(1,Y,T,HEATCP,CPMASS,CONT)
C
        HEATR(1)=-90840.+CONT(1)
        HEATR(2)=41270.+CONT(2)
        RETURN
        END
C
C       ------------------------------------------------------------------
C
C
        SUBROUTINE INTER2(TO,UO,CGO,TEST,X1,X2,T,CG,U)
C
C       CALCULATES THE CONCENTRATIONS,TEMPERATURE AND GAS VELOCITY
C       FOR A GIVEN SET OF CONVERSIONS
C
C       TO   :INLET TEMPERATURE FOR THE CATALYST BED (K)
C       UO   :INLET SUPERFICIAL GAS VELOCITY (M/S)
C       CGO   :INLET GAS CONCENTRATIONS (KMOL/M**3)
C       P   :PRESSURE (ATM)
C       TEST   :ESTIMATED TEMPERATURE (K)
C       X1   :CONVERSION FOR METHANOL SYNTHESIS REACTION
C       X2   :CONVERSION FOR CO2 REACTION
C       T   :TEMPERATURE (K)
C       CG   :CONCENTRATION (KMOL/M**3)
C       U   :GAS VELOCITY (M/S)
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DIMENSION CGO(7),CG(7),YO(7),Y(7),HEATR(2),CONT(2)
C
        R=0.082
C
        CTOTO=0
C
        DO 10 I=1,7
```

```
10      CTOTO=CTOTO+CGO(I)
C
        DO 15 I=1,7
15      YO(I)=CGO(I)/CTOTO
C
        DENO=1./CTOTO
        CALL CPGAS(0,YO,TO,HEATCP,CPMASS,CONT)
        CPO=HEATCP
C
        T1=TEST
C
30      TET1=(T1-TO)/TO
        BET=(1.+TET1)*(1.-2.*YO(1)*X1)
C
        CG(1)=CGO(1)=(1.-X1+X2)
        CG(2)=CGO(2)-CGO(1)*X2
        CG(3)=CGO(3)-CGO(1)=(2.*X1+X2)
        CG(4)=CGO(4)+CGO(1)*X1
        CG(5)=CGO(5)+CGO(1)*X2
        CG(6)=CGO(6)
        CG(7)=CGO(7)
C
        CTOT=0.
        DO 20 I=1,7
        CG(I)=CG(I)/BET
20      CTOT=CTOT+CG(I)
C
        DO 40 I=1,7
40      Y(I)=CG(I)/CTOT
C
        DENG=1./CTOT
        CALL CPGAS(0,Y,T1,HEATCP,CPMASS,CONT)
        CP=HEATCP
        CALL RHEAT(T1,HEATR)
        TET=CPO*DENO/BET/CP/DENG-1.-(HEATR(1)*X1+HEATR(2)*X2)/BET/
     * CP/TO*CGO(1)/DENG
C
        T=TO*(1.+TET)
        IF(DABS((T1-T)/T).LE.0.01) GO TO 50
        T1=(T1+T)/2.
        GO TO 30
C
50      CONTINUE
        U=BET*UO
        RETURN
        END
C
C       ------------------------------------------------------------
C
C
        SUBROUTINE DEN(P,T,Y,DENGAS)
C
C       CALCULATES THE GAS DENSITY OF METHANOL SYNTHESIS MIXTURE
C
C       P   :PRESSURE (ATM)
C       T   :TEMPERATURE (K)
C       Y   :MOL FRACTION
C       DENGAS   :DENSITY (KG/M**3)
C
        IMPLICIT REAL*8(A-H,O-Z)
```

```
C
      DIMENSION AM(7),Y(7)
      DATA AM/28.,44.,2.,32.,18.,28.,16./
C
      R=.082
      AMEAN=0.
      DO 10 I=1,7
10    AMEAN=AMEAN+Y(I)*AM(I)
C
      DENGAS=P*AMEAN/R/T
      RETURN
      END
C
C
C
      SUBROUTINE INTBED(TQ,YQ,UQ,TN,YN,UN,TNP,YNP,UNP)
C
C     CALCULATES TEMPERATURE,COMPOSITION AND GAS FLOW RATE
C     FOR THE FEED TO NEXT BED IN A METHANOL SYNTHESIS REACTOR
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION YQ(7),YN(7),YNP(7),CONT(2)
C
      TNP1=TQ
      CALL CPGAS(0,YQ,TQ,CPQ,CPMASS,CONT)
      CALL CPGAS(0,YN,TN,CPN,CPMASS,CONT)
      CPNP=CPN
C
10    UNP=(CPQ*UQ+CPN*UN)/CPNP
      TNP=UNP/(UQ/TQ+UN/TN)
      DO 20 I=1,7
20    YNP(I)=TNP/UNP*(UQ*YQ(I)/TQ+UN*YN(I)/TN)
      IF(DABS((TNP-TNP1)/TNP).LT.0.001) GO TO 30
      TNP1=TNP
      CALL CPGAS(0,YNP,TNP,CPNP,CPMASS,CONT)
      GO TO 10
30    RETURN
      END
C
```

I-C-5 Sample Output from Fixed Bed Reactor Simulation

****

SIMULATION OF A FIXED-BED ADIABATIC REACTOR

FOR

METHANOL SYNTHESIS

****

SUMMARY OF THE INPUT DATA

********** FEED CHARACTERISTICS **********

INLET TEMPERATURE = 470.00000 Deg. K

PRESSURE = 80.00000 atm

GAS COMPOSITION

Component	Mole fraction
CO	0.25000
CO2	0.10000
H2	0.50000
CH3OH	0.00000
H2O	0.00000
N2	0.01000
CH4	0.14000

VOLUMETRIC GAS VELOCITY = 0.58437D+02 N.m**3/Sec

SUPERFICIAL GAS VELOCITY = 0.40000 m/sec

******** REACTOR CHARACTERISTICS ********

DIAMETER = 2.00000 m

LENGTH = 0.80000 m
BED VOID FRACTION = 0.40000
BED NUMBER = 1

******** CATALYST CHARACTERISTICS *********

CATALYST DIAMETER = 0.00500 m
DENSITY = 1980.00000(Kg/m**3)
POROSITY = 0.30000
TORTOUSITY = 7.00000
THERMAL CONDUCTIVITY = 0.00418 KJ/m-sec-K

TEMPERATURE = 450.0000

PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
0.000E+00	0.208E+00	0.102E+00	0.461E+00	0.740E-01	0.555E-03	0.000E+00	0.505E-27	0.450E+03
0.100E+00	0.208E+00	0.102E+00	0.461E+00	0.732E-01	0.554E-03	-0.555E-01	-0.166E-03	0.450E+03
0.200E+00	0.209E+00	0.102E+00	0.462E+00	0.710E-01	0.548E-03	-0.111E+00	-0.352E-03	0.450E+03
0.300E+00	0.212E+00	0.102E+00	0.464E+00	0.674E-01	0.539E-03	-0.168E+00	-0.583E-03	0.450E+03
0.400E+00	0.215E+00	0.102E+00	0.467E+00	0.622E-01	0.524E-03	-0.224E+00	-0.898E-03	0.450E+03
0.500E+00	0.218E+00	0.102E+00	0.471E+00	0.556E-01	0.502E-03	-0.282E+00	-0.136E-02	0.450E+03
0.600E+00	0.223E+00	0.101E+00	0.475E+00	0.474E-01	0.469E-03	-0.341E+00	-0.208E-02	0.450E+03
0.700E+00	0.229E+00	0.101E+00	0.480E+00	0.378E-01	0.418E-03	-0.401E+00	-0.326E-02	0.450E+03
0.800E+00	0.235E+00	0.101E+00	0.486E+00	0.267E-01	0.339E-03	-0.463E+00	-0.525E-02	0.450E+03
0.900E+00	0.242E+00	0.100E+00	0.492E+00	0.142E-01	0.213E-03	-0.527E+00	-0.870E-02	0.450E+03
0.100E+01	0.250E+00	0.100E+00	0.500E+00	0.968E-04	0.203E-05	-0.592E+00	-0.148E-01	0.450E+03

EFF RATE 1 = .2984E-09
EFF RATE 2 = .8227E-11
EFF1 = .9585E+00
EFF2 = .4015E+00

TEMPERATURE = 455.0000
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
0.000E+00	0.200E+00	0.103E+00	0.453E+00	0.880E-01	0.639E-03	0.000E+00	0.000E+00	0.455E+03
0.100E+00	0.200E+00	0.103E+00	0.454E+00	0.872E-01	0.637E-03	-0.653E-01	-0.206E-03	0.455E+03
0.200E+00	0.202E+00	0.103E+00	0.455E+00	0.845E-01	0.630E-03	-0.131E+00	-0.434E-03	0.455E+03
0.300E+00	0.204E+00	0.102E+00	0.458E+00	0.802E-01	0.618E-03	-0.197E+00	-0.710E-03	0.455E+03
0.400E+00	0.208E+00	0.102E+00	0.461E+00	0.740E-01	0.600E-03	-0.264E+00	-0.108E-02	0.455E+03
0.500E+00	0.212E+00	0.102E+00	0.465E+00	0.661E-01	0.573E-03	-0.333E+00	-0.161E-02	0.455E+03
0.600E+00	0.218E+00	0.102E+00	0.470E+00	0.565E-01	0.534E-03	-0.403E+00	-0.242E-02	0.455E+03
0.700E+00	0.224E+00	0.101E+00	0.476E+00	0.450E-01	0.475E-03	-0.475E+00	-0.374E-02	0.455E+03
0.800E+00	0.232E+00	0.101E+00	0.483E+00	0.318E-01	0.385E-03	-0.549E+00	-0.597E-02	0.455E+03
0.900E+00	0.240E+00	0.100E+00	0.491E+00	0.169E-01	0.240E-03	-0.626E+00	-0.984E-02	0.455E+03

0.100E+01	0.250E+00	0.100E+00	0.500E+00	0.115E-03	0.229E-05	-0.708E+00	-0.167E-01	0.455E+03

EFF RATE 1 = .3553E-09
EFF RATE 2 = .9295E-11
EFF1 = .9507E+00
EFF2 = .4009E+00

TEMPERATURE = 460.0000
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
0.000E+00	0.190E+00	0.103E+00	0.445E+00	0.104E+00	0.735E-03	0.000E+00	0.000E+00	0.460E+03
0.100E+00	0.191E+00	0.103E+00	0.445E+00	0.103E+00	0.733E-03	-0.762E-01	-0.259E-03	0.460E+03
0.200E+00	0.193E+00	0.103E+00	0.447E+00	0.100E+00	0.724E-03	-0.153E+00	-0.539E-03	0.460E+03
0.300E+00	0.196E+00	0.103E+00	0.450E+00	0.949E-01	0.710E-03	-0.230E+00	-0.872E-03	0.460E+03
0.400E+00	0.200E+00	0.103E+00	0.454E+00	0.876E-01	0.687E-03	-0.309E+00	-0.130E-02	0.460E+03
0.500E+00	0.205E+00	0.102E+00	0.459E+00	0.783E-01	0.655E-03	-0.390E+00	-0.191E-02	0.460E+03
0.600E+00	0.212E+00	0.102E+00	0.465E+00	0.668E-01	0.608E-03	-0.473E+00	-0.282E-02	0.460E+03
0.700E+00	0.220E+00	0.101E+00	0.472E+00	0.533E-01	0.539E-03	-0.558E+00	-0.430E-02	0.460E+03
0.800E+00	0.229E+00	0.101E+00	0.480E+00	0.377E-01	0.435E-03	-0.647E+00	-0.678E-02	0.460E+03
0.900E+00	0.239E+00	0.100E+00	0.489E+00	0.200E-01	0.271E-03	-0.739E+00	-0.111E-01	0.460E+03
0.100E+01	0.250E+00	0.100E+00	0.500E+00	0.137E-03	0.258E-05	-0.836E+00	-0.189E-01	0.460E+03

EFF RATE 1 = .4209E-09
EFF RATE 2 = .1048E-10
EFF1 = .9417E+00
EFF2 = .4003E+00

TEMPERATURE = 465.0000
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
0.000E+00	0.180E+00	0.104E+00	0.435E+00	0.123E+00	0.849E-03	0.000E+00	0.000E+00	0.465E+03
0.100E+00	0.181E+00	0.104E+00	0.436E+00	0.121E+00	0.845E-03	-0.882E-01	-0.328E-03	0.465E+03
0.200E+00	0.183E+00	0.104E+00	0.438E+00	0.118E+00	0.834E-03	-0.177E+00	-0.678E-03	0.465E+03
0.300E+00	0.186E+00	0.103E+00	0.441E+00	0.112E+00	0.816E-03	-0.267E+00	-0.108E-02	0.465E+03

0.400E+00	0.191E+00	0.103E+00	0.445E+00	0.103E+00	0.788E-03	-0.359E+00	-0.159E-02	0.465E+03
0.500E+00	0.197E+00	0.103E+00	0.451E+00	0.922E-01	0.748E-03	-0.453E+00	-0.228E-02	0.465E+03
0.600E+00	0.205E+00	0.102E+00	0.458E+00	0.787E-01	0.692E-03	-0.551E+00	-0.331E-02	0.465E+03
0.700E+00	0.214E+00	0.102E+00	0.467E+00	0.628E-01	0.612E-03	-0.652E+00	-0.495E-02	0.465E+03
0.800E+00	0.225E+00	0.101E+00	0.476E+00	0.444E-01	0.492E-03	-0.757E+00	-0.770E-02	0.465E+03
0.900E+00	0.237E+00	0.101E+00	0.487E+00	0.235E-01	0.306E-03	-0.868E+00	-0.125E-01	0.465E+03
0.100E+01	0.250E+00	0.100E+00	0.500E+00	0.161E-03	0.290E-05	-0.985E+00	-0.212E-01	0.465E+03

EFF RATE 1 = .4961E-09
EFF RATE 2 = .1178E-10
EFF1 = .9316E+00
EFF2 = .3999E+00

TEMPERATURE = 469.6773
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
**********	**********	**********	**********	**********	**********	**********	**********	**********
0.000E+00	0.169E+00	0.105E+00	0.425E+00	0.142E+00	0.972E-03	0.000E+00	0.000E+00	0.470E+03
0.100E+00	0.170E+00	0.105E+00	0.426E+00	0.140E+00	0.968E-03	-0.999E-01	-0.411E-03	0.470E+03
0.200E+00	0.172E+00	0.104E+00	0.428E+00	0.136E+00	0.954E-03	-0.201E+00	-0.844E-03	0.470E+03
0.300E+00	0.176E+00	0.104E+00	0.432E+00	0.129E+00	0.931E-03	-0.303E+00	-0.133E-02	0.470E+03
0.400E+00	0.182E+00	0.104E+00	0.437E+00	0.119E+00	0.897E-03	-0.408E+00	-0.191E-02	0.470E+03
0.500E+00	0.189E+00	0.103E+00	0.443E+00	0.107E+00	0.849E-03	-0.516E+00	-0.269E-02	0.470E+03
0.600E+00	0.198E+00	0.103E+00	0.451E+00	0.912E-01	0.783E-03	-0.628E+00	-0.382E-02	0.470E+03
0.700E+00	0.209E+00	0.102E+00	0.461E+00	0.729E-01	0.690E-03	-0.745E+00	-0.560E-02	0.470E+03
0.800E+00	0.221E+00	0.101E+00	0.472E+00	0.517E-01	0.554E-03	-0.868E+00	-0.857E-02	0.470E+03
0.900E+00	0.234E+00	0.101E+00	0.485E+00	0.277E-01	0.348E-03	-0.998E+00	-0.138E-01	0.470E+03
0.100E+01	0.250E+00	0.100E+00	0.499E+00	0.704E-03	0.149E-04	-0.114E+01	-0.232E-01	0.470E+03

EFF RATE 1 = .5727E-09
EFF RATE 2 = .1291E-10
EFF1 = .9214E+00
EFF2 = .4010E+00

TEMPERATURE = 477.3469

PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
0.000E+00	0.150E+00	0.106E+00	0.408E+00	0.174E+00	0.121E-02	0.000E+00	0.000E+00	0.478E+03
0.100E+00	0.151E+00	0.106E+00	0.408E+00	0.173E+00	0.121E-02	-0.119E+00	-0.600E-03	0.478E+03
0.200E+00	0.154E+00	0.105E+00	0.411E+00	0.167E+00	0.119E-02	-0.240E+00	-0.122E-02	0.478E+03
0.300E+00	0.159E+00	0.105E+00	0.416E+00	0.159E+00	0.115E-02	-0.362E+00	-0.188E-02	0.478E+03
0.400E+00	0.166E+00	0.105E+00	0.422E+00	0.147E+00	0.110E-02	-0.489E+00	-0.264E-02	0.478E+03
0.500E+00	0.175E+00	0.104E+00	0.430E+00	0.131E+00	0.104E-02	-0.620E+00	-0.359E-02	0.478E+03
0.600E+00	0.186E+00	0.104E+00	0.440E+00	0.112E+00	0.949E-03	-0.758E+00	-0.491E-02	0.478E+03
0.700E+00	0.199E+00	0.103E+00	0.452E+00	0.900E-01	0.830E-03	-0.903E+00	-0.695E-02	0.477E+03
0.800E+00	0.214E+00	0.102E+00	0.466E+00	0.640E-01	0.663E-03	-0.106E+01	-0.103E-01	0.477E+03
0.900E+00	0.231E+00	0.101E+00	0.481E+00	0.344E-01	0.415E-03	-0.122E+01	-0.162E-01	0.477E+03
0.100E+01	0.249E+00	0.100E+00	0.499E+00	0.128E-02	0.271E-04	-0.140E+01	-0.269E-01	0.477E+03

EFF RATE 1 = .7258E-09
EFF RATE 2 = .1538E-10
EFF1 = .9038E+00
EFF2 = .4058E+00

TEMPERATURE = 474.4258
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
0.000E+00	0.157E+00	0.105E+00	0.414E+00	0.162E+00	0.112E-02	0.000E+00	0.000E+00	0.475E+03
0.100E+00	0.158E+00	0.105E+00	0.415E+00	0.160E+00	0.111E-02	-0.112E+00	-0.519E-03	0.475E+03
0.200E+00	0.161E+00	0.105E+00	0.417E+00	0.156E+00	0.109E-02	-0.224E+00	-0.106E-02	0.475E+03
0.300E+00	0.165E+00	0.105E+00	0.421E+00	0.148E+00	0.107E-02	-0.339E+00	-0.164E-02	0.475E+03
0.400E+00	0.172E+00	0.105E+00	0.427E+00	0.137E+00	0.102E-02	-0.457E+00	-0.232E-02	0.475E+03
0.500E+00	0.180E+00	0.104E+00	0.435E+00	0.122E+00	0.965E-03	-0.579E+00	-0.319E-02	0.475E+03
0.600E+00	0.190E+00	0.103E+00	0.444E+00	0.105E+00	0.887E-03	-0.707E+00	-0.442E-02	0.475E+03
0.700E+00	0.202E+00	0.103E+00	0.455E+00	0.840E-01	0.780E-03	-0.841E+00	-0.632E-02	0.475E+03
0.800E+00	0.216E+00	0.102E+00	0.467E+00	0.599E-01	0.628E-03	-0.983E+00	-0.947E-02	0.475E+03
0.900E+00	0.232E+00	0.101E+00	0.482E+00	0.326E-01	0.400E-03	-0.113E+01	-0.150E-01	0.474E+03

0.100E+01	0.240E+00	0.100E+00	0.498E+00	0.192E-02	0.407E-04	-0.130E+01	-0.250E-01	0.474E+03

EFF RATE 1 = .6559E-09
EFF RATE 2 = .1394E-10
EFF1 = .9107E+00
EFF2 = .4047E+00

TEMPERATURE = 482.3610
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
**********	**********	**********	**********	**********	**********	**********	**********	**********
0.000E+00	0.136E+00	0.107E+00	0.394E+00	0.199E+00	0.141E-02	0.000E+00	0.000E+00	0.483E+03
0.100E+00	0.137E+00	0.107E+00	0.395E+00	0.197E+00	0.140E-02	-0.132E+00	-0.776E-03	0.483E+03
0.200E+00	0.140E+00	0.106E+00	0.398E+00	0.191E+00	0.138E-02	-0.266E+00	-0.156E-02	0.483E+03
0.300E+00	0.146E+00	0.106E+00	0.403E+00	0.181E+00	0.133E-02	-0.404E+00	-0.238E-02	0.483E+03
0.400E+00	0.154E+00	0.106E+00	0.410E+00	0.168E+00	0.127E-02	-0.545E+00	-0.328E-02	0.483E+03
0.500E+00	0.164E+00	0.105E+00	0.420E+00	0.150E+00	0.119E-02	-0.694E+00	-0.435E-02	0.483E+03
0.600E+00	0.176E+00	0.104E+00	0.431E+00	0.129E+00	0.108E-02	-0.850E+00	-0.580E-02	0.483E+03
0.700E+00	0.191E+00	0.103E+00	0.444E+00	0.103E+00	0.943E-03	-0.102E+01	-0.797E-02	0.483E+03
0.800E+00	0.208E+00	0.102E+00	0.460E+00	0.739E-01	0.752E-03	-0.120E+01	-0.115E-01	0.482E+03
0.900E+00	0.227E+00	0.101E+00	0.477E+00	0.403E-01	0.477E-03	-0.139E+01	-0.178E-01	0.482E+03
0.100E+01	0.249E+00	0.100E+00	0.497E+00	0.258E-02	0.541E-04	-0.160E+01	-0.292E-01	0.482E+03

EFF RATE 1 = .8312E-09
EFF RATE 2 = .1673E-10
EFF1 = .8909E+00
EFF2 = .4101E+00

TEMPERATURE = 479.7400
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
**********	**********	**********	**********	**********	**********	**********	**********	**********
0.000E+00	0.143E+00	0.107E+00	0.400E+00	0.187E+00	0.131E-02	0.000E+00	0.000E+00	0.480E+03
0.100E+00	0.144E+00	0.106E+00	0.401E+00	0.185E+00	0.130E-02	-0.126E+00	-0.681E-03	0.480E+03
0.200E+00	0.147E+00	0.106E+00	0.404E+00	0.180E+00	0.128E-02	-0.252E+00	-0.137E-02	0.480E+03
0.300E+00	0.152E+00	0.106E+00	0.409E+00	0.171E+00	0.124E-02	-0.382E+00	-0.210E-02	0.480E+03

0.400E+00	0.159E+00	0.105E+00	0.415E+00	0.158E+00	0.119E-02	-0.516E+00	-0.292E-02	0.480E+03
0.500E+00	0.189E+00	0.105E+00	0.424E+00	0.142E+00	0.111E-02	-0.655E+00	-0.391E-02	0.480E+03
0.600E+00	0.181E+00	0.104E+00	0.434E+00	0.121E+00	0.102E-02	-0.802E+00	-0.526E-02	0.480E+03
0.700E+00	0.194E+00	0.103E+00	0.447E+00	0.976E-01	0.892E-03	-0.957E+00	-0.731E-02	0.480E+03
0.800E+00	0.210E+00	0.102E+00	0.462E+00	0.700E-01	0.718E-03	-0.112E+01	-0.107E-01	0.480E+03
0.900E+00	0.228E+00	0.101E+00	0.478E+00	0.386E-01	0.463E-03	-0.130E+01	-0.165E-01	0.480E+03
0.100E+01	0.248E+00	0.101E+00	0.497E+00	0.333E-02	0.690E-04	-0.149E+01	-0.273E-01	0.480E+03

EFF RATE 1 = .7595E-09
EFF RATE 2 = .1527E-10
EFF1 = .8977E+00
EFF2 = .4092E+00

TEMPERATURE = 488.0361
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
**********	**********	**********	**********	**********	**********	**********	**********	**********
0.000E+00	0.118E+00	0.108E+00	0.378E+00	0.229E+00	0.168E-02	0.000E+00	0.000E+00	0.488E+03
0.100E+00	0.120E+00	0.108E+00	0.379E+00	0.227E+00	0.167E-02	-0.148E+00	-0.105E-02	0.488E+03
0.200E+00	0.123E+00	0.108E+00	0.382E+00	0.220E+00	0.163E-02	-0.298E+00	-0.209E-02	0.488E+03
0.300E+00	0.130E+00	0.107E+00	0.388E+00	0.209E+00	0.158E-02	-0.452E+00	-0.314E-02	0.488E+03
0.400E+00	0.139E+00	0.107E+00	0.396E+00	0.194E+00	0.150E-02	-0.612E+00	-0.423E-02	0.488E+03
0.500E+00	0.150E+00	0.106E+00	0.407E+00	0.174E+00	0.139E-02	-0.781E+00	-0.547E-02	0.488E+03
0.600E+00	0.165E+00	0.105E+00	0.420E+00	0.149E+00	0.126E-02	-0.961E+00	-0.707E-02	0.488E+03
0.700E+00	0.181E+00	0.104E+00	0.435E+00	0.120E+00	0.109E-02	-0.115E+01	-0.939E-02	0.488E+03
0.800E+00	0.201E+00	0.103E+00	0.453E+00	0.861E-01	0.865E-03	-0.136E+01	-0.132E-01	0.488E+03
0.900E+00	0.223E+00	0.102E+00	0.473E+00	0.475E-01	0.553E-03	-0.159E+01	-0.198E-01	0.488E+03
0.100E+01	0.248E+00	0.101E+00	0.496E+00	0.410E-02	0.838E-04	-0.184E+01	-0.321E-01	0.488E+03

EFF RATE 1 = .9635E-09
EFF RATE 2 = .1849E-10
EFF1 = .8750E+00
EFF2 = .4154E+00

TEMPERATURE = 485.7808

PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
0.000E+00	0.125E+00	0.108E+00	0.383E+00	0.218E+00	0.158E-02	0.000E+00	0.000E+00	0.486E+03
0.100E+00	0.126E+00	0.108E+00	0.384E+00	0.216E+00	0.157E-02	-0.142E+00	-0.937E-03	0.486E+03
0.200E+00	0.129E+00	0.108E+00	0.388E+00	0.210E+00	0.154E-02	-0.285E+00	-0.187E-02	0.486E+03
0.300E+00	0.136E+00	0.107E+00	0.393E+00	0.199E+00	0.148E-02	-0.433E+00	-0.282E-02	0.486E+03
0.400E+00	0.144E+00	0.107E+00	0.401E+00	0.184E+00	0.141E-02	-0.586E+00	-0.383E-02	0.486E+03
0.500E+00	0.155E+00	0.106E+00	0.411E+00	0.165E+00	0.132E-02	-0.746E+00	-0.499E-02	0.486E+03
0.600E+00	0.168E+00	0.105E+00	0.423E+00	0.142E+00	0.119E-02	-0.917E+00	-0.650E-02	0.486E+03
0.700E+00	0.184E+00	0.104E+00	0.437E+00	0.115E+00	0.104E-02	-0.110E+01	-0.871E-02	0.486E+03
0.800E+00	0.203E+00	0.103E+00	0.454E+00	0.825E-01	0.832E-03	-0.130E+01	-0.123E-01	0.486E+03
0.900E+00	0.224E+00	0.102E+00	0.473E+00	0.460E-01	0.541E-03	-0.151E+01	-0.186E-01	0.486E+03
0.100E+01	0.248E+00	0.101E+00	0.495E+00	0.498E-02	0.101E-03	-0.174E+01	-0.303E-01	0.486E+03

EFF RATE 1 = .8912E-09
EFF RATE 2 = .1701E-10
EFF1 = .8814E+00
EFF2 = .4148E+00

TEMPERATURE = 494.5298
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
0.000E+00	0.966E-01	0.109E+00	0.357E+00	0.266E+00	0.207E-02	0.000E+00	0.000E+00	0.495E+03
0.100E+00	0.981E-01	0.109E+00	0.359E+00	0.264E+00	0.206E-02	-0.165E+00	-0.150E-02	0.495E+03
0.200E+00	0.102E+00	0.109E+00	0.363E+00	0.256E+00	0.201E-02	-0.333E+00	-0.296E-02	0.495E+03
0.300E+00	0.110E+00	0.109E+00	0.369E+00	0.244E+00	0.192E-02	-0.507E+00	-0.437E-02	0.495E+03
0.400E+00	0.120E+00	0.108E+00	0.379E+00	0.226E+00	0.181E-02	-0.690E+00	-0.575E-02	0.495E+03
0.500E+00	0.133E+00	0.107E+00	0.391E+00	0.203E+00	0.167E-02	-0.884E+00	-0.722E-02	0.495E+03
0.600E+00	0.150E+00	0.106E+00	0.406E+00	0.174E+00	0.149E-02	-0.109E+01	-0.898E-02	0.495E+03
0.700E+00	0.169E+00	0.105E+00	0.423E+00	0.141E+00	0.128E-02	-0.132E+01	-0.115E-01	0.495E+03
0.800E+00	0.192E+00	0.104E+00	0.444E+00	0.101E+00	0.101E-02	-0.157E+01	-0.155E-01	0.495E+03
0.900E+00	0.218E+00	0.102E+00	0.468E+00	0.565E-01	0.648E-03	-0.185E+01	-0.227E-01	0.495E+03

0.100E+01	0.247E+00	0.101E+00	0.494E+00	0.590E-02	0.117E-03	-0.215E+01	-0.361E-01	0.495E+03

EFF RATE 1 = .1132E-08
EFF RATE 2 = .2081E-10
EFF1 = .8550E+00
EFF2 = .4222E+00

TEMPERATURE = 492.7230
PRESSURE = 80.0000

X	CO	CO2	H2	CH3OH	H2O	SLOPE 1	SLOPE 2	TEMPERATURE(K)
0.000E+00	0.102E+00	0.109E+00	0.362E+00	0.257E+00	0.197E-02	0.000E+00	0.000E+00	0.493E+03
0.100E+00	0.103E+00	0.109E+00	0.363E+00	0.254E+00	0.195E-02	-0.161E+00	-0.137E-02	0.493E+03
0.200E+00	0.107E+00	0.109E+00	0.367E+00	0.247E+00	0.191E-02	-0.324E+00	-0.271E-02	0.493E+03
0.300E+00	0.115E+00	0.109E+00	0.374E+00	0.235E+00	0.183E-02	-0.492E+00	-0.401E-02	0.493E+03
0.400E+00	0.124E+00	0.108E+00	0.382E+00	0.218E+00	0.173E-02	-0.668E+00	-0.531E-02	0.493E+03
0.500E+00	0.137E+00	0.107E+00	0.394E+00	0.196E+00	0.160E-02	-0.855E+00	-0.670E-02	0.493E+03
0.600E+00	0.153E+00	0.106E+00	0.408E+00	0.169E+00	0.144E-02	-0.106E+01	-0.839E-02	0.493E+03
0.700E+00	0.172E+00	0.105E+00	0.425E+00	0.136E+00	0.124E-02	-0.127E+01	-0.108E-01	0.493E+03
0.800E+00	0.194E+00	0.104E+00	0.445E+00	0.984E-01	0.983E-03	-0.151E+01	-0.147E-01	0.493E+03
0.900E+00	0.219E+00	0.103E+00	0.468E+00	0.554E-01	0.640E-03	-0.177E+01	-0.215E-01	0.493E+03
0.100E+01	0.247E+00	0.101E+00	0.493E+00	0.694E-02	0.136E-03	-0.206E+01	-0.343E-01	0.493E+03

EFF RATE 1 = .1062E-08
EFF RATE 2 = .1936E-10
EFF1 = .8608E+00
EFF2 = .4220E+00

SUMMARY OF THE OUTPUT DATA

OUTPUT TEMPERATURE = 496.60337 Deg. K

PRESSURE = 80.00000 atm

GAS COMPOSITION

Component	Mole fraction
CO	0.24636
CO2	0.10137
H2	0.49227

CH3OH	0.00759
H2O	0.00015
N2	0.01015
CH4	0.14212

CONVERSION 1 = .29297E-01
CONVERSION 2 = .00000E+00
OVERALL CONV. = .29887E-01

VOLUMETRIC GAS VELOCITY = 0.61196D+02 N.m**3/Sec

SPACE VELOCITY = 0.70458E+02 Nm**3/kg-hr
SPACE TIME YIELD = 0.52644E+00 NM**3 Gas Converted/kg-hr

LENGTH DIMENSIONLESS	ACTUAL (m)	EFF. RATE 1	EFF. RATE 2
0.10000	0.08000	0.45475E-02	0.10801E-03
0.20000	0.16000	0.52504E-02	0.11834E-03
0.30000	0.24000	0.66534E-02	0.14095E-03
0.40000	0.32000	0.60132E-02	0.12782E-03
0.50000	0.40000	0.76200E-02	0.15337E-03
0.60000	0.48000	0.69622E-02	0.13998E-03
0.70000	0.56000	0.88327E-02	0.16947E-03
0.80000	0.64000	0.81701E-02	0.15598E-03
0.90000	0.72000	0.10381E-01	0.19081E-03
1.00000	0.80000	0.97349E-02	0.17746E-03

LENGTH DIMENSIONLESS	ACTUAL (m)	EFF.FACTOR 1	EFF.FACTOR 2
0.10000	0.08000	0.93160E+00	0.39986E+00
0.20000	0.16000	0.92136E+00	0.40096E+00
0.30000	0.24000	0.90381E+00	0.40575E+00
0.40000	0.32000	0.91074E+00	0.40472E+00
0.50000	0.40000	0.89091E+00	0.41007E+00
0.60000	0.48000	0.89771E+00	0.40924E+00
0.70000	0.56000	0.87497E+00	0.41539E+00
0.80000	0.64000	0.88137E+00	0.41484E+00
0.90000	0.72000	0.85496E+00	0.42219E+00
1.00000	0.80000	0.86057E+00	0.42205E+00

LENGTH		GAS FLOW RATE	
DIMENSIONLESS	ACTUAL (m)	DIMENSIONLESS	ACTUAL (m/s)
0.00000	0.00000	0.10000E+01	0.40000
0.10000	0.08000	0.10002E+01	0.40009
0.20000	0.16000	0.10089E+01	0.40355
0.30000	0.24000	0.10082E+01	0.40329
0.40000	0.32000	0.10168E+01	0.40674
0.50000	0.40000	0.10167E+01	0.40670
0.60000	0.48000	0.10258E+01	0.41031
0.70000	0.56000	0.10263E+01	0.41052
0.80000	0.64000	0.10358E+01	0.41433
0.90000	0.72000	0.10371E+01	0.41483
1.00000	0.80000	0.10472E+01	0.41889

LENGTH		TEMPERATURE	
DIMENSIONLESS	ACTUAL (m)	DIMENSIONLESS	ACTUAL (K)
**********	**********	**********	**********
0.00000	0.00000	0.00000E+00	0.47000E+03
0.10000	0.08000	0.11205E-01	0.47527E+03
0.20000	0.16000	0.41294E-02	0.47194E+03
0.30000	0.24000	0.20437E-01	0.47961E+03
0.40000	0.32000	0.14845E-01	0.47698E+03
0.50000	0.40000	0.31722E-01	0.48491E+03
0.60000	0.48000	0.26894E-01	0.48264E+03
0.70000	0.56000	0.44546E-01	0.49094E+03
0.80000	0.64000	0.40670E-01	0.48911E+03
0.90000	0.72000	0.59295E-01	0.49787E+03
1.00000	0.80000	0.56603E-01	0.49660E+03

LENGTH				
DIMENSIONLESS	ACTUAL (m)	CONVERSION 1	CONVERSION 2	OVERALL CONV.
0.00000	0.00000	0.00000E+00	0.00000E+00	0.00000E+00
0.10000	0.08000	0.19709E-02	0.45847E-04	0.20168E-02
0.20000	0.16000	0.40155E-02	0.92304E-04	0.41078E-02
0.30000	0.24000	0.66029E-02	0.14756E-03	0.67505E-02
0.40000	0.32000	0.89545E-02	0.19792E-03	0.91524E-02
0.50000	0.40000	0.11929E-01	0.25825E-03	0.12187E-01
0.60000	0.48000	0.14664E-01	0.31363E-03	0.14977E-01
0.70000	0.56000	0.18125E-01	0.38056E-03	0.18505E-01
0.80000	0.64000	0.21350E-01	0.44258E-03	0.21792E-01
0.90000	0.72000	0.25434E-01	0.51830E-03	0.25953E-01
1.00000	0.80000	0.29297E-01	0.58930E-03	0.29887E-01

LENGTH		GAS PHASE MOLE FRACTIONS						
DIMENSIONLESS	ACTUAL (m)	CO	CO2	H2	CH3OH	H2O	N2	CH4
**********	**********	**********	**********	**********	**********	**********	**********	**********
0.00000	0.00000	.25000E+00	.10000E+00	.50000E+00	.00000E+00	.00000E+00	.10000E-01	.14000E+00
0.10000	0.08000	.24976E+00	.10009E+00	.49948E+00	.50470E-03	.11473E-04	.10010E-01	.14014E+00
0.20000	0.16000	.24951E+00	.10018E+00	.49895E+00	.10291E-02	.23124E-04	.10021E-01	.14029E+00
0.30000	0.24000	.24919E+00	.10030E+00	.49827E+00	.16933E-02	.37015E-04	.10034E-01	.14047E+00
0.40000	0.32000	.24880E+00	.10041E+00	.49765E+00	.22086E-02	.49708E-04	.10046E-01	.14064E+00
0.50000	0.40000	.24853E+00	.10055E+00	.49687E+00	.30854E-02	.64958E-04	.10061E-01	.14086E+00
0.60000	0.48000	.24819E+00	.10068E+00	.49615E+00	.37726E-02	.78999E-04	.10075E-01	.14106E+00
0.70000	0.56000	.24776E+00	.10084E+00	.49523E+00	.46805E-02	.96027E-04	.10093E-01	.14131E+00
0.80000	0.64000	.24738E+00	.10099E+00	.49438E+00	.55081E-02	.11186E-03	.10110E-01	.14154E+00
0.90000	0.72000	.24684E+00	.10118E+00	.49330E+00	.65735E-02	.13128E-03	.10131E-01	.14184E+00
1.00000	0.80000	.24636E+00	.10137E+00	.49227E+00	.75850E-02	.14956E-03	.10152E-01	.14212E+00

I-C-6 Program Listing - SLURRY DAT

```
C
C
C       THIS IS AN INTERACTIVE PROGRAM THAT RECEIVES THE INPUT
C       DATA FOR THE SIMULATION OF ADIBATIC BUBBLE COLUMN
C       SLURRY REACTOR FOR METHANOL SYNTHESIS.
C       THE DATA ARE THEN STORED IN A FILE NAMED
C       INPUT1.DAT  AND USED IN THE SIMULATOR.
C
C       THE USER CAN GET A COMPLETE LIST OF INPUT DATA
C       FROM THE FILE NAMED  CHECK1.DAT
C
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DIMENSION YF(7),XF(5)
C
        OPEN (UNIT=12,FILE='INPUT1.DAT')
        OPEN (UNIT=13,FILE='CHECK1.DAT')
C
        WRITE(06,10)
10      FORMAT(///,5X,'************************************************',
     * //,9X,'BUBBLE COLUMN SLURRY REACTOR SIMULATION',/,5X,
     * '                    FOR',/,5X,
     * '             METHANOL  SYNTHESIS',//,5X,
     * '************************************************',//)
C
C
        WRITE(06,15)
15      FORMAT(5X,'INSTRUCTIONS',///,5X,
     * 'THIS PROGRAM SIMULATES  A ADIABATIC BUBBLE COLUMN ',/,5X,
     * 'SLURRY REACTOR FOR METHANOL SYNTHESIS. ',/,5X,
     * 'PLUG FLOW AND AXIAL DISPERSION MODEL IS USED FOR GAS',/,5X,
     * 'AND SLURRY PHASES RESPECTIVELY .',/,5X,
     * 'INPUT VARIABLES INCLUDING FEED,REACTOR AND CATALYST',/,5X,
     * 'CHARACTERISTICS ARE PROVIDED BY THE USER VIA THIS',/,5X,
     * 'INTERACTIVE PACKAGE.THE SIMULATOR THEN EVALUATES ',/,5X,
     * 'TEMPERATURE AND CONCENTRATION PROFILES TOGETHER WITH',/,5X,
     * 'CONVERSIONS,AND CATALYST CONCENTRATION ',///,5X,
     * 'TO RUN THE SIMULATOR ,PLEASE ENTER THE FOLLOWING DATA',/,5X,
     * 'IN FREE FORMAT',//)
C
        WRITE(06,20)
        WRITE(13,20)
20      FORMAT(5X,'********** REACTOR CHARACTERISTICS ************',
     * //,5X,'DIAMETER (m) = ? ')
        READ(05,*) DC
        WRITE(12,*) DC
        WRITE(13,*) DC
C
        WRITE(06,30)
        WRITE(13,30)
30      FORMAT(5X,'LENGHT (m) = ?')
        READ(05,*) AL
        WRITE(12,*) AL
        WRITE(13,*) AL
C
        WRITE(06,40)
        WRITE(13,40)
40      FORMAT(/,5X,'******** OPERATING CONDITIONS ************',//,
     *  5X,'PRESSURE (atm) = ?')
```

```
      READ(05,*) P
      WRITE(12,*) P
      WRITE(13,*) P
C
      WRITE(06,50)
      WRITE(13,50)
50    FORMAT(5X,'FEED TEMPERATURE (K) = ?')
      READ(05,*) TF
      WRITE(12,*)TF
      WRITE(13,*) TF
C
      WRITE(06,60)
      WRITE(13,60)
60    FORMAT(5X,'INLET GAS FLOW RATE (Nm**3/sec) = ?')
      READ(05,*) QFG
      WRITE(12,*) QFG
      WRITE(13,*) QFG
C
      WRITE(06,70)
      WRITE(13,70)
70    FORMAT(5X,'SLURRY FLOW RATE (m**3/sec) = ?')
      READ(05,*) QFL
      WRITE(12,*) QFL
      WRITE(13,*) QFL
C
      WRITE(06,80)
      WRITE(13,80)
80    FORMAT(/,5X,'INLET GAS COMPOSITION',/,5X,
     * 'ENTER THE MOLE FRACTIONS. THE SQUENCE IS :',/,5X,
     * '1:CO  2:CO2  3:H2  4:CH3OH  5:H2O  6:N2  7:CH4')
      READ(05,*) (YF(I),I=1,7)
      WRITE(12,*) (YF(I),I=1,7)
      WRITE(13,*) (YF(I),I=1,7)
C
      WRITE(06,90)
      WRITE(13,90)
90    FORMAT(/,5X,'INLET LIQUID COMPOSITION',/,5X,
     * 'ENTER THE MOLE FRACTIONS. THE SQUENCE IS :',/,5X,
     *  '1:CO  2:CO2  3:H2  4:CH3OH  5:H2O')
      READ(05,*) (XF(I),I=1,5)
      WRITE(12,*) (XF(I),I=1,5)
      WRITE(13,*) (XF(I),I=1,5)
C
      WRITE(06,100)
      WRITE(13,100)
100   FORMAT(/,5X,'CATALYST LOADING ',/,5X,
     * 'WEIGHT FRACTION IN SLURRY (kg cat/kg slurry) = ?')
      READ(05,*) WCAT
      WRITE(12,*) WCAT
      WRITE(13,*) WCAT
C
C
      WRITE(06,110)
      WRITE(13,110)
110   FORMAT(5X,'CATALYST DENSITY (kg/m**3) = ?')
      READ(05,*) DENCAT
      WRITE(12,*) DENCAT
      WRITE(13,*) DENCAT
C
      WRITE(06,120)
```

```
      WRITE(13,120)
120   FORMAT(5X,'PARTICLE DIAMETER (m) = ?')
      READ(05,*) DP
      WRITE(12,*) DP
      WRITE(13,*) DP
C
      WRITE(06,130)
      WRITE(13,130)
130   FORMAT(5X,'CATALYST HEAT CAPACITY = ?',/,5X,
     *  'IF NO INFORMATION IS AVAILABLE ENTER ZERO ')
      READ(05,*) CPCAT
      WRITE(12,*) CPCAT
      WRITE(13,*) CPCAT
C
      WRITE(06,140)
140   FORMAT(//,5X,'END OF DATA **********',/,5X,
     * 'INPUT DATA ARE STORED IN THE FILE NAMED  INPUT1.DAT',/,5X,
     * 'PLEASE CHECK YOUR DATA FROM THE FILE NAMED  CHECK1.DAT')
C
      STOP
      END
```

I-C-7 Sample Run Showing Interactive Input

```
**************************************************

    BUBBLE COLUMN SLURRY REACTOR SIMULATION
                    FOR
              METHANOL  SYNTHESIS

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


INSTRUCTIONS


THIS PROGRAM SIMULATES  A ADIABATIC BUBBLE COLUMN
SLURRY REACTOR FOR METHANOL SYNTHESIS.
PLUG FLOW AND AXIAL DISPERSION MODEL IS USED FOR GAS
AND SLURRY PHASES RESPECTIVELY
INPUT VARIABLES INCLUDING FEED,REACTOR AND CATALYST
CHARACTERISTICS ARE PROVIDED BY THE USER VIA THIS
INTERACTIVE PACKAGE.THE SIMULATOR THEN EVALUATES
TEMPERATURE AND CONCENTRATION PROFILES TOGETHER WITH
CONVERSIONS,AND CATALYST CONCENTRATION


TO RUN THE SIMULATOR ,PLEASE ENTER THE FOLLOWING DATA
IN FREE FORMAT


********** REACTOR CHARACTERISTICS **********

DIAMETER (m) = ?
>4.0
LENGHT (m) = ?
>8.0

********* OPERATING CONDITIONS **********

PRESSURE (atm) = ?
>70.
FEED TEMPERATURE (K) = ?
>500.
INLET GAS FLOW RATE (Nm**3/sec) = ?
>48.064
SLURRY FLOW RATE (m**3/sec) = ?
>0.31416

INLET GAS COMPOSITION
ENTER THE MOLE FRACTIONS. THE SQUENCE IS :
1:CO  2:CO2  3:H2  4:CH3OH  5:H2O  6:N2  7:CH4
>0.25 0.1 0.5 0.0 0.0 0.01 0.14

INLET LIQUID COMPOSITION
ENTER THE MOLE FRACTIONS. THE SQUENCE IS :
1:CO  2:CO2  3:H2  4:CH3OH  5:H2O
>0.0 0.0 0.0 0.0 0.0

CATALYST LOADING
```

```
WEIGHT FRACTION IN SLURRY (kg cat/kg slurry) = ?
>0.3
CATALYST DENSITY (kg/m**3) = ?
>1980.
PARTICLE DIAMETER (m) = ?
>0.00005
CATALYST HEAT CAPACITY = ?
>0.0
IF NO INFORMATION IS AVAILABLE ENTER ZERO


END OF DATA **********
INPUT DATA ARE STORED IN THE FILE NAMED  INPUT1.DAT
PLEASE CHECK YOUR DATA FROM THE FILE NAMED  CHECK1.DAT
```

I-C-8 Program Listing - SLURRY BED

```
C
C       ************************************************************************
C
C       MAIN PROGRAM FOR SLURRY REACTOR DESIGN FOR METHANOL SYNTHESIS
C
C       THIS PROGRAM SIMULATES AN ADIABATIC BUBBLE COLUMN SLURRY REACTOR
C       FOR METHANOL SYNTHESIS.
C
C       THE CONVERSION, TEMPERATURE AND CONCENTRATION PROFILES ARE
C       CALCULATED FOR A SET OF DESIGN AND OPERATION CONDITIONS.
C       THE KINETIC DATA AND THE PHYSICOCHEMICAL AND THERMODYNAMICAL
C       PROPERTIES OF THE SYSTEM ARE SUPPLIED BY SEPARETE SUBROUTINES
C       SO THAT THE USER CAN ACCOMADATE HIS OWN DATA BY SIMPLE UPDATE
C       PROCEDURE. THE PROGRAM NORMALLY EMPLOYS THE DATA ON WITCO-40
C       AS A SOLVENT AND A Cu/Zn/Cr2O3 CATALYST( United Catalyst T-2370 )
C
C       ************************************************************************
C
C       VARIABLE LIST
C
C       AL   :COLUMN LENGTH (m)
C       BOL   :LIQUID PHASE BODENSTEIN NUMBER (-)
C       BOLO   :LIQUID PHASE BODENSTEIN NUMBER AT THE COLUMN INLET (-)
C       BOS   :SOLID PHASE BODENSTEIN NUMBER (-)
C       BOLST :LIQUID PHASE BODENSTEIN NUMBER FOR SEDIMENTATION (-)
C       CCATF   :FEED CATALST CONCENTRATION (kg/m**3)
C       CF   :FEED LIQUID PHASE CONCENTRATION (kmol?/m**3)
C       CL   :LIQUID PHASE CONCENTRATION (kmol/m**3)
C       CPCAT   :CATALYST HEAT CAPACITY (kJ/kg-K)
C       DC   :COLUMN DIAMETER (m)
C       DENCAT,DENC   :CATALYST DENSITY (kg/m**3)
C       DP   :PARTICLE DIAMETER (m)
C       EG   :GAS HOLDUP (-)
C       HENRY   :HENRY'S CONSTANT (atm-M**3/kmol)
C       NAME   :NAME VECTOR FOR THE COMPONENTS
C       P   :PRESSURE (atm)
C       PE   :PECLET NUMBER FOR HEAT TRANSFER (-)
C       PED   :PECLET NUMBER FOR HEAT TRANSFER AT THE COLUMN INLET   (-)
C       Q   :FLOW RATE RATIO (slurry/gas), (-)
C       QFG   :VOLUMETRIC GAS FLOW RATE (Nm**3/sec)
C       QFL   :VOLUMETRIC SLURRY FLOW RATE (m**3/sec)
C       STG   :GAS PHASE STANTON NUMBER (-)
C       STL   :LIQUID PHASE STANTON NUMBER (-)
C       STY   :SPACE TIME YIELD (NM**3 gas converted/kg Cat-hr)
C       TF   :FEED TEMPERATURE (K)
C       UGO   :SUPERFICIAL GAS VELOCITY (m/sec)
C       VCAT   :VOLUME FRACTION OF CATALYST IN THE SUSPENSION (-)
C       WCAT   :WEIGHT FRACTION OF CATALYST IN THE SUSPENSION (-)
C       WHSV   :WEIGHT HOURLY SPACE VELOCITY (Nm**3/kg Cat-hr)
C       XF,XF1   :FEED LIQUID PHASE CONCENTRATION (mole fraction)
C       X1   :LIQUID PHASE DIMENSIONLESS CONCENTRATION (-)
C       XO   :LIQUID PHASE FEED DIMENSIONLESS CONCENTRATION (-)
C       YF,YF1   :GAS PHASE FEED CONCENTRATIONS (mole fractions)
C
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        COMMON/PAR1/QFG,QFL
        COMMON/PAR2/YF1(7),XF1(5),DENC
        COMMON/PAR5/P,TF,AL,UGO,DP,WCAT,CPCAT,DC,STG(5),STL(5),BOL,PE
```

```
      COMMON/PAR6/Q,DENCAT,CCATF,EG,HENRY(5),YF(7),XF(7),CF(7),XO(5)
      COMMON/PAR7/BOLO,PEO
      COMMON/PAR8/VCAT
      COMMON/PAR9/BOS,BOLST
      DIMENSION FSPACE(40000),ZETA(17),TOL(11),Z(17),X1(5),CL(5)
      DIMENSION ISPACE(2000),M(11),IPAR(11),LTOL(11),NAME(5)
      EXTERNAL FSUB,DFSUB,GSUB,DGSUB,SOLUTN
      DATA NAME/' CO  ',' CO2 ',' H2  ','CH3OH',' H2O '/
C
      OPEN (UNIT=30,FILE='TEMP.PRO')
      OPEN (UNIT=31,FILE='CONC.GAS')
      OPEN (UNIT=32,FILE='CONC.LIQ')
      OPEN (UNIT=33,FILE='CONV.PRO')
      OPEN (UNIT=34,FILE='OUTPUT.SUM')
      OPEN (UNIT=35,FILE='DIMCON.LIQ')
      OPEN (UNIT=36,FILE='CAT.PRO')
      CALL INPUT1
C
      SA=3.1416/4.*DC**2.
      UGO=QFG*TF/P/273.2/SA
C
      UL=QFL/SA
C
      Q=UL/UGO


C
      DO 110 I=1,7
110   YF(I)=YF1(I)
C
      DO 120 I=1,5
120   XF(I)=XF1(I)
C
      DENCAT=DENC
      IF(CPCAT.EQ.0.0D00) CPCAT=2.5
C
      TET=0.
      CALL INTER(P,TF,XF,TET,CL,T)
C
C
      WRITE(34,130)
130   FORMAT(///,10X,
     *  '*******************************************************',
     *  //,14X,'ADIABATIC BUBBLE-COLUMN SLURRY REACTOR SIMULATION',//,
     *  34X,'FOR',//,25X,'METHANOL SYNTHESIS',//,10X,
     *  '*******************************************************',//)
      WRITE(34,140)
140   FORMAT(/,5X,'SUMMARY OF THE INPUT DATA',///)
      WRITE(34,150) DC
150   FORMAT(5X,'************ REACTOR CHARACTERISTICS ***********',//,
     *  5X,'DIAMETER = ',F10.5,' m')
      WRITE(34,160) AL
160   FORMAT(5X,'LENGTH = ',F10.5,' m')
      WRITE(34,170) TF,P
170   FORMAT(//,5X,'********** FEED CHARACTERISTICS **********',
     *  //,5X,'INLET TEMPERATURE = ',F10.5,' K',/,5X,'PRESSURE = ',
     *  F10.5,' atm')
      WRITE(34,180) QFG,QFL
180   FORMAT(5X,'GAS FLOW RATE = ',E10.5,' Nm**3/sec',/,5X,
     *  'SLURRY FLOW RATE = ',E10.5,' m**3/sec')
```

```
      WRITE(34,190) UGO,Q
190   FORMAT(5X,'SUPERFICIAL GAS VELOCITY = ',F10.5,' m/sec',/,5X,
     * 'FLOW RATE RATIO (slurry/gas) = ',F10.5)
      WRITE(34,220)
220   FORMAT(/,5X,'FEED COMPOSITIONS ',/,5X,'COMPONENT ',9X,
     * 'GAS',15X,'SLURRY',/,24X,'mole frac.',7X,'(kmol/m**3)',/,
     * 3(5X,12('*')))
      WRITE(34,230) (NAME(I),YF(I),CL(I),I=1,5)
230   FORMAT(9X,A5,3X,5X,E12.5,5X,E12.5)
C
      WCAT1=100.*WCAT
C
      WRITE(34,240) WCAT1,DENCAT,DP
240   FORMAT(//,5X,'**CATALYST CHARACTERISTICS**',/,5X,
     * 'CATALYST LOADING = ',F10.5,' % WEIGHT',
     * /,14X,'DENSITY = ',F10.5,' kg/m**3',/,14X,'DIAMETER = ',E10.5,
     * ' m')

      IF(TF.GT.450.) GO TO 700
      NI=1
      GO TO 720

700   NI=(TF-450.)/5.+1

      TF=450.
720   CONTINUE
C
C
      R=.082D00
C
C
C     PARAMETERS FOR COLSYS
C
      NCOMP=11
      DO 10 I=1,5
10    M(I)=1
      DO 20 I=6,11
20    M(I)=2
C
      DO 30 I=1,11
30    ZETA(I)=0.D00
      DO 40 I=12,17
40    ZETA(I)=1.D00
C
      DO 50 I=1,11
50    IPAR(I)=0
C
      IPAR(1)=1
      IPAR(4)=11
      IPAR(5)=40000
      IPAR(6)=2000
      IPAR(7)=1
      IPAR(9)=1
C
      DO 60 I=1,6
60    LTOL(I)=I
      LTOL(7)=8
      LTOL(8)=10
      LTOL(9)=12
      LTOL(10)=14
```

```
      LTOL(11)=16
C
      DO 70 I=1,11
70    TOL(I)=1.D-03
C
      DO 144 IP=1,NI
C
      IF(IP.EQ.1) GO TO 88
      TF=TF+5.
C
C
      IPAR(9)=3
      IPAR(3)=ISPACE(1)
C
88    CONTINUE
      CALL DIMPAR(TF,DENSL,CPSL)
      CALL COLSYS(NCOMP,M,0.,1.,ZETA,IPAR,LTOL,TOL,FIXPNT,ISPACE,
     * FSPACE,IFLAG,FSUB,DFSUB,GSUB,DGSUB,SOLUTN)
C
144   CONTINUE
C
      ALPCO=Q*CF(1)+YF(1)*P/R/TF
      ALPM=Q*CF(4)+YF(4)*P/R/TF
      ALPH2=Q*CF(5)+YF(5)*P/R/TF
C
      ACAT=SA*AL*(1.-EG)*DENCAT=VCAT
C
C
      WRITE(30,200)
200   FORMAT(//,15X,'LENGTH',24X,'TEMPERATURE',/,5X,'DIMENSIONLESS'
     *  3X,'ACTUAL (m) ',5X,'DIMENSIONLESS',3X,'ACTUAL (K) ',/,5X,
     *  12('*'),3X,12('*'),5X,12('*'),3X,12('*'))
C
      WRITE(36,500)
500   FORMAT(//,15X,'LENGTH',20X,'CATALYST CONCENTRATION',/,5X,
     *  'DIMENSIONLESS',3X,'ACTUAL (m) ',5X,'DIMENSIONLESS',3X,
     *  'ACTUAL(% WEIGHT)',/,5X,12('*'),3X,12('*'),5X,12('*'),3X,
     *  12('*'))
C
      WRITE(31,300) (NAME(I),I=1,5)
300   FORMAT(//,14X,'LENGTH',25X,'GAS PHASE MOLE FRACTIONS',/,3X,
     *  'DIMENSIONLESS',2X,'ACTUAL (m) ',5(8X,A5),/,5X,10('*'),3X,
     *  10('*'),2X,5(3X,10('*')))
C
      WRITE(32,400) (NAME(I),I=1,5)
400   FORMAT(//,14X,'LENGTH',22X,
     *  'LIQUID PHASE CONCENTRATIONS (kmol/m**3)',
     *  /,3X,'DIMENSIONLESS',2X,'ACTUAL (m) ',5(8X,A5),/,5X,10('*'),3X,
     *  10('*'),2X,5(3X,10('*')))
C
      WRITE(35,405) (NAME(I),I=1,5)
405   FORMAT(//,14X,'LENGTH',22X,
     *  'DIMENSIONLESS LIQUID PHASE CONCENTRATIONS',
     *  /,3X,'DIMENSIONLESS',2X,'ACTUAL (m) ',5(8X,A5),/,5X,10('*'),3X,
     *  10('*'),2X,5(3X,10('*')))
C
      WRITE(33,600)
600   FORMAT(//,15X,'LENGTH',/,5X,'DIMENSIONLESS',3X,'ACTUAL (m) ',5X,
     *  'CONVERSION 1',3X,'CONVERSION 2',/,5X,12('*'),3X,12('*'),2X,
     *  2(3X,12('*')))
```

```
C
      DO 55 I=1,11
      X=(I-1.)*.1
      CALL APPSLN(X,Z,FSPACE,ISPACE)
C
      ALEN=AL*X
      TET=Z(16)
      X1(1)=Z(6)
      X1(2)=Z(8)
      X1(3)=Z(10)
      X1(4)=Z(12)
      X1(5)=Z(14)
C
      CALL INTER(P,TF,X1,TET,CL,T)
C
      CGM=Z(4)*P/R/T
      CGH2=Z(5)*P/R/T
C
      CONV1=((Q*CL(4)+CGM)-ALPM)/ALPCO
C
      CONV2=((Q*CL(5)+CGH2)-ALPH2)/ALPCO
C
      CONV1=CONV1-CONV2
C
      WRITE(30,210) X,ALEN,TET,T
210   FORMAT(5X,F12.5,3X,F12.5,5X,E12.5,3X,F12.5)
C
      WRITE(31,310) X,ALEN,(Z(K),K=1,5)
310   FORMAT(5X,F10.4,3X,F10.4,2X,5(3X,E10.4))
C
      WRITE(32,310) X,ALEN,(CL(K),K=1,5)
C
      WRITE(35,310) X,ALEN,(X1(K),K=1,5)
C
      WRITE(33,410) X,ALEN,CONV1,CONV2
410   FORMAT(5X,F12.5,3X,F12.5,2X,2(3X,E12.5))
C
      CALL CATCON(X,CATDIM)
      CATCL=CATDIM*WCAT*100.
C
      WRITE(36,510) X,ALEN,CATDIM,CATCL
510   FORMAT(5X,F12.5,3X,F12.5,5X,E12.5,3X,F12.5)
C
55    CONTINUE
C
      WHSV=QFG/ACAT*3600.
      STY=QFG*YF(1)*CONV1/ACAT*3600.
C
C     WRITE(34,433) TF
C433  FORMAT(//,5X,' TF = ',F10.5,//)
C
      WRITE(34,250) CONV1,CONV2,T,WHSV,STY
250   FORMAT(//,5X,'OUTPUT SUMMARY',///,5X,'CONVERSION 1 = ',
     *  E10.5,/,5X,'CONVERSION 2 = ',E10.5,/,5X,'OUTLET TEMPERATURE = ',
     *  F10.5,' K',/,5X,'SPACE VELOCITY = ',E10.5,
     *  ' Nm**3/kg-hr',/,5X,'SPACE TIME YIELD = ',E10.5,
     *  ' Nm**3 gas converted/kg-hr')
C
      STOP
      END
```

```
C
C     ------------------------------------------------------------------
C
      SUBROUTINE FSUB(X,Z,F)
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      COMMON/PARE/P,TF,AL,UGO,DP,WCAT,CPCAT,DC,STG(5),STL(5),BOL,PE
      COMMON/PAR6/Q,DENCAT,CCATF,EG,HENRY(5),YF(7),XF(7),CF(7),XO(5)
      COMMON/PAR7/BOLO,PEO
      COMMON/PAR3/VCAT
      COMMON/PAR9/BOS,BOLST
      DIMENSION Z(17),F(11),RATE(2),X1(5),CL(5),HEATR(2)
C
      TET=Z(16)
      X1(1)=Z(6)
      X1(2)=Z(8)
      X1(3)=Z(10)
      X1(4)=Z(12)
      X1(5)=Z(14)
C
      CALL INTER(P,TF,X1,TET,CL,T)
      CALL DIMPAR(T,DENSL,CPSL)
C
      F(1)=-STG(1)*(Z(1)-Z(6))*(1.+Z(16))
      F(2)=-STG(2)*(Z(2)-Z(8))*(1.+Z(16))
      F(3)=-STG(3)*(Z(3)-Z(10))*(1.+Z(16))
      F(4)=-STG(4)*(Z(4)-Z(12))*(1.+Z(16))
      F(5)=-STG(5)*(Z(5)-Z(14))*(1.+Z(16))
C
      CALL CATCON(X,CATDIM)
      CALL RHEAT(T,HEATR)
      CALL REAC1(T,CL,RATE)
C
      PARA=CATDIM*(1.-EG)*CCATF*AL/P/UGO
C
      F(6)=BOL*(Q*Z(7)-STL(1)*(Z(1)-Z(6))+PARA*HENRY(1)*(RATE(1)-
     * RATE(2)))
C
      F(7)=BOL*(Q*Z(9)-STL(2)*(Z(2)-Z(8))+PARA*HENRY(2)*RATE(2))
C
      F(8)=BOL*(Q*Z(11)-STL(3)*(Z(3)-Z(10))+PARA*HENRY(3)*(2.*RATE(1)+
     * RATE(2)))
C
      F(9)=BOL*(Q*Z(13)-STL(4)*(Z(4)-Z(12))-PARA*HENRY(4)*RATE(1))
C
      F(10)=BOL*(Q*Z(15)-STL(5)*(Z(5)-Z(14))-PARA*HENRY(5)*RATE(2))
C
      PARA1=PARA*P/TF/DENSL/CPSL
C
      F(11)=PE*(Q*Z(17)+PARA1*(HEATR(1)*RATE(1)+HEATR(2)*RATE(2)))
C
      RETURN
      END
C
C     ------------------------------------------------------------------
C
      SUBROUTINE DFSUB(X,Z,DF)
C
      IMPLICIT REAL*8(A-H,O-Z)
```

```
C
      DIMENSION Z(17),DF(11,17),WORK1(11),WORK2(11)
C
      EPS=1.D-07
      DO 10 J=1,17
      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=1,11
10    DF(I,J)=(WORK1(I)-WORK2(I))*.5/EPS
      RETURN
      END
C
C     ------------------------------------------------------------
C
      SUBROUTINE GSUB(I,Z,G)
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      COMMON/PAR5/P,TF,AL,UGO,DP,WCAT,CPCAT,DC,STG(5),STL(5),BOL,PE
      COMMON/PAR6/Q,DENCAT,CCATF,EG,HENRY(5),YF(7),XF(7),CF(7),XO(5)
      COMMON/PAR7/BOLO,PEO
      DIMENSION Z(17)
C
      GO TO(1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17),I
C
1     G=Z(1)-YF(1)
      RETURN
2     G=Z(2)-YF(2)
      RETURN
3     G=Z(3)-YF(3)
      RETURN
4     G=Z(4)-YF(4)
      RETURN
5     G=Z(5)-YF(5)
      RETURN
6     G=Z(6)-XO(1)-Z(7)/Q/BOLO
      RETURN
7     G=Z(8)-XO(2)-Z(9)/Q/BOLO
      RETURN
8     G=Z(10)-XO(3)-Z(11)/Q/BOLO
      RETURN
9     G=Z(12)-XO(4)-Z(13)/Q/BOLO
      RETURN
10    G=Z(14)-XO(5)-Z(15)/Q/BOLO
      RETURN
11    G=Z(16)-Z(17)/Q/PEO
      RETURN
12    G=Z(7)
      RETURN
13    G=Z(9)
      RETURN
14    G=Z(11)
      RETURN
15    G=Z(13)
      RETURN
16    G=Z(15)
      RETURN
```

```
17      G=Z(17)
        RETURN
        END
C
C       ------------------------------------------------------------------
C
        SUBROUTINE DGSUB(I,X,DG)
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        COMMON/PARS/P,TF,AL,UGO,DP,WCAT,CPCAT,DC,STG(5),STL(5),BOL,PE
        COMMON/PARS/Q,DENCAT,CCATF,EG,HENRY(5),YF(7),XF(7),CF(7),XO(5)
        COMMON/PAR7/BOLO,PEO
        DIMENSION DG(17),Z(17)
C
        DO 20 J=1,17
20      DG(J)=0.DCO
C
        GO TO(1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17),I
C
1       DG(1)=1.
        RETURN
2       DG(2)=1.
        RETURN
3       DG(3)=1.
        RETURN
4       DG(4)=1.
        RETURN
5       DG(5)=1.
        RETURN
6       DG(6)=1.
        DG(7)=-1./Q/BOLO
        RETURN
7       DG(8)=1.
        DG(9)=-1./Q/BOLO
        RETURN
8       DG(10)=1.
        DG(11)=-1./Q/BOLO
        RETURN
9       DG(12)=1.
        DG(13)=-1./Q/BOLO
        RETURN
10      DG(14)=1.
        DG(15)=-1./Q/BOLO
        RETURN
11      DG(16)=1.
        DG(17)=-1./Q/PEO
        RETURN
12      DG(7)=1.
        RETURN
13      DG(9)=1.
        RETURN
14      DG(11)=1.
        RETURN
15      DG(13)=1.
        RETURN
16      DG(15)=1.
        RETURN
17      DG(17)=1.
        RETURN
```

```
      END
C
C     ------------------------------------------------------------------
C
      SUBROUTINE SOLUTN(X,Z,DMVAL)
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      COMMON/PAR5/P,TF,AL,UGO,DP,WCAT,CPCAT,DC,STG(5),STL(5),BOL,PE
      COMMON/PAR6/Q,DENCAT,CCATF,EG,HENRY(5),YF(7),XF(7),CF(7),XO(5)
      COMMON/PAR7/BOLO,PEO
C
      DIMENSION Z(17),DMVAL(10),Y1(5),Y2(5),Y3(5)
C
      DO 10 I=1,17
10    Z(I)=0.D00
C
      CALL CALPRO(5,YF,XO,Q,STG,STL,BOLO,X,Y1,Y2,Y3)
C
      DO 20 I=1,5
20    Z(I)=Y1(I)
      Z(6)=Y2(1)
      Z(8)=Y2(2)
      Z(10)=Y2(3)
      Z(12)=Y2(4)
      Z(14)=Y2(5)
C
      Z(7)=Y3(1)
      Z(9)=Y3(2)
      Z(11)=Y3(3)
      Z(13)=Y3(4)
      Z(15)=Y3(5)
C
      RETURN
      END
C
C     ------------------------------------------------------------------
C
      SUBROUTINE DIMPAR(T,DENSL,CPSL)
C
C     EVALUATES DIMENSIONLESS PARAMETERS FOR MODEL EQUATIONS
C
C     T   :TEMPERATURE (K)
C     STG  :GAS PHASE STANTON NUMBER
C     STL  :LIQUID PHASE STANTON NUMBER
C     PE   :PECLET NUMBER FOR HEAT TRANSFER
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      COMMON/PAR5/P,TF,AL,UGO,DP,WCAT,CPCAT,DC,STG(5),STL(5),BOL,PE
      COMMON/PAR6/Q,DENCAT,CCATF,EG,HENRY(5),YF(7),XF(7),CF(7),XO(5)
      COMMON/PAR7/BOLO,PEO
      COMMON/PAR8/VCAT
      COMMON/PAR9/BOS,BOLST
C
      DIMENSION DIF(5),AKLA(5)
C
      CALL LIQPRO(T,AMLIQ,DENL,CPL,VISL,STEN)
C
      CALL SOLUB(T,HENRY)
```

```
C
      CALL DIFCF(AMLIQ,T,VISL,DIF)
C
      CALL SLUPRO(WCAT,DENL,DENCAT,VISL,CPL,CPCAT,DENSL,VISSL,CPSL)
C
      CALL MASSTR(5,UGO,DC,DENSL,STEN,VISSL,DIF,AKLA)
C
      R=.082
C
      DO 10 I=1,5
      STG(I)=AKLA(I)*AL*R*TF/UGO/HENRY(I)
10    STL(I)=AKLA(I)*AL/UGO
C
      CALL HOLDUP(UGO,DC,DENSL,STEN,VISSL,EG)
C
      CALL LIQDIF(UGO,DC,DL)
C
      BOL=UGO*AL/(1.-EG)/DL
C
      CALL HEATDF(DENSL,CPSL,DL,DH)
C
      PE=UGO*DENSL*CPSL*AL/(1.-EG)/DH
C
      CCATF=WCAT*DENSL
C
      DO 20 I=1,5
20    CF(I)=XF(I)*DENL/AMLIQ
C
      DO 30 I=1,5
30    XO(I)=HENRY(I)*CF(I)/P
C
      CALL TERVEL(DENL,DENCAT,WCAT,DP,VISL,UTER)

C
      WCATP=100./DENSL
      VCAT1=DENL*WCATP/(DENCAT-WCATP*(DENCAT-DENL))
C
      USS=1.2*UTER*(UGO/UTER)**.25*((1.-VCAT)/(1.-VCAT1))**2.5
C
      CALL SOLDIF(UGO,DC,DS)
      BOS=USS*AL/DS
      BOLST=UGO*Q*AL/DS/(1.-EG)
C
C


      IF(T.NE.TF) RETURN
      BOLO=BOL
      PEO=PE
      RETURN
      END
C
C     ------------------------------------------------------------------
C
      SUBROUTINE LIQPRO(T,AMLIQ,DENL,CPLIQ,VISL,STEN)
C
C     LIQUID PHASE PHYSICAL PROPERTIES FOR WITCO-40
C
C     T  :TEMPERATURE (K)
C
      IMPLICIT REAL*8(A-H,O-Z)
```

```
C
C       MOLECULAR WEIGHT
        AMLIQ=250.
C       DENSITY ,KG/M**3
        DENL=620.
C
C       HEAT CAPACITY ,KJ/KG-K
        CPLIQ=2.75
C       VISCOSITY ,KG/M-SEC
C
        A=777.4*(1./T-1./385.D00)
        VISL=10.D0**A*1.D-03
C
C       SURFACE TENSION  N/M
        STEN=.016
C
        RETURN
        END
C
C       ---------------------------------------------------------------
C
        SUBROUTINE DIFCF(AMLIQ,T,VISL,DIF)
C
C       DIFFUSIVITIES ARE ESTIMATED BY WILKE-CHANG EQUATION
C
C       AMLIQ  :LIQUID MOLECULAR WEIGHT
C       T  :TEMPERATURE (K)
C       VISL  :VISCOSITY (kg/m-s)
C       DIF  :DIFFUSIVITY (m**2/s)
C
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DIMENSION DIF(5),VG(5)
C
        VG(1)=.0307
        VG(2)=.0340
        VG(3)=.0143
        VG(4)=.0259
        VG(5)=.0189
        DO 10 I=1,5
10      DIF(I)=1.173E-16*AMLIQ**(.5)*T/(VISL*VG(I)**(.6))
C
        RETURN
        END
C
C       ---------------------------------------------------------------
C
        SUBROUTINE SOLUB(T,HENRY)
C
C
C       THIS SUBROUTINE SUPPLIES THE SOLUBILITY DATA
C
C       THE FORM IS  HENRY(I)=A(I)*EXP(B(I)/T)
C
C       UNITS ARE  A : ATM*M**3/KMOL     B  : K
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DIMENSION A(5),B(5),HENRY(5)
```

```
C
      A(1)=20.73
      A(2)=818.39
      A(3)=11.25
      A(4)=35224S.19
      A(5)=993094.75
C
      B(1)=1015.5
      B(2)=-849.1
      B(3)=1289.5
      B(4)=-4307.
      B(5)=-4890.
C
      DO 10 I=1,5
10    HENRY(I)=A(I)*DEXP(B(I)/T)
C
      RETURN
      END
C
C     ----------------------------------------------------------------
C
C
      SUBROUTINE CPGAS(N,Y,T,HEATCP,CPMASS,CONT)
C
C     THIS SUBROUTINE PROVIDES HEAT CAPACITY DATA
C     FOR METHANOL SYNTHESIS,
C     ALSO USED TO CALCULATE HEAT OF REACTION DATA
C
C     N  :CONTROL VARIABLE
C           0:ONLY HEAT CAPACITY IS TO BE CALCULATED
C           1:ONLY HEAT OF REACTION IS TO BE CALCULATED
C     Y  :MOLE FRACTIONS
C     T  :TEMPERATURE (K)
C     HEATCP  :MOLAL HEAT CAPACITY (KJ/KMOL-K)
C     CPMASS  :MASS HEAT CAPACITY (KJ/KG-K)
C     CONT  :CONTRIBUTION TO REACTION ENTHALPIES
C
C     CP(I,J) ARE THE CONSTANTS FOR HEAT CAPACITY EQUATION
C
C     CPGAS(I)=CP(I,1)+CP(I,2)*TC+CP(I,3)*TC**2+CP(I,4)*TC**3
C
C     UNITS ARE   CPGAS:KJ/KMOL-K,   T:K
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION CP(7,4),CONT(2),AM(7),SUM(7),Y(7)
C
      DATA AM/28.,44.,2.,32.,18.,28.,16./
C
C     CO
C
      CP(1,1)=28.98
      CP(1,2)=.411E-02
      CP(1,3)=.3548E-05
      CP(1,4)=-2.22E-09
C
C     CO2
C
      CP(2,1)=36.11
      CP(2,2)=4.233E-02
      CP(2,3)=-2.887E-05
      CP(2,4)=7.465E-09
```

```
C
C       H2
C
        CP(3,1)=28.84
        CP(3,2)=.00765E-02
        CP(3,3)=.3288E-05
        CP(3,4)=-.8698E-09
C
C       CH3OH
C
        CP(4,1)=42.93
        CP(4,2)=8.301E-02
        CP(4,3)=-1.89E-05
        CP(4,4)=-8.03E-09
C
C       H2O
C
        CP(5,1)=33.46
        CP(5,2)=.688E-02
        CP(5,3)=.7604E-05
        CP(5,4)=-3.593E-09
C
C       N2
C
        CP(6,1)=29.
        CP(6,2)=.2199E-02
        CP(6,3)=.5723E-05
        CP(6,4)=-2.871E-09
C
C       CH4
C
        CP(7,1)=34.33
        CP(7,2)=5.711E-02
        CP(7,3)=.3363E-05
        CP(7,4)=11.0092E-09
C
        TC=T-273.15
C
        IF(N.EQ.1) GO TO 40
        DO 20 I=1,7
        SUM(I)=0.
20      CONTINUE
        DO 10 I=1,7
        SUM(I)=SUM(I)+CP(I,1)+CP(I,2)*TC+CP(I,3)*TC**2.+CP(I,4)*TC**3.
10      CONTINUE
C
        HEATCP=0.
        CPMASS=0.
        DO 30 I=1,7
        CPMASS=CPMASS+SUM(I)*Y(I)/AM(I)
30      HEATCP=HEATCP+SUM(I)*Y(I)
C
        RETURN
C
40      A1=CP(4,1)-2.*CP(3,1)-CP(1,1)
        A2=CP(4,2)-2.*CP(3,2)-CP(1,2)
        A3=CP(4,3)-2.*CP(3,3)-CP(1,3)
        A4=CP(4,4)-2.*CP(3,4)-CP(1,4)
C
        B1=CP(5,1)+CP(1,1)-CP(3,1)-CP(2,1)
```

```
      B2=CP(5,2)+CP(1,2)-CP(3,2)-CP(2,2)
      B3=CP(5,3)+CP(1,3)-CP(3,3)-CP(2,3)
      B4=CP(5,4)+CP(1,4)-CP(3,4)-CP(2,4)
C
      CONT(1)=A1*(TC-25.)+A2*(TC**2.-25.**2.)*.5+
     * A3/3.*(TC**3.-25.**3.)+A4/4.*(TC**4.-25.**4.)
C
      CONT(2)=B1*(TC-25.)+B2*(TC**2.-25.**2.)*.5+
     * B3/3.*(TC**3.-25.**3.)+B4/4.*(TC**4.-25.**4.)
      RETURN
      END
C
C     ---------------------------------------------------------------
C
      SUBROUTINE RHEAT(T,HEATR)
C
C     PROVIDES HEAT OF REACTION DATA FOR METHANOL
C     SYNTHESIS.
C
C     T  :TEMPERATURE , K
C     HEATR  :HEAT OF REACTION , KJ/KMOL
C             1:METHANOL FORMATION
C             2:CO2 REACTION
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION HEATR(2),Y(7),CONT(2)
C
      CALL CPGAS(1,Y,T,HEATCP,CPMASS,CONT)
C
      HEATR(1)=-98920.+CONT(1)
      HEATR(2)=41270.+CONT(2)
      RETURN
      END
C
C     ---------------------------------------------------------------
C
      SUBROUTINE HOLDUP(UG,DC,DEN,STEN,VIS,EG)
C
C     EVALUATES GAS HOLDUP VALUE FOR BUBBLE-COLUMN
C     USING  AKITA-YOSHIDA'S CORRELATION
C
C     UG  :SUPERFICIAL GAS VELOCITY (m/s)
C     DC  :COLUMN DIAMETER (m)
C     DEN  :DENSITY (kg/m**3)
C     STEN  :SURFACE TENSION (N/m-s)
C     VIS  :VISCOSITY (kg/m-s)
C     EG  :GAS HOLUP (-)
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      G=9.8
      VISK=VIS/DEN
      A=(G*DC**2.*DEN/STEN)**(.125)
      B=(G*DC**3./VISK**2.)**(1./12.)
      C=UG/DSQRT(G*DC)
      D=.2*A*B*C
C
      EG1=D
20    EG=(1-EG1)**4.*D
```

```
      IF(DABS((EG-EG1)/EG).LT..01) GO TO 10
      EG1=(EG1+EG)/2.
      GO TO 20
10    RETURN
      END
C
C     ---------------------------------------------------------------
C
      SUBROUTINE MASSTR(N,UG,DC,DEN,STEN,VIS,DIF,AKLA)
C
C     EVALUATES THE VOLUMETRIC MASS TRANSFER COEFFICIENTS
C     IN BUBBLE-COLUMN SLURRY REACTOR
C
C     N   :NUMBER OF COMPONENTS
C     UG   :SUPERFICIAL GAS VELOCITY (m/s)
C     DC   :COLUMN DIAMETER (m)
C     DEN   :DENSITY (kg/m**3)
C     STEN   :SURFACE TENSION (N/m-s)
C     VIS   ;VISCOSITY (kg/m-s)
C     DIF   :DIFFUSIVITY OF THE SPECIES (m**2/s)
C     AKLA   :VOLUMETRIC MASS TRANSFER COEFFICIENTS (1./s)
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      DIMENSION DIF(N),AKLA(N)
C
      CALL HOLDUP(UG,DC,DEN,STEN,VIS,EG)
C
      G=9.8
      VISK=VIS/DEN
      A=(G*DC**2.*DEN/STEN)**(.62)
      B=(G*DC**3./VISK**2.)**(.31)
C
      DO 10 I=1,N
10    AKLA(I)=.6*DIF(I)*DSQRT(VISK/DIF(I))*A*B*EG**(1.1)/DC**2.
      RETURN
      END
C
C     ---------------------------------------------------------------
C
      SUBROUTINE HEATDF(DEN,CP,DL,DH)
C
C     HEAT DISPERSION COEFFICIENT
C
C     DEN   :DENSITY (kg/m**3)
C     CP   :HEAT CAPACITY  (kJ/kg-K)
C     DL   :LIQUID PHASE AXIAL DIFFUSIVITY  (m**2/s)
C     DH   :HEAT DIFFUSION COEFFICIENT  (kJ/m-s-K)
C
      DH=DL*DEN*CP
C
      RETURN
      END
C
C     ---------------------------------------------------------------
C
      SUBROUTINE SLUPRO(WCAT,DENL,DENCAT,VISL,CPL,CPCAT,DENSL,VISSL,
     * CPSL)
C
C     EVALUATES SLURRY PHYSICAL PROPERTIES
```

```
C
C       WCAT  :CATALYST WEIGHT FRACTION
C       DENL  :LIQUID DENSITY (kg/m**3)
C       DENCAT  :CATALYST DENSITY (kg/m**3)
C       VISL  :LIQUID VISCOSITY (kg/m-s)
C       CPL  :LIQUID HEAT CAPACITY (kJ/kg-K)
C       CPCAT  :CATALYST HEAT CAPACITY (kJ/kg-K)
C       DENSL  :SLURRY DENSITY (kg/m**3)
C       VISSL  :SLURRY VISCOSITY (kg/m-s)
C       CPSL  :SLURRY HEAT CAPACITY (kJ/kg-K)
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        COMMON/PARS/VCAT
C
        VCAT=(DENL*WCAT)/(DENCAT-WCAT*(DENCAT-DENL))
C
        DENSL=VCAT*DENCAT+(1.-VCAT)*DENL
C
        VISSL=VISL*(1.+4.5*VCAT)
C
        CPSL=WCAT*CPCAT+(1-WCAT)*CPL
C
        RETURN
        END
C
C       ------------------------------------------------------------
C
        SUBROUTINE LIQDIF(UG,DC,DL)
C
C       EVALUATES LIQUID PHASE DISPERSION COEFFICIENT
C       USING SHAH-DECKWER'S CORRELATION
C
C       UG  :SUPERFICIAL GAS VELOCITY (m/s)
C       DC  :COLUMN DIAMETER (m)
C       DL  :LIQUID PHASE DISPERSION COEFFICIENT (m**2/s)
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DL=.768*UG**(.32)*DC**(1.34)
C
        RETURN
        END
C
C       ------------------------------------------------------------
C
        SUBROUTINE SOLDIF(UG,DC,DS)
C
C       EVALUATES SOLID PHASE DISPERSION COEFFICIENT
C       USING KATO EL.AL.'S CORRELATION
C
C       UG  :SUPERFICIAL GAS VELOCITY (m/s)
C       DC  :COLUMN DIAMETER (m)
C       DS  :SOLID PHASE DISPERSION COEFFICIENT (m**2/s)
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        G=9.8
        FR=UG/DSQRT(G*DC)
C
```

```
      BOC=13.*FR/(1.+8.*FR**(.85))
C
      DS=UG*DC/BOC
C
      RETURN
      END
C
C     ------------------------------------------------------------
C
      SUBROUTINE REAC1(T,C,RATE)
C
C     CALCULATES THE REACTION RATES BY BERTY'S EQUATIONS
C
C     T   :TEMPERATURE (K)
C     C   :CONCENTRATIONS VECTOR (kmol/m**3)
C           1 :CO  2 :CO2  3 :H2  4 :CH3OH  5 :H2O
C
C     RATE  :REACTION RATE  (kmol/kg-sec)
C           1 :Methanol reaction
C           2  :Shift reaction
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION C(7),RATE(2)
C
      R=.082
C
      AKK1=3.27D-11*EXP(11678./T)*(R*T)**2
      AKK2=1.17D+02*EXP(-4827./T)
      AK1=39.144*EXP(-7488.7/T)
      AK2=.01189*EXP(-5068.4/T)
C
C
      RATE(1)=AK1*(C(3)-C(4)/(AKK1*C(3)*C(1)))
      RATE(2)=AK2*(C(3)-C(1)*C(5)/(AKK2*C(2)))
C
      RETURN
      END
C
C     ------------------------------------------------------------------
C
      SUBROUTINE CATCON(X,CATDIM)
C
C     EVALUATES CATALYST CONCENTRATION
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/PAR9/BOS,BOLST
C
C
      A=BOS*DEXP((BOS-BOLST)*(1.-X))-BOLST
      B=BOS-BOLST
      CATDIM=A/B
C
      RETURN
      END
C
C     ------------------------------------------------------------
C
      SUBROUTINE INTER(P,TF,X,TET,CLIQ,T)
C
C     CALCULATES ACTUAL CONCENTRATIONS AND TEMPERATURE FORE     ROM
```

```
C       DIMENSIONLESS VALUES
C
C       OP  P  :PRESSURE (atm)
C       TF  :T FEED TEMPR ERATURE (k)  K)
C       X  :DIMENSIONLESS CO  LIQUID PHASE CONCENTRATION (-)
C       TET  :DIMENSIONLESS TEMPERATURE (-)
C       CLIQ  :LIQUID PHASE CONCENTRATION (kmol/m**# 3)
C       T  :TEMPERATURE (K)
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DIMENSION HENRY(5),X(5),CLIQ(5)
        T=TF*(1.+TET)
C
        CALL SOLUB(T,HENRY)
C
        DO 10 I=1,5
10      CLIQ(I)=P*X(I)/HENRY(I)
C
        RETURN
        END
C
C
C       ---------------------------------------------------------
C
        SUBROUTINE CALPRO(N,YO,XO,Q,STG,STL,BOL,Z,Y,X,DERX)
C
C       PROVIDES A SOLUTION ANALYTICAL SOLUTION TO THE PROBLEM
C       N  :NO OF COMPONENT
C       YO  :GAS FEED CONCENTRATION (mole fraction)
C       XO  :LIQUID FEED CONCENTRATION (dimensionless)
C       Q  :FLOW RATE RATIO (liquid/gas)
C       STG  :GAS PHASE STANTON NUMBER
C       STL  :LIQUID PHASE STANTON NUMBER
C       BOL  :LIQUID PHASE BODENSTEIUN NUMBER
C       Z  :AXIAL COORDINATE (dimensionless)
C       Y  :GAS PHASE CONCENTRATION
C       X  :LIQUID PHASE CONCENTRATION
C       DERX  :DERIVATIVE VALUE  dX/dZ
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        DIMENSION YO(N),XO(N),STG(N),STL(N),Y(N),X(N),DERX(N)
C
C
        DO 1CO I=1,N
        AL=STG(I)-Q*BOL
        BET=BOL*(STG(I)*Q+STL(I))
        GAM=BOL*(STL(I)*YO(I)+STG(I)*Q*XO(I))
        R1=-.5*(AL+DSQRT(AL**2.+4.*BET))
        R2=.5*(-AL+DSQRT(AL**2.+4.*BET))
        A=(R1*Q*BOL*XO(I)+GAM)*DEXP(R1)
        B=(R2*Q*BOL*XO(I)+GAM)*DEXP(R2)
        C=R1*(R1+Q*BOL+AL)*DEXP(R1)
        D=R2*(R2+Q*BOL+AL)*DEXP(R2)
C
        A=(A-B)/(C-D)
        C1=-GAM/R1/R2
        IF(Q.NE.O.) GO TO 21
        A=R1*(R1+AL)*DEXP(R1)-R2*(R2+AL)*DEXP(R2)
```

```
      A=GAM*(DEXP(R1)-DEXP(R2))/A
      C2=(R1*A*(R1+AL)-GAM)/(R1-R2)/R1
      C3=(R2*A*(R2+AL)-GAM)/(R2-R1)/R2
      GO TO 41
21    CONTINUE
C
      C2=R1*(A*(R1+Q*BOL+AL)-Q*BOL*XO(I))-GAM
      C2=C2/R1/(R1-R2)
C
      C3=R2*(A*(R2+Q*BOL+AL)-Q*BOL*XO(I))-GAM
      C3=C3/R2/(R2-R1)
C
41    CONTINUE
      X(I)=C1+C2*DEXP(R1*Z)+C3*DEXP(R2*Z)
C
      DERX(I)=C2*R1*DEXP(R1*Z)+C3*R2*DEXP(R2*Z)
C
      Y(I)=YO(I)+STG(I)/STL(I)*(DERX(I)/BOL-Q*(X(I)-XO(I)))
100   CONTINUE
C
      RETURN
      END
C
C     ---------------------------------------------------------------
C
      SUBROUTINE INPUT1
C
C
C
C     THIS SUBROUTINE PROVIDES THE INPUT DATA TO THE BUBBLE-COLUMN
C     SLURRY REACTOR FOR METHANOL SYNTHESIS SIMULATOR.
C
      IMPLICIT REAL*8(A-H,O-Z)
C
      COMMON/PAR1/QFG,QFL
      COMMON/PAR2/YF1(7),XF1(5),DENC
      COMMON/PAR5/P,TF,AL,UGO,DP,WCAT,CPCAT,DC,STG(5),STL(5),BOL,PE
C
      OPEN (UNIT=12,FILE='INPUT1.DAT')
C
      READ(12,*) DC
      READ(12,*) AL
      READ(12,*) P
      READ(12,*) TF
      READ(12,*) QFG
      READ(12,*) QFL
      READ(12,*) (YF1(I),I=1,7)
      READ(12,*) (XF1(I),I=1,5)
      READ(12,*) WCAT
      READ(12,*) DENC
      READ(12,*) DP
      READ(12,*) CPCAT
C
      RETURN
      END
C
C     ------------------------------------------------
C
      SUBROUTINE TERVEL(DENL,DENCAT,WCAT,DP,VISL,UTER)
C
```

```
C       EVALUARTES TERMINAL VELOSITY CITY FOR A PARTICLE IN THE SWARM
C
C       DENL   :LIQUID DENSITY (kg/M**3)
C       DENCAT  :CATALYST DENSITY (kg/m**#3)
C       WCAT   :CATALYST WEIGHT FRACTION
C       DP   :PARTICLE DIAMETER (m)
C       VISL  :VISCOSITY (kg/m-sec)
C       UTER   :TERNMINAL VELOCITY (m/sec)
C
        IMPLICIT REAL*8(A-H,O-Z)
C
        G=9.8
C
        ITER=0
C
        AR=DENL*(DENCAT-DENL)*G*DP**3./VISL**2.
        RE=AR/18.
30      IF(RE.LE..5000) GO TO 20
        RE=(AR/13.9)**.7
        IF(RE.GT..5000) GO TO 20
        IF(ITER.GT.20) GO TO 20
        ITER=ITER+1
        GO TO 30
20      UTER=VISL*RE/DP/DENL
        RETURN
        END
```

I-C-9 Sample Output from Bubble Column Slurry Reactor Simulation

****

ADIABATIC BUBBLE-COLUMN SLURRY REACTOR SIMULATION

FOR

METHANOL SYNTHESIS

****

SUMMARY OF THE INPUT DATA

********** REACTOR CHARACTERISTICS **********

DIAMETER = 4.00000 m
LENGTH = 8.00000 m

********** FEED CHARACTERISTICS **********

INLET TEMPERATURE = 500.00000 K
PRESSURE = 70.00000 atm
GAS FLOW RATE = .48064E+02 Nm**3/sec
SLURRY FLOW RATE = .31416E+00 m**3/sec
SUPERFICIAL GAS VELOCITY = 0.10000 m/sec
FLOW RATE RATIO (slurry/gas) = 0.25000

FEED COMPOSITIONS

COMPONENT	GAS mole frac.	SLURRY (kmol/m**3)
CO	0.25000E+00	0.00000E+00
CO2	0.10000E+00	0.00000E+00
H2	0.50000E+00	0.00000E+00
CH3OH	0.00000E+00	0.00000E+00
H2O	0.00000E+00	0.00000E+00

CATALYST CHARACTERISTICS
CATALYST LOADING = 30.00000 % WEIGHT
DENSITY = 1980.00000 kg/m**3
DIAMETER = .50000E-04 m

OUTPUT SUMMARY

CONVERSION 1 = .12194E+00
CONVERSION 2 = .23833E-02
OUTLET TEMPERATURE = 510.49245 K
SPACE VELOCITY = .90359E+01 Nm**3/kg-hr
SPACE TIME YIELD = .27546E+00 Nm**3 gas converted/kg-hr

LENGTH		GAS PHASE MOLE FRACTIONS				
DIMENSIONLESS	ACTUAL (m)	CO	CO2	H2	CH3OH	H2O
**********	**********	**********	**********	**********	**********	**********
0.0000	0.0000	.2500E+00	.1000E+00	.5000E+00	.2700E-28	.6141E-30
0.1000	0.8000	.2234E+00	.9256E-01	.4381E+00	.1944E-01	.3926E-03
0.2000	1.6000	.2166E+00	.9156E-01	.4274E+00	.2152E-01	.4229E-03
0.3000	2.4000	.2137E+00	.9140E-01	.4227E+00	.2287E-01	.4459E-03
0.4000	3.2000	.2117E+00	.9135E-01	.4190E+00	.2408E-01	.4662E-03
0.5000	4.0000	.2099E+00	.9133E-01	.4156E+00	.2513E-01	.4837E-03
0.6000	4.8000	.2084E+00	.9130E-01	.4127E+00	.2604E-01	.4985E-03
0.7000	5.6000	.2071E+00	.9128E-01	.4102E+00	.2678E-01	.5104E-03
0.8000	6.4000	.2061E+00	.9127E-01	.4082E+00	.2735E-01	.5194E-03
0.9000	7.2000	.2053E+00	.9126E-01	.4069E+00	.2773E-01	.5253E-03
1.0000	8.0000	.2049E+00	.9125E-01	.4061E+00	.2790E-01	.5279E-03

LENGTH		LIQUID PHASE CONCENTRATIONS (kmol/m**3)				
DIMENSIONLESS	ACTUAL (m)	CO	CO2	H2	CH3OH	H2O
**********	**********	**********	**********	**********	**********	**********
0.0000	0.0000	.9947E-01	.5444E-01	.2130E+00	.1798E-01	.3939E-03
0.1000	0.8000	.9950E-01	.5465E-01	.2127E+00	.1899E-01	.4153E-03
0.2000	1.6000	.9876E-01	.5465E-01	.2110E+00	.2026E-01	.4401E-03
0.3000	2.4000	.9794E-01	.5462E-01	.2091E+00	.2143E-01	.4622E-03
0.4000	3.2000	.9715E-01	.5459E-01	.2075E+00	.2247E-01	.4817E-03
0.5000	4.0000	.9644E-01	.5456E-01	.2059E+00	.2338E-01	.4983E-03
0.6000	4.8000	.9582E-01	.5454E-01	.2046E+00	.2415E-01	.5123E-03
0.7000	5.6000	.9531E-01	.5453E-01	.2036E+00	.2477E-01	.5233E-03
0.8000	6.4000	.9492E-01	.5451E-01	.2027E+00	.2522E-01	.5314E-03
0.9000	7.2000	.9467E-01	.5451E-01	.2022E+00	.2551E-01	.5364E-03
1.0000	8.0000	.9458E-01	.5450E-01	.2020E+00	.2561E-01	.5382E-03

LENGTH		DIMENSIONLESS LIQUID PHASE CONCENTRATIONS				
DIMENSIONLESS	ACTUAL (m)	CO	CO2	H2	CH3OH	H2O
**********	**********	**********	**********	**********	**********	**********
0.0000	0.0000	.2158E+00	.9099E-01	.4292E+00	.1944E-01	.3828E-03
0.1000	0.8000	.2158E+00	.9137E-01	.4284E+00	.2057E-01	.4043E-03
0.2000	1.6000	.2141E+00	.9139E-01	.4246E+00	.2198E-01	.4292E-03
0.3000	2.4000	.2122E+00	.9136E-01	.4208E+00	.2327E-01	.4514E-03
0.4000	3.2000	.2105E+00	.9134E-01	.4173E+00	.2443E-01	.4710E-03
0.5000	4.0000	.2089E+00	.9131E-01	.4141E+00	.2544E-01	.4878E-03
0.6000	4.8000	.2075E+00	.9129E-01	.4114E+00	.2630E-01	.5019E-03
0.7000	5.6000	.2064E+00	.9127E-01	.4091E+00	.2699E-01	.5131E-03
0.8000	6.4000	.2055E+00	.9126E-01	.4074E+00	.2750E-01	.5213E-03
0.9000	7.2000	.2049E+00	.9125E-01	.4063E+00	.2782E-01	.5263E-03
1.0000	8.0000	.2048E+00	.9125E-01	.4060E+00	.2793E-01	.5281E-03

LENGTH		TEMPERATURE	
DIMENSIONLESS	ACTUAL (m)	DIMENSIONLESS	ACTUAL (K)
**********	**********	**********	**********
0.00000	0.00000	0.19945E-01	509.97264
0.10000	0.80000	0.20143E-01	510.07142
0.20000	1.60000	0.20320E-01	510.15976
0.30000	2.40000	0.20475E-01	510.23769
0.40000	3.20000	0.20610E-01	510.30522
0.50000	4.00000	0.20725E-01	510.36236
0.60000	4.80000	0.20818E-01	510.40913
0.70000	5.60000	0.20891E-01	510.44554
0.80000	6.40000	0.20943E-01	510.47158
0.90000	7.20000	0.20974E-01	510.48722
1.00000	8.00000	0.20985E-01	510.49245

LENGTH			
DIMENSIONLESS	ACTUAL (m)	CONVERSION 1	CONVERSION 2
**********	**********	**********	**********
0.00000	0.00000	0.10298E-01	0.23072E-03
0.10000	0.80000	0.85574E-01	0.17827E-02
0.20000	1.60000	0.94314E-01	0.19158E-02
0.30000	2.40000	0.10019E+00	0.20187E-02
0.40000	3.20000	0.10541E+00	0.21092E-02
0.50000	4.00000	0.11000E+00	0.21875E-02
0.60000	4.80000	0.11392E+00	0.22533E-02
0.70000	5.60000	0.11714E+00	0.23064E-02
0.80000	6.40000	0.11958E+00	0.23462E-02
0.90000	7.20000	0.12121E+00	0.23721E-02
1.00000	8.00000	0.12194E+00	0.23833E-02

LENGTH		CATALYST CONCENTRATION	
DIMENSIONLESS	ACTUAL (m)	DIMENSIONLESS	ACTUAL (% WEIGHT)
0.00000	0.00000	0.10494E+01	31.48071
0.10000	0.80000	0.10445E+01	31.33611
0.20000	1.60000	0.10397E+01	31.19075
0.30000	2.40000	0.10348E+01	31.04463
0.40000	3.20000	0.10299E+01	30.89774
0.50000	4.00000	0.10250E+01	30.75007
0.60000	4.80000	0.10201E+01	30.60163
0.70000	5.60000	0.10151E+01	30.45240
0.80000	6.40000	0.10101E+01	30.30239
0.90000	7.20000	0.10051E+01	30.15159
1.00000	8.00000	0.10000E+01	30.00000

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APPENDIX I-D

```
NEW
;
REPORT NOPROPERTIES BLOCKS STREAMS FLOWSHEET
HISTORY MSG-LEVEL PROPERTIES=2 STREAMS=6
;       DEFINE THE PROBLEM
;
TITLE 'SIMULATION OF DIRECT COAL LIQUEFACTION REACTOR AND PREHEATER'
DESCRIPTION "THIS IS AN EXAMPLE FOR ADAPTING USER WRITTEN MODELS
             TO THE ASPEN SIMULATOR. THE PROGRAM CHOSEN IS THE
             DIRECT COAL LIQUEFACTION ONE. THE ONLY PIECES OF
             EQUIPMENT ENCOUNTERED IN THE FLOWSHEET ARE THE PREHEATER
             AND REACTOR, WHICH ARE LUMPED INTO ONE BLOCK CALLED PR."
;
;       SELECT UNITS OF MEASUREMENT
;
IN-UNITS SI
OUT-UNITS SI
;
;       SPECIFY FLOWSHEET CONNECTIVITY
;
FLOWSHEET
        BLOCK PR IN=GASIN SLURRYIN OUT=GASOUT SLURRYOUT
SIM-OPTIONS ENERGY-BAL=0
FLOWSHEET-REPORT DESCRIPTION NOTOTBAL
BLOCK-REPORT TOTBAL
STREAM-REPORT MOLE-FLOW
PROP-DATA COMP-LIST    SP1 SP2 SP3
          CVAL MW 1 1 100. 60. 50.
;
;       SPECIFY THE COMPONENTS
;
COMPONENTS H2 HYDROGEN/N2 NITROGEN/SP1 SP1/SP2 SP2/SP3 SP3
;
;       SPECIFY FEED STREAMS
;
STREAM GASIN TEMP=400 PRES=15.2E06 FLASH-OPTION=NOFLASH
             MOLE-FLOW H2 0.0013375/N2 0.0013375
STREAM SLURRYIN TEMP=400 PRES=15.2E06 FLASH-OPTION=NOFLASH
             MASS-FLOW SP1 0.3159
;
;       SPECIFY BLOCK DATA
;
BLOCK PR USER                    ;USER INDICATES USER WRITTEN MODULE
        BLOCK-OPTIONS ENERGY-BAL=0
        SUBROUTINE USRDCL USRDCL
        PARAM NREAL=23 NINT=12
        INT 3 3 2 2 1 2 2 3 1 2 2 3    ;
        REAL 4000. 700. 3.81 30.48 407. .89 .45 1.2 .0000513 &
             20. 1.3 3213. 21000. 5850. 770.   &
             24. 12200. 24. 12200. 24. 12200. 24. 12200.
```

```
;
;DEFINITION OF PARAMETERS IN REAL AND INTEGER ARRAYS
;REAL ARRAY
;  1 - Length of preheater [cm]
;  2 - Length of reactor [cm]
;  3 - Diameter of preheater [cm]
;  4 - Diameter of reactor [cm]
;  5 - Temperature of furnace [deg C]
;  6 - Specific heat of gas [cal/gm/deg C]
;  7 - Weighted average specific heat of slurry [cal/gm/deg C]
;  8 - Preexponential factor for Hydrogen solubility temperature
;        dependance.
;  9 - Diffusivity of gas [sq.cm/sec]
;  10 - Surface tension of slurry [dyne/cm]
;  11 - Density of slurry [gm/cc]
;  12 - Preexponential factor for Hydrogen consumption kinetics [1/s]
;  13 - Activation energy for hydrogen consumption kinetics [cal/gmole]
;14 - Heat of reaction for hydrogen consumption [cal/gm]
;15 - Heat of dissolution [cal/gm]
;16- Arrhenius factor for reaction 1 in preheater [1/s]
;17 - Activation energy for reaction 1 in preheater [cal/gmole]
;18 - same as 16 for rxn 2 in preheater[1/s]
;19 - same as 17 for rxn 2 in preheater [cal/gmole]
;20 - same as 16 for rxn 1 in reactor [1/s]
;21 - same as 17 for rxn 1 in reactor [cal/gmole]
;22 - same as 16 for rxn 2 in reactor [1/s]
;23 - same as 17 for rxn 2 in reactor [cal/gmole]
;
;  INTEGER ARRAY
;  1 - No. of species reacting in preheater
;  2 - No. of species reacting in reactor
;  3 - No. of reactions in preheater
;  4 - No. of reactions in reactor
;  5 - Code of reactant for rxn 1 in preheater
;  6 - Code of product for rxn 1 in preheater
;  7 - Code of reactant for rxn 2 in preheater
;  8 - Code of product for rxn 2 in preheater
;  9 - Code of reactant for rxn 1 in reactor
;10 - Code of product for rxn 1 in reactor
;11 - Code of reactant for rxn 2 in reactor
;12 - Code of product for rxn 2 in reactor
;
;        IMPOSE DESIGN SPECIFICATIONS AND RUN TIME CRITERIA HERE
;
```

USER Model Subroutine USRDCL

```
      SUBROUTINE USRDCL (NSIN, NINFI, SIN1, SIN2, SIN3, SIN4,
     *                   SINFI, NSOUT, NINFO, SOUT1, SOUT2, SOUT3, SOUT4,
     *                   SINFO, NSUBS, IDXSUB, ITYPE, NINT, INT, NREAL,
     *                   REAL, IDS, NPO, NBOPST, NIW, IW, NW, W, NSIZE, SIZE)

      IMPLICIT REAL*8(A-H,O-Z)
      DOUBLE PRECISION L,KBARP,KBARR
      DIMENSION SIN1(1), SIN2(1), SIN3(1), SIN4(1),
     *          SINFI(1), SOUT1(1), SOUT2(1), SOUT3(1),
     *          SOUT4(1), SINFO(1), IDXSUB(NSUBS), ITYPE(NSUBS),
     *          INT(NINT), REAL(NREAL), IDS(2,13), NBOPST(3,NPO),
     *          IW(NIW), W(NW), SIZE(NSIZE)
      DIMENSION VG(5),VL(5),L(5),D(5)
      DIMENSION GAMMA(5),GAMS(5),GAMR(5),
     *  FLUX(5),HT(5),ALFA(5),TIME(5)
      DIMENSION RL(5),RP(5),CPO(10)
      DIMENSION ZKLA(5),EG(5)
      DIMENSION KBARP(20,20),KBARR(20,20),COEFFP(20,20)
      DIMENSION COEFFR(20,20),ECP(20,20),ECR(20,20),CPI(10)

      COMMON /USER/ RMISS, IMISS, NGBAL, IPASS, IRESTR, ICONVG,
     *              LMSG, LPMSG, KFLAG, NHSTRY, NRPT, NTRMNL, ISIZE
      COMMON /NCOMP/ NCC, NNCC
      COMMON /IDSCC/ IDSCC(2,1)
      COMMON /IDSNCC/ IDSNCC(2,1)
      COMMON /IDXNCC/ IDXNCC(1)
      COMMON /IDXCC/ IDXCC(1)
      COMMON /MW/ XMW(1)
      COMMON /RPTGLB/ IREPFL, ISUB(10)
      COMMON/Z1/ KBARP,ECP,COEFFP
      COMMON/Z11/ KBARR,ECR,COEFFR
      COMMON/Z2/ CPI
      COMMON /A/ VG,VL,L,D
      COMMON /B/ TIL,HIL,CGI,AGPI,ALPI,TEMPI,TEMW
      COMMON /C/ RHOA,RHOG,DI,SIG,R,G
      COMMON /D/ CPG,CPBAR,E,DHR,DHS,ZKBAR
      COMMON/DD/ HBAR
      COMMON /DDD/ DHSTAR,ESTAR,GAMMA,GAMS,GAMR,RL,RP
     *  ,FLUX,HT,ALFA
      COMMON /E/ ZKLA,EG
      COMMON/Z5/ TIME
      COMMON/Z15/ TEMPA,AGPA,ALPA,TEMPO,AGPO,ALPO
      COMMON/Z16/ ZRTEMP,ZRAG,ZRAL
      COMMON/Z6/ NSPH,NSPR
      COMMON/Z7/ CPO
```

```
      DO 1 J=1,20
      DO 1 I=1,20
      KBARP(I,J)=0.0
      KBARR(I,J)=0.0
      ECP(I,J)=0.0
      ECR(I,J)=0.0
      COEFFP(I,J)=0.0
      COEFFR(I,J)=0.0
    1 CONTINUE

      NSPH=INT(1)
      NSPR=INT(2)
      NKP=INT(3)
      NKR=INT(4)
      K=5
      KK=16
      DO 20 I=1,NKP
      II=INT(K)
      JJ=INT(K+1)
      COEFFP(II,JJ)=1.0
      KBARP(II,JJ)=REAL(KK)
      ECP(II,JJ)=REAL(KK+1)
      ECP(II,JJ)=ECP(II,JJ)/R/TIL
      K=K+2
      KK=KK+2
   20 CONTINUE

      DO 21 I=1,NKR
      II=INT(K)
      JJ=INT(K+1)
      COEFFR(II,JJ)=1.0
      KBARR(II,JJ)=REAL(KK)
      ECR(II,JJ)=REAL(KK+1)
      ECR(II,JJ)=ECR(II,JJ)/R/TIL
      K=K+2
      KK=KK+2
   21 CONTINUE

      CALL PHEATR
      CALL PHEATC
      CALL REATEM
      CALL REACTC
      CALL STEADY

C     .....Supply output
```

```
      RR=82.057
      R=1.987
      G=981.0
      TIL=SIN1(NCC+2)
      L(1)=REAL(1)
      L(2)=REAL(2)
      D(1)=REAL(3)
      D(2)=REAL(4)
      TH=REAL(5)
      CPG=REAL(6)
      CPBAR=REAL(7)
      HBAR=REAL(8)
      DI=REAL(9)
      SIG=REAL(10)
      RHOA=REAL(11)
      ZKBAR=REAL(12)
      E=REAL(13)
      DHR=REAL(14)
      DHS=REAL(15)
      TOT=SIN2(NCC+1)*SIN2(NCC+9)
      CPI(1)=SIN2(3)*XMW(3)/TOT
      CPI(2)=SIN2(4)*XMW(4)/TOT
      CPI(3)=SIN2(5)*XMW(5)/TOT
      WRITE(NTRMNL,*) ' CP1 =',CPI(1),'CP2 =',CPI(2),'CP3=',CPI(3)
      P=SIN1(NCC+3)/0.1013E06
      VOLG=SIN1(NCC+1)*1000.*RR*TIL/P
      TH=TH+273.
      VOLL=SIN2(NCC+1)*1000./RHOA*XMW(3)
      WRITE(NTRMNL,*) 'VOLL=',VOLL,'VOLG=',VOLG
      DO 10 I=1,2
      VG(I)=VOLG/(D(I)**2.0*0.786)
      VL(I)=VOLL/(D(I)**2.0*0.786)
10    CONTINUE

      CGI=P/(RR*TIL)*XMW(1)*SIN1(1)/SIN1(NCC+1)
      RHOG=CGI
      AGPI=1.0
      ALPI=0.0
      TEMPI=0.0
      TEMW=(TH-TIL)/TIL
      DHSTAR=DHS/(R*TIL)
      ESTAR=E/(R*TIL)
      HIL=HBAR*(EXP(-DHSTAR))
      CALL HYDRO(2)
      DO 11 I=1,2
      RL(I)=ZKLA(I)*L(I)*HIL/VG(I)
      GAMMA(I)=VL(I)/VG(I)
      RP(I)=ZKBAR*(1-EG(I))*L(I)/VG(I)
      TIME(I)=L(I)*(1.-EG(I))/VL(I)
      FLUX(I)=VG(I)*RHOG*CPG+VL(I)*RHOA*CPBAR
      GAMS(I)=(CGI*VG(I)*DHS)/TIL/FLUX(I)
      GAMR(I)=(CGI*VG(I)*DHR)/TIL/FLUX(I)
      BETA=0.00+5
      HT(I)=BETA*VL(I)**0.8/D(I)**0.2
      ALFA(I)=HT(I)/D(I)*L(I)/FLUX(I)
11    CONTINUE
```

```
      SOUT1(1)=VOLG*ZRAG*1.0E-03
      SOUT2(1)=VOLL*ZRAL*1.0E-03
      SOUT1(2)=SIN1(2)*XMW(2)
      SOUT2(2)=0.0
      DO 30 I=3,NCC
      SOUT1(I)=0.0
      SOUT2(I)=VOLL*RHOA*CP0(I-2)*1.0E-03
30    CONTINUE
      SUM1=0.0
      SUM2=0.0
      SUM3=0.0
      SUM4=0.0
      DO 31 I=1,NCC
      SUM1=SUM1+SOUT1(I)
      SUM2=SUM2+SOUT2(I)
      SOUT1(I)=SOUT1(I)/XMW(I)
      SOUT2(I)=SOUT2(I)/XMW(I)
      SUM3=SUM3+SOUT1(I)
      SUM4=SUM4+SOUT2(I)
31    CONTINUE
      AM1=SUM1/SUM3
      AM2=SUM2/SUM4
      SOUT1(NCC+9)=AM1
      SOUT2(NCC+9)=AM2
      SOUT1(NCC+1)=SUM1/AM1
      SOUT2(NCC+1)=SUM2/AM2
      SOUT1(NCC+2)=ZRTEMP
      SOUT1(NCC+3)=SIN1(NCC+3)
      SOUT2(NCC+2)=ZRTEMP
      SOUT2(NCC+3)=SIN2(NCC+3)

      RETURN
      END
```

ASPEN Generated Output

DESCRIPTION

THIS IS AN EXAMPLE FOR ADAPTING USER WRITTEN MODELS TO THE ASPEN SIMULATOR. THE PROGRAM CHOSEN IS THE DIRECT COAL LIQUEFACTION ONE. THE ONLY PIECES OF EQUIPMENT ENCOUNTERED IN THE FLOWSHEET ARE THE PREHEATER AND REACTOR, WHICH ARE LUMPED INTO ONE BLOCK CALLED PR.

RUN CONTROL INFORMATION

TYPE OF RUN: NEW

INPUT FILE NAME: INPUT

INPUT PROBLEM DATA FILE NAME: RUN1 UPDATE NO. 0

MAIN CALLING PROGRAM NAME: RUN1

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

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SIMULATION OF DIRECT COAL LIQUEFACTION REACTOR AND PREHEATER
FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
GASOUT	PR	----	SLURRYOU	PR	----
GASIN	----	PR	SLURRYIN	----	PR

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
PR	GASIN SLURRYIN	GASOUT SLURRYOU

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:
PR

OVERALL FLOWSHEET BALANCE

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
H2	0.133750E-02	0.623289E-03	0.533990
N2	0.133750E-02	0.133750E-02	0.000000E+00
SP1	0.315900E-02	0.816233E-04	0.974162
SP2	0.000000E+00	0.268106E-03	-1.00000
SP3	0.000000E+00	0.583303E-02	-1.00000
TOTAL BALANCE			
MOLE(KMOL/SEC)	0.583400E-02	0.814354E-02	-0.283604
MASS(KG/SEC)	0.356064	0.354624	0.404380E-02
ENTHALPY(WATT	0.356064E+30	0.354624E+30	0.404380E-02

SIMULATION OF DIRECT COAL LIQUEFACTION REACTOR AND PREHEATER
U-O-S BLOCK SECTION

USER-MODEL (USER): PR
INPUT STREAMS GASIN SLURRYIN
OUTPUT STREAMS GASOUT SLURRYOU
PROPERTY OPTION SET SYSOP0

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/SEC)			
H2	0.133750E-02	0.623289E-03	0.533990
N2	0.133750E-02	0.133750E-02	0.000000E+00
SP1	0.315900E-02	0.816233E-04	0.974162
SP2	0.000000E+00	0.268106E-03	-1.00000
SP3	0.000000E+00	0.583303E-02	-1.00000
TOTAL BALANCE			
MOLE(KMOL/SEC)	0.583400E-02	0.814354E-02	-0.283604
MASS(KG/SEC)	0.356064	0.354624	0.404380E-02
ENTHALPY(WATT	0.356064E+30	0.354624E+30	0.404380E-02

DESCRIPTION OF STREAM CLASS CONVEN

STREAM CLASS : CONVEN
SUBSTREAMS : MIXED
SUBSTRM CLASS: MIXED

GASOUT SLURRYOU GASIN SLURRYIN

STREAM ID		GASOUT	SLURRYOU	GASIN	SLURRYIN
FROM :		PR	PR		
TO :				PR	PR
CLASS:		CONVEN	CONVEN	CONVEN	CONVEN
SUBSTREAM: MIXED		STRUCTURE: CONVENTIONAL			
H2	KMOL/SEC	.48227-03	.14102-03	0.0013	0.0
N2	KMOL/SEC	0.0013	0.0	0.0013	0.0
SP1	KMOL/SEC	0.0	.81623-04	0.0	0.0031
SP2	KMOL/SEC	0.0	.26811-03	0.0	0.0
SP3	KMOL/SEC	0.0	0.0058	0.0	0.0
TOTAL	KMOL/SEC	0.0018	0.0063	0.0026	0.0031
TEMP	K	743.6546	743.6546	400.0000	400.0000
PRES	N/SQM	.15200+08	.15200+08	.15200+08	.15200+08
ENTHALPY	J/KMOL	MISSING	MISSING	MISSING	MISSING
VFRAC		MISSING	MISSING	MISSING	MISSING
LFRAC		MISSING	MISSING	MISSING	MISSING
AVG MW		21.1233	49.9992	15.0145	100.0000

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