Appendix I-A

CONTENTS

I-A-1 User Manual for MTG

Use of Simulator

a. Fluidized Bed Reactor Model

This manual describes the use of the simulators. To use the simulator, the user must provide the following information:

- Design Parameters and Operating Conditions

  Length of reactor (cm)

  Diameter of reactor (cm)

  Reactor Pressure (psig)

  Reactor Temperature (deg F)

  Charge rate of methanol (ml/hr)

- Catalyst Properties

  Voidage at minimum fluidization

  velocity at minimum fluidization (cm/sec)

- Physico-Chemical Parameter

  Diffusivity of gas (cm^2/sec)

The above input data are entered via an interactions program, INPUT.FOR. A file called FB.DAT is created on executing this program. Then the main program, FBMODL.FOR can be executed in a batch mode. Since the software package, COLSYS.FOR (Ascher et al. (1981)), which currently resides in the mathematical library at the University of Pittsburgh is used, the program is executed by invoking the command, EX FBMODL.FOR, MTH:COLSYS.REL.

The following subroutines are used in the simulator

SUBROUTINE	PURPOSE
INPUT	Reads input data, calculates transfer coefficients.
FSUB	Evaluates the differential equations
DFSUB	Evaluates the Jacobian of the differential equation
GSUB	Evaluates the boundary conditions
DGSUB	Evaluates the partials of the boundary condition

The subroutines, FSUB, DFSUB, GSUB and DBSUB are user supplied subroutines that are needed by COLSYS.

The output from the simulator is contained in a file called OUTPUT.DAT. It includes concentration profiles along the length of the reactor, conversion of methanol and dimensionless concentrations of A (methanol and dimethylether), B (olefins) and C (paraffins and aromatics) at the exit. A typical run showing both input and output is given.

b. Fixed Bed Reactor Model

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

.Design parameters and operating conditions

Length of reactor (m)

Diameter of reactor (m)

Reactor pressure (psig)

Inlet temperaure to MTG reactor (deg F)

Inlet temperature to dehydration reaction (deg F)

Charge rate of methanol (kg/sec)

The kinetic data are stored in a file called MIH.DAT and the specific heats and heats of formation are stored in a file called PROP.DAT. The user does not have to input this information. The design parameters and operating conditions are entered via an interactive program, INPUT1.FOR and a file, DGN.DAT, containing this data is created on running this program. After creation of DGN.DAT, the main program, FXBR.FOR can be executed in a batch mode. The program is executed by invoking the command

EX FXBR.FOR, MTH:DLSODE.REL

The software package, DLSODE.FOR, resides in the mathematical library at the University of Pittsburgh and is used for solving the system of stiff differential equations.

The following subroutines are used in the simulator

SUBROUTINE NAME	PURPOSE
INPUT	reads in input data
FCN1	Evaluates the differential equations
HEAT	Evaluates the heat of formation and specific heats of reacting species at reaction temperature
DHYDN	Evaluates the equilibrium conversion and outlet tempertaure from the dehydration reactor.

The subroutine FCN1 is a user supplied subroutine that is needed by DLSODE.

The output from the simulator is contained in the following files:

Dehydration reactor results: DHYDN.DAT

MTG reactor resutls: OUTPT1.DAT

Input data: DATA.DAT

Physico-chemical and kinetic data: PARAM.DAT

Note that the reactor can be simulated either as an isothermal or an adiabatic reactor.

I-A-2 Program Listing - Input Data to Fluidized Bed Reactor Module

```
C     ------------------------------------------------------------
C           This program is used to input data to the main simulation
C     routine. It is interactive and creates an input file called FB.DAT
C     on execution. Input data are entered in free format.
C     ------------------------------------------------------------

      IMPLICIT REAL*8(A-H,O-Z)
      CHARACTER*20 NAME
      OPEN (UNIT=20,FILE='FB.DAT')

      WRITE(6,10)
 10   FORMAT(5X,'ENTER THE RUN NUMBER FROM THE MOBIL REPORT ' $)
      READ(5,20) NAME
      WRITE(20,20) NAME
 20   FORMAT(A20)
      WRITE(6,50)
 50   FORMAT(//5X,'ENTER THE FOLLOWING PARAMETERS IN FREE FORMAT',/,
     * 5X,'LENGTH OF REACTOR (cm) ',/,
     * 5X,'DIAMETER OF REACTOR (cm) ',/,
     * 5X,'DIFFUSIVITY OF GAS (cm**2/sec)',/)
      READ(5,*) AL,DT,DG
      WRITE(6,100)
100   FORMAT(//5X,'ENTER THE FOLLOWING PARAMETERS IN FREE FORMAT',/,
     * 5X,'VOIDAGE AT MINIMUM FLUIDIZATION',/,
     * 5X,'VELOCITY AT MINIMUM FLUIDIZATION (cm/sec) ',/,
     * 5X,'REACTOR PRESSURE (psig)',/,
     * 5X,'REACTOR TEMPERATURE (deg F) ',/,
     * 5X,'CHARGE RATE (ml/hr) ',/)
      READ(5,*) EMF,UMF,PT,TEMP,CHG
      PT=(PT+14.7)/14.7
      TEMP=(TEMP-32.)*5./9.+273.
      RHOM=0.792              ! DENSITY OF METHANOL AT METERING CONDITIONS
      CHG=CHG*RHOM/3600.      ! CONVERT CHARGE RATE TO gm/sec
      RHOV=PT*32./82.06/TEMP ! DENSITY OF VAPOR AT REACTOR CONDITIONS
      PI=3.1416
      AREA=PI*DT**2./4.
      U=CHG/RHOV/AREA
      CAO=RHOV/32.
      A=EXP(16.2083)
      AK1=A*DEXP(-10333./TEMP)
      AK2=0.98
      WRITE(20,*) U,UMF,EMF,AL,DG,AK1,AK2,DT,CAO,TEMP,PT
      WRITE(6,99)
99    FORMAT(//5X,'INPUT DATA HAVE BEEN ENTERED IN FILE FB.DAT',/,
     * 5X,'FLUIDIZED BED MODEL CAN NOW BE RUN',//)
      CLOSE(UNIT=20)
      STOP
      END
```

I-A-3 Sample Run Showing Interactive Input

```
ENTER THE RUN NUMBER FROM THE MOBIL REPORT >CT-231-1-2

ENTER THE FOLLOWING PARAMETERS IN FREE FORMAT
LENGTH OF REACTOR (cm)
DIAMETER OF REACTOR (cm)
DIFFUSIVITY OF GAS (cm**2/sec)

>762. 10.12 0.18

ENTER THE FOLLOWING PARAMETERS IN FREE FORMAT
VOIDAGE AT MINIMUM FLUIDIZATION
VELOCITY AT MINIMUM FLUIDIZATION (cm/sec)
REACTOR PRESSURE (psig)
REACTOR TEMPERATURE (deg F)
CHARGE RATE (ml/hr)

>0.53 0.15 25. 751. 22463.

INPUT DATA HAVE BEEN ENTERED IN FILE FB.DAT
FLUIDIZED BED MODEL CAN NOW BE RUN
```

I-A-4 Program Listing - Fluidized Bed Reactor Module

```
C     ------------------------------------------------------------
C           FLUIDIZED BED REACTOR MODEL USING FRYER-POTTER'S
C                 COUNTERCURRENT BACKMIXING MODEL
C     ------------------------------------------------------------

C           The boundary value ODE's are solved using the software
C     package COLSYS. For details on COLSYS and its parameters the
C     reader is referred to the paper by Christianson et. al. (ACM
C     Transactions on Mathematical Software, vol.2, 229(1981)).

      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION FSPACE(20000),ZETA(9),TOL(9),Z(9),ISPACE(2000),
     *          M(9),IPAR(11),LTOL(9)
      EXTERNAL FSUB,DFSUB,GSUB,DGSUB,DUMMY
      COMMON /HYD/ EPS2,FN,UO,UG2O,UGCO,UGPO
      COMMON /CN/ CAO,CBO,CCO,AL

      OPEN (UNIT=25,FILE='OUTPUT.DAT')
      CALL INPUT
      NCOMP=3
      DO 10 I=1,NCOMP
10    M(I)=1
      ALEFT=0.DO
      ARIGHT=1.DO
      DO 12 I=1,6
12    ZETA(I)=0.DO
      DO 13 I=7,9
13    ZETA(I)=1.DO

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

      IPAR(4)=9
      IPAR(5)=20000
      IPAR(6)=2000
      IPAR(7)=1

      DO 4 I=1,9
      LTOL(I)=I
4     TOL(I)=1.0D-4

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

      IF(IFLAG.NE.1) GO TO 99
      WRITE(25,29)
29    FORMAT('1',5X,'DIMENSIONLESS CONCENTRATION PROFILES OF A,B & C',
     *       ///,T10,'X',T20,'CA',T30,'CB',T40,'CC',//)
      X=0.0
      DO 31 I=1,11
      CALL APPSLN(X,Z,FSPACE,ISPACE)
      WRITE(25,27) X,Z(1),Z(4),Z(7)
      X=X+0.1
31    CONTINUE
      CA=(UG2O*Z(1)+(UO-UG2O)*Z(2))/UO
      CB=(UG2O*Z(4)+(UO-UG2O)*Z(5))/UO
      CC=(UG2O*Z(7)+(UO-UG2O)*Z(8))/UO
      CONVN=(CAO-CA)/CAO
      WRITE(25,28) CA,CB,CC,CONVN
28    FORMAT(//5X,'EXIT CONCENTRATIONS OF A,B AND C',/,5X,3(X,F12.8),
```

```
     *        //,5X,'CONVERSION OF METHANOL = ',F12.6)
              CLOSE (UNIT=25)
              STOP
88            FORMAT(2(2X,E12.5))
27            FORMAT(T10,F6.2,T20,F9.6,T30,F9.6,T40,F9.6)
99            WRITE(6,*) 'IFLAG = ',IFLAG
              STOP
              END

              SUBROUTINE FSUB(X,Z,F)
              IMPLICIT REAL*8(A-H,O-Z)
              DIMENSION Z(9),F(9)
              COMMON /AK/ AK1,AKBC,AKCP,AK2,ALPHA
              COMMON /HYD/ EPSB,FW,UO,UGBO,UGCO,UGPO
              COMMON /CN/ CAO,CBO,CCO,AL

              F(1)=-(AKBC*(Z(1)-Z(2)))*AL*EPSB/UGBO
              F(2)=-(AKBC*(Z(2)-Z(1))+AKCP*(Z(2)-Z(3))+AK1*Z(2)*FW)*EPSB*AL/UGCO
              F(3)=-(AKCP*(Z(3)-Z(2))*EPSB+AK1*Z(3)*(1.-EPSB*(1.+FW)))*AL/UGPO
              F(4)=-(AKBC*(Z(4)-Z(5)))*AL*EPSB/UGBO
              F(5)=-(AKBC*(Z(5)-Z(4))+AKCP*(Z(5)-Z(6))-AK1*Z(2)*FW+AK2*Z(5)*FW)
     *             *EPSB*AL/UGCO
              F(6)=-(AKCP*(Z(6)-Z(5))*EPSB-AK1*Z(3)*(1.-EPSB*(1.+FW))
     *             +AK2*Z(6)*(1.-EPSB*(1.+FW)))*AL/UGPO
              F(7)=-(AKBC*(Z(7)-Z(8)))*AL*EPSB/UGBO
              F(8)=-(AKBC*(Z(8)-Z(7))+AKCP*(Z(8)-Z(9))-AK2*Z(5)*FW)*EPSB*AL/UGCO
              F(9)=-(AKCP*(Z(9)-Z(8))*EPSB-AK2*Z(6)*(1.-EPSB*(1.+FW)))*AL/UGPO

              RETURN
              END

              SUBROUTINE DFSUB(X,Z,DF)
              IMPLICIT REAL*8(A-H,O-Z)
              DIMENSION DF(9,9),WORK1(9),WORK2(9),Z(9)

              EPS=1.D-7

              DO 10 J=1,9
              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=1,9
10            DF(I,J)=(WORK1(I)-WORK2(I))*.5/EPS
              RETURN
              END

              SUBROUTINE GSUB(I,Z,G)
              IMPLICIT REAL*8(A-H,O-Z)
              DIMENSION Z(9)
              COMMON /CN/ CAO,CBO,CCO,AL
              COMMON /HYD/ EPSB,FW,UO,UGBO,UGCO,UGPO

              GO TO (10,20,30,40,50,60,70,80,90),I
10            G=Z(1)-CAO
              RETURN
20            G=(UO-UGBO)*CAO-UGPO*Z(3)-UGCO*Z(2)
              RETURN
30            G=Z(4)-CBO
```

```
      RETURN
40    G=UGPO*Z(6)+UGCO*Z(5)-(UO-UG3O)*C3O
      RETURN
50    G=Z(7)-CCO
      RETURN
60    G=UGPO*Z(9)+UGCO*Z(8)-(UO-UG3O)*C3O
      RETURN
70    G=Z(2)-Z(3)
      RETURN
80    G=Z(5)-Z(6)
      RETURN
90    G=Z(8)-Z(9)
      RETURN
      END

      SUBROUTINE DGSUB(I,Z,DG)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Z(9),DG(9)
      COMMON /HYD/ EPS3,FW,UO,UG3O,UGCO,UGPO

      DO 11 J=1,9
11    DG(J)=0.0

      GO TO (10,20,30,40,50,60,70,80,90),I
10    DG(1)=1.0
      RETURN
20    DG(2)=-UGCO
      DG(3)=-UGPO
      RETURN
30    DG(4)=1.0
      RETURN
40    DG(6)=UGPO
      DG(5)=UGCO
      RETURN
50    DG(7)=1.0
      RETURN
60    DG(8)=UGCO
      DG(9)=UGPO
      RETURN
70    DG(2)=1.0
      DG(3)=-1.0
      RETURN
80    DG(5)=1.0
      DG(6)=-1.0
      RETURN
90    DG(8)=1.0
      DG(9)=-1.0
      RETURN
      END

      SUBROUTINE DUMMY
      RETURN
      END

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

C     List of parameters:
C     -------------------
```

```
C       AK1,AK2 - First order kinetic rate constants (1/s)
C       AKBC    - Transfer coefficient from bubble to cloud-wake (1/s)
C       AKCP    - Transfer coefficient from cloud-wake to emulsion (1/s)
C       AL - length of reactor (cm)
C       CAO,CBO,CCO - Initial concentrations of A,B,C.
C       DB - bubble diameter (cm)
C       DG - diffusivity of gas
C       DT - diameter of reactor (cm)
C       EMF - Voidage at minimum fluidization
C       EPSB - Bubble phase voidage
C       FW - solid fraction
C       UO - superficial gas velocity (cm/sec)
C       UGBO - superficial velocity of bubble phase (cm/sec)
C       UGCO - superficial velocity of cloud-wake phase (cm/sec)
C       UGPO - superficial velocity of particulate phase (cm/sec)
C       UMF - superficial velocity at minimum fluidization
C       ----------------------------------------------------------------

        COMMON /AK/ AK1,AKBC,AKCP,AK2,ALPHA
        COMMON /CN/ CAO,CBO,CCO,AL
        COMMON /HYD/ EPSB,FW,UO,UGBO,UGCO,UGPO
        CHARACTER*20 NAME

        OPEN(UNIT=20,FILE='FB.DAT')
        READ(20,20) NAME
20      FORMAT(A20)
        READ(20,*) UO,UMF,EMF,AL,DG,AK1,AK2,DT,CACTO,TEMP,PT
        CAO=1.0
        CBO=0.0
        CCO=0.0
        G=981.0
        FW=1.0
        DB=7.5
        ALPHA=1.0
        UBR=0.71*(G*DB)**.5
        IDUM=0
23      T1=UO+UMF*FW+UBR
        T2=4.*UMF*UBR*(1.+FW)

        UA=(T1+SQRT(T1**2.-T2))/2.
        UGBO=(UO-UMF)/(1.-UMF*(1.+FW)/UA)
        EPSB=UGBO/UA
        IF(IDUM.EQ.1) GO TO 22
        IF(EPSB.LT.(1./3.)) GO TO 22
        FW=(1.-EPSB)/2./EPSB
        IDUM=1
        GO TO 23
22      CONTINUE
        UGCO=FW*EMF*UGBO
        UGPO=UMF*(1.-EPSB*(1.+FW))*(1.+EMF*FW)-UO*FW*EMF
        AKBC=4.5*UMF/DB+5.85*G**.25*DG**.5/DB**1.25
        AKCP=6.78*(EMF*DG*UA/DB**3.)**.5

        WRITE(25,30) NAME
30      FORMAT(T30,'SIMULATION OF MTG RUN # ',A20)
        WRITE(25,100) TEMP,PT,UO,UGBO,UGCO,UGPO,UA,EPSB,FW,AKBC,AKCP
     *                ,AK1,AK2
100     FORMAT(///,5X,'LIST OF INPUT DATA:',///,
     *  5X,'TEMPERATURE OF FLUID BED (K) ',T50,F8.4,//,
     *  5X,'OPEARTING PRESSURE (atm) ',T50,F8.4,//,
```

```
*  5X,'SUPERFICIAL GAS VELOCITY (cm/sec)  ',T50,F8.4,//,
*  5X,'BUBBLE PHASE VELOCITY (cm/sec)',T50,F8.4,//,
*  5X,'CLOUD PHASE VELOCITY (cm/sec)',T50,F8.4,//,
*  5X,'PARTICULATE PHASE VELOCITY (cm/sec)',T50,F8.4,//,
*  5X,'BUBBLE RISE VELOCITY (cm/sec)',T50,F8.4,//,
*  5X,'BUBBLE PHASE VOIDAGE',T50,F8.4,//,
*  5X,'SOLID FRACTION',T50,F8.4,//,
*  5X,'MASS TRANSFER COEFNT (B-TO-C) (1/sec) ',T50,F8.4,//,
*  5X,'MASS TRANSFER COEFNT (C-TO-P) (1/sec)',T50,F8.4,//,
*  5X,'FIRST ORDER KINETIC CONSTANT k1 (1/sec)',T50,F8.4,//,
*  5X,'FIRST ORDER KINETIC CONSTANT k2 (1/sec)',T50,F8.4,/)


   CLOSE(UNIT=20)
   RETURN
   END
```

I-A-5 Sample Output from Simulation of Fluidized Bed Reactor

SIMULATION OF MTG RUN # CT-231-1-2

LIST OF INPUT DATA:

TEMPERATURE OF FLUID BED (K)	672.4444
OPEARTING PRESSURE (atm)	2.7007
SUPERFICIAL GAS VELOCITY (cm/sec)	39.2286
BUBBLE PHASE VELOCITY (cm/sec)	39.1830
CLOUD PHASE VELOCITY (cm/sec)	16.1333
PARTICULATE PHASE VELOCITY (cm/sec)	-16.0877
BUBBLE RISE VELOCITY (cm/sec)	100.0839
BUBBLE PHASE VOIDAGE	0.3915
SOLID FRACTION	0.7769
MASS TRANSFER CFFNT (B-TO-C) (1/sec)	1.2091
MASS TRANSFER CFFNT (C-TO-P) (1/sec)	1.0200
FIRST ORDER KINETIC CONSTANT k1 (1/sec)	2.2058
FIRST ORDER KINETIC CONSTANT k2 (1/sec)	0.9800

DIMENSIONLESS CONCENTRATION PROFILES OF A,B & C

X	CA	CB	CC
0.00	1.000000	0.000000	0.000000
0.10	0.536803	0.138476	0.324721
0.20	0.299958	0.182407	0.517635
0.30	0.167623	0.170766	0.661611
0.40	0.093674	0.140452	0.765874
0.50	0.052348	0.107941	0.839711
0.60	0.029254	0.079585	0.891161
0.70	0.016343	0.057083	0.926574
0.80	0.009134	0.040145	0.950721
0.90	0.005106	0.027847	0.967047
1.00	0.002874	0.019535	0.977590

EXIT CONCENTRATIONS OF A,B AND C

0.002872 0.019528 0.977600

CONVERSION OF METHANOL = 0.997128

I-A-6 Program Listing - Input Data to Fixed Bed Reactor Module

```
C     ------------------------------------------------------------
C     This program is used to input the design parameters required
C     for the simulation of the fixed bed reactor.
C     ------------------------------------------------------------

      IMPLICIT REAL*8(A-H,O-Z)
      OPEN (UNIT=23,FILE='DGN.DAT')
      WRITE(6,10)
 10   FORMAT(5X,'IF SIMULATION OF DEHYDRATION REACTOR AND MTG',/,
     *       5X,'REACTOR DESIRED, SPECIFY IND=2. IF ONLY MTG',/,
     *       5X,'REACTOR PRESENT, SPECIFY IND=1.',/,
     *       5X,'WHAT IS THE VALUE OF IND ? '$)
      READ(5,*) IND
      WRITE(6,21)
 21   FORMAT(//5X,'IF PRINTING OF PHYSICO-CHEMICAL PROPERTIES',/,
     * 5X,'AND KINETIC PARAMETERS IS TO BE SUPPRESSED, SPECIFY',/,
     * 5X,'IPRINT=0,OTHERWISE SET IPRINT=1',/,
     * 5X,'WHAT IS THE VALUE OF IPRINT ? '$)
      READ(5,*) IPRINT
      WRITE(6,31)
 31   FORMAT(//5X,'FOR ISOTHERMAL OPERATION SPECIFY ISO=1',/,
     * 5X,'OTHERWISE ISO=0',/,
     * 5X,'WHAT IS THE VALUE OF ISO ? '$)
      READ(5,*) ISO
      WRITE(23,*)IND,IPRINT,ISO
      WRITE(6,11)
 11   FORMAT(//5X,'LIST OF DESIGN PARAMETERS:',//,
     * 5X,'SPECIFY THE FOLLWING PARAMETERS IN FREE FORMAT',//,
     * 5X,'INLET TEMPERATURE TO DEHYDRATION REACTOR (deg F)',/,
     * 5X,'INLET TEMPERATURE TO MTG REACTOR (deg F)',/,
     * 5X,'OPERATING PRESSURE OF MTG REACTOR (psig)',/,
     * 5X,'RECYCLE RATIO (mol recycle gas/mol methanol fed)',/,
     * 5X,'FEED RATE OF METHANOL (kg/sec)',/,
     * 5X,'FEED RATE OF WATER (kg/sec)',/,
     * 5X,'LENGTH OF MTG REACTOR (m) ',/,
     * 5X,'DIAMETER OF MTG REACTOR (m)',///)
      READ(5,*) TIN,TINR,PT,RCYCL,FMEOH,FH2O,AL,DT
      TIN=(TIN-32.)*5./9.+273.15
      TINR=(TINR-32.)*5./9.+273.15
      PT=(PT+14.7)/14.7
      WRITE(23,*) TIN,TINR,PT,RCYCL,FMEOH,FH2O,AL,DT

      WRITE(6,12)
 12   FORMAT(5X,'SPECIFY COMPOSITION OF RECYCLE GAS IN TERMS',/,
     * 5X,'OF MOLE FRACTIONS',//)
      WRITE(6,13)
 13   FORMAT(5X,'MOLE FRACTION OF METHANE ',/,
     * 5X,'MOLE FRACTION OF HYDROGEN',/,
     * 5X,'MOLE FRACTION OF CARBON MONOXIDE',/,
     * 5X,'MOLE FRACTION OF PROPYLENE',/,
     * 5X,'MOLE FRACTION OF PROPANE',/,
     * 5X,'MOLE FRACTION OF ETHYLENE',/,
     * 5X,'MOLE FRACTION OF ETHANE',///)
      READ(5,*) C1,C2,C3,C4,C5,C6,C7
      WRITE(23,*) C1,C2,C3,C4,C5,C6,C7

      WRITE(6,14)
 14   FORMAT(//5X,'INPUT DATA HAVE BEEN ENTERED IN FILE DGN.DAT',/,
     * 5X,'FIXED BED REACTOR MODEL CAN BE RUN IN BATCH MODE ',///)
      CLOSE (UNIT=23)
```

```
STOP
END
```

I-A-7 Sample Run Showing Interactive Input

```
IF SIMULATION OF DEHYDRATION REACTOR AND MTG
REACTOR DESIRED, SPECIFY IND=2. IF ONLY MTG
REACTOR PRESENT, SPECIFY IND=1.
WHAT IS THE VALUE OF IND ? >2

IF PRINTING OF PHYSICO-CHEMICAL PROPERTIES
AND KINETIC PARAMETERS IS TO BE SUPPRESSED, SPECIFY
IPRINT=0,OTHERWISE SET IPRINT=1
WHAT IS THE VALUE OF IPRINT ? >1

FOR ISOTHERMAL OPERATION SPECIFY ISO=1
OTHERWISE ISO=0
WHAT IS THE VALUE OF ISO ? >0

LIST OF DESIGN PARAMETERS:

SPECIFY THE FOLLWING PARAMETERS IN FREE FORMAT

INLET TEMPERATURE TO DEHYDRATION REACTOR (deg F)
INLET TEMPERATURE TO MTG REACTOR (deg F)
OPERATING PRESSURE OF MTG REACTOR (psig)
RECYCLE RATIO (mol recycle gas/mol methanol fed)
FEED RATE OF METHANOL (kg/sec)
FEED RATE OF WATER (kg/sec)
LENGTH OF MTG REACTOR (m)
DIAMETER OF MTG REACTOR (m)

>608. 704. 300. 4.5 5.88E-05 1.204E-05 0.2395 0.033


SPECIFY COMPOSITION OF RECYCLE GAS IN TERMS
OF MOLE FRACTIONS


MOLE FRACTION OF METHANE
MOLE FRACTION OF HYDROGEN
MOLE FRACTION OF CARBON MONOXIDE
MOLE FRACTION OF PROPYLENE
MOLE FRACTION OF PROPANE
MOLE FRACTION OF ETHYLENE
MOLE FRACTION OF 1-BUTENE

>0.4 0.1 0.1 0.1 0.1 0.1 0.1


INPUT DATA HAVE BEEN ENTERED IN FILE DGN.DAT
FIXED BED REACTOR MODEL CAN BE RUN IN BATCH MODE
```

I-A-8 Program Listing - Fixed Bed Reactor Module

```
C     ---------------------------------------------------------------
C             ONE-DIMENSIONAL PSEUDO-HOMOGENEOUS FIXED BED
C                       REACTOR MODEL
C     ---------------------------------------------------------------

C           This program models the fixed bed reactor used in the MTG
C     process with a one-dimensional pseudo-homogeneous model. The
C     reaction scheme is that of Mihail et. al (1983b). The continuity
C     equations for the species comprise a set of stiff first-order
C     differential equations. The software package MTH:DLSODE.REL is
C     used for the solution of these equations.
C     ---------------------------------------------------------------

C     Definition of components:
C     CH3OH -1 CH3OCH3 -4 H2O -5 CO -2 H2 -3
C     OLEFINS -7 8 9 10 11 12
C     PARAFFINS - 13 19 21 22 23
C     AROMATICS - 26 27 28 29 31 32 33 34 35 36 37
C     DIENES & CYCLODIENES - 18 20 24 25
C     ---------------------------------------------------------------

      IMPLICIT REAL*8(A-H,O-Z)
      CHARACTER*30 NAM1(45)
      DIMENSION Y(45),ATOL(45),RWORK(2452),IWORK(65),XMW(45),WT(45)
      EXTERNAL FCN1,DUMMY

      COMMON /NAME/ NAM1
      COMMON /INT1/ NR,NSP
      COMMON /INT2/ IND
      COMMON /AINP/ TIN,PT,FMEOH,FH2O
      COMMON /DGN/ AL,AREA
      COMMON /DGN1/ TINR,FT,PA
      COMMON /RC/ FC1,FC2,FC3,FC4,FC5,FC6,FC7
      COMMON /AW/ XMW

      CALL INPUT
      FDME=0.0
      IF(IND.EQ.1) GO TO 33
      CALL DMYDN(TIN,FMEOH,FH2O,FDME,ADT,CONVN)
      OPEN (UNIT=23,FILE='DMYDN.DAT')
      WRITE(23,41) ADT,CONVN*100.,FMEOH,FDME,FH2O
33    FT=FMEOH+FH2O+FDME+FC1+FC2+FC3+FC4+FC5+FC6+FC7
      PA=(FMEOH+FH2O+FDME)*PT/FT

      NEQ=NSP+1
      T=0.0D0
      DO 11 I=1,NEQ
11    Y(I)=0.0D0

      Y(1)=FMEOH/FT
      Y(2)=FC3/FT
      Y(3)=FC2/FT
      Y(4)=FDME/FT
      Y(5)=FH2O/FT
      Y(7)=FC6/FT
      Y(8)=FC4/FT
      Y(19)=FC7/FT
      Y(13)=FC1/FT
      Y(21)=FC5/FT
```

```
 55     FORMAT(////,5X,'HYDROCARBON DISTRIBUTION ON WATER FREE BASIS'
     *  ,//,5X,'WT. PERCENT OLEFINS ',T50,F12.5,/,
     *  5X,'WT. PERCENT PARAFFINS ',T50,F12.5,/,
     *  5X,'WT. PERCENT AROMATICS ',T50,F12.5,//)
        WRITE(6,751)
 751    FORMAT(///5X,'SIMULATION OF FIXED BED COMPLETE',/,
     *  5X,'OUTPUT CAN BE FOUND IN THE FOLLOWING FILES:',//,
     *  5X,'DEHYDRATION REACTOR RESULTS       : DHYDN.DAT',/,
     *  5X,'MTG REACTOR RESULTS               : OUTPT1.DAT',/,
     *  5X,'INPUT DATA                        : DATA.DAT',/,
     *  5X,'PHYSICO-CHEMICAL & KINETIC DATA   : PARAM.DAT',///)
        CLOSE (UNIT=25)
        CLOSE (UNIT=26)
        STOP

 20     WRITE(6,90) ISTATE
 90     FORMAT(////5X,'ERROR HALT... ISTATE = ',I3)
 41     FORMAT(5X,'CONDITIONS AT EXIT OF DEHYDRATION REACTOR:',//,
     *  5X,'EXIT TEMPERATURE FROM DEHYDRATION REACTOR (K)',T70,F9.5,//,
     *  5X,'EQUILIBRIUM METHANOL CONVERSION IN DEHYDRATION REACTOR (%)',
     *  T70,F9.5,//,
     *  5X,'FLOW RATE OF METHANOL (kmol/s) ',T70,E12.7,//,
     *  5X,'FLOW RATE OF DME (kmol/s) ',T70,E12.7,//
     *  5X,'FLOW RATE OF WATER (kmol/s)',T70,E12.7,//)
 45     FORMAT('1',5X,'TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG',
     *  ' REACTOR LENGTH',//,5X,'X = ',F8.3,5X,'TEMPERATURE = ',F9.5,
     *  1X,'K',//,5X,'SPECIES NAME ',15X,'WEIGHT PERCENT',//)
 44     FORMAT(5X,A30,2X,F9.5)

        STOP
        END

        SUBROUTINE DHYDN(TIN,FMEOH,FH2O,FDME,ADT,CONVN)

C       This subroutine evaluates the equilibrium conversion and outlet
C       temperature from the dehydration reactor.

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

        FMO=FMEOH
        IF(FH2O.EQ.0.0) GO TO 11
        CONVN=(-0.042*TIN+101.80)/100.
        ADT=0.833*TIN+193.62
        GO TO 21
 11     CONVN=(-0.0315*TIN+99.788)/100.
        ADT=0.8165*TIN+225.14
 21     FMEOH=FMO*(1.-CONVN)
        FH2O=FH2O+FMO*CONVN/2.0
        FDME=FMO*CONVN/2.0
        RETURN
        END

        SUBROUTINE DUMMY
        RETURN
        END

        SUBROUTINE FCN1(NEQ,T,Y,YDOT)

C       This subroutine provides the definition of the differential equations
C       required for LSODE.
```

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

      DIMENSION Y(NEQ),YDOT(NEQ)
      DIMENSION A(60,45),IOR(60,45),AK(60),E(60),R(60)
      DIMENSION DELHF(45),DELHR(60),CP(45)

      COMMON /A/ A,AK,E
      COMMON /INT/ IOR
      COMMON /INT1/ NR,NSP
      COMMON /DGN/ AL,AREA
      COMMON /DGN1/ TINR,FT,PA
      COMMON /AINP/ TIN,PT,FHEOH,FH2O
      COMMON /HT/ DELHF,CP
      COMMON /MODE/ ISO

      AKA=1.5
      RR=0.082057
      RG=1.987
      SUM=0.0D0

      DO 41 I=1,NSP
   41 SUM=SUM+Y(I)

      TEMP=TINR*(1.0+Y(NEQ))

C     .....Define reaction rates for the various species.
      DO 21 J=1,NR
      PROD=1.0D0

      DO 31 I=1,NSP
      CONC=Y(I)*PT/(RR*TEMP*SUM)
      IF(IOR(J,I).EQ.0) GO TO 31
      TER=CONC**IOR(J,I)
   33 PROD=PROD*TER
   31 CONTINUE

      AKONS=AK(J)*DEXP(-E(J)/RG/TEMP)
      R(J)=AKONS*PROD*(1.+AKA)/(1.+AKA*PA)
   21 CONTINUE

      CALL HEAT(TEMP,NSP)

      SUM1=0.0D0
      DO 71 I=1,NSP
   71 SUM1=SUM1+Y(I)*CP(I)
      SUM1=SUM1*FT

C     .....calculate heats of reaction for the various reactions.
      DO 81 J=1,NR
      SUM2=0.0
      DO 80 I=1,NSP
   80 SUM2=SUM2+A(J,I)*DELHF(I)
      DELHR(J)=-SUM2
   81 CONTINUE

      SUM3=0.0D0
      DO 91 I=1,NR
      SUM3=SUM3+R(I)*DELHR(I)
   91 CONTINUE
```

```
C       ......The following parameters are required as part of MTH:DLSODE.REL

        TOUT=0.01D0
        ISTATE=1
        IOPT=0
        ITOL=2
        RTOL=1.D-4
        ITASK=1
        MF=22
        LRW=2452
        LIW=65

        DO 12 I=1,NEQ
 12     ATOL(I)=1.0D-6

C       ......Tolerances for reactants and ionic species are specified
C       smaller than those for products.

        ATOL(1)=1.0D-10
        ATOL(4)=1.0D-10
        ATOL(5)=1.0D-10
        ATOL(14)=1.0D-10
        ATOL(15)=1.0D-10
        ATOL(16)=1.0D-10
        ATOL(17)=1.0D-10

        OPEN (UNIT=26,FILE='OUTPT1.DAT')
        DO 21 K=1,11
        TOUT=0.1D0*DFLOAT(K-1)
        CALL LSODE(FCN1,NEQ,Y,T,TOUT,ITOL,RTOL,ATOL,ITASK,ISTATE,IOPT,
     *          RWORK,LRW,IWORK,LIW,DUMMY,MF)
        IF(ISTATE.LT.0) GO TO 20

        DO 88 I=1,NSP
 88     WT(I)=Y(I)*FT

        SUM=0.0D0
        DO 91 I=1,NSP
        WT(I)=WT(I)*XMW(I)
 91     SUM=SUM+WT(I)

        WRITE(26,45) TOUT,Y(NEQ)*TINR+TINR
        DO 101 I=1,NSP
        WT(I)=WT(I)/SUM*100.
        IF(I.EQ.6) GO TO 101
        IF(I.EQ.14) GO TO 101
        IF(I.EQ.15) GO TO 101
        IF(I.EQ.16) GO TO 101
        IF(I.EQ.17) GO TO 101
        WRITE(26,44) NAM1(I),WT(I)
101     CONTINUE
        WFREE=100.-WT(5)
        OLFNS=(WT(7)+WT(8)+WT(9)+WT(10)+WT(11)+WT(12)+WT(18)+WT(20)
     *                  +WT(24)+WT(25))*100./WFREE
        PRFNS= (WT(13)+WT(19)+WT(21)+WT(22)+WT(23))*100./WFREE
        ARMTCS=(WT(26)+WT(27)+WT(28)+WT(29)+WT(31)+WT(32)+WT(33)+
     *          WT(34)+WT(35)+WT(36)+WT(37))*100./WFREE
        WRITE(26,55) OLFNS,PRFNS,ARMTCS

21      CONTINUE
```

```
      DO 51 I=1,NSP
      SUM=0.0D0

      DO 61 J=1,NR
   61 SUM=SUM+A(J,I)*R(J)

   51 YDOT(I)=SUM*AREA*AL/FT
      IF(ISO.EQ.1) GO TO 22
      YDOT(NEQ)=AREA*SUM3/SUM1*AL/TIME
      RETURN
   22 YDOT(NEQ)=0.0D0
      RETURN
      END

      SUBROUTINE HEAT(TEMP,NSP)

C     This subroutine evaluates the heats of formation and the specific
C     heats of the species at the reaction temperature.

      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION CPA(45),CPB(45),CPC(45),CPD(45),DELHG(45),CP(45)
      DIMENSION DELH(45)
      COMMON /PROP/ CPA,CPB,CPC,CPD,DELHG
      COMMON /HT/ DELH,CP

      TR=298.15
      A=TEMP-TR
      B=TEMP**2-TR**2
      C=TEMP**3-TR**3
      D=TEMP**4-TR**4
      DO 11 I=1,NSP
      AINT=CPA(I)*A+CPB(I)*B/2.+CPC(I)*C/3.+CPD(I)*D/4.
      DELH(I)=DELHG(I)+AINT
   11 CP(I)=CPA(I)+CPB(I)*TEMP+CPC(I)*TEMP**2+CPD(I)*TEMP**3

      RETURN
      END

      SUBROUTINE INPUT

C     This is the input subroutine that reads in the input data.

C     List of variables:
C     ------------------
C     A(I,J) - Stoichiometric coefficient of jth species in the
C              ith reaction.
C     AK     - Arrhenius frequency factor, 1/s or m**3/kmol s
C              depending on the order of the reaction.
C     AL - Length of reactor, m
C     AREA - Cross-sectional area of reactor, m**2
C     CPA,CPB,CPC,CPD - polynomial coefficients of specific heat in the
C                       form CP=CPA+CPB*T+CPC*T**2+CPD*T**3
C     DELHG - Standard heat of formation (298.15 K) kcal/kmol
C     E - Activation energy, kcal/kmol
C     FMEOH - Feed rate of methanol, kmol/s
C     FH2O - Feed rate of water, kmol/s
C     IOR(I,J) - order of ith reaction with respect to jth species. All
C                orders are whole numbers since all reactions are
C                elementary.
C     NR - Number of reactions
```

```
C       NSP - Number of species
C       PT - Operating pressure, atm
C       RCYCL - Recycle ratio, (mol recycle gas/mol methanol feed)
C       TIN - Inlet temperature to dehydration reactor, K
C       TINR - Inlet temperature to MTG reactor, K
C       XMW - Molecular weights
C       ------------------------------------------------------------------

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

        CHARACTER*7 NAME(45)
        CHARACTER*30 NAM1(45)
        DIMENSION A(60,45),AK(60),E(60),IOR(60,45),II(4),IA(60,45)
        DIMENSION CPA(45),CPB(45),CPC(45),CPD(45),DELHG(45),XMW(45)

        COMMON /PROP/ CPA,CPB,CPC,CPD,DELHG
        COMMON /NAME/ NAM1
        COMMON /A/ A,AK,E
        COMMON /INT/ IOR
        COMMON /INT1/ NR,NSP
        COMMON /INT2/ IND
        COMMON /AM/ XMW
        COMMON /AINP/ TIN,PT,FMEOH,FH2O
        COMMON /DGN/ AL,AREA
        COMMON /DGN1/ TINR,FT,PA
        COMMON /RC/ FC1,FC2,FC3,FC4,FC5,FC6,FC7
        COMMON /MODE/ ISO

        OPEN (UNIT=23,FILE='DGN.DAT')
        READ(23,*) IND,IPRINT,ISO
        READ(23,*) TIN,TINR,PT,RCYCL,FMEOH,FH2O,AL,DT
        READ(23,*) C1,C2,C3,C4,C5,C6,C7
        CLOSE (UNIT=23)
        OPEN (UNIT=24,FILE='DATA.DAT')
        WRITE(24,81) TIN,TINR,PT,RCYCL,FMEOH,FH2O,AL,DT
        WRITE(24,82) C1,C2,C3,C4,C5,C6,C7
 81     FORMAT(//5X,'LIST OF INPUT DATA:',//,
     *  5X,'INLET TEMPERATURE TO DEHYDRATION REACTOR (K)',T60,F9.5,/,
     *  5X,'INLET TEMPERATURE TO MTG REACTOR (K)',T60,F9.5,/,
     *  5X,'OPERATING PRESSURE (atm)',T60,F9.5,/,
     *  5X,'RECYCLE RATIO (mol recycle gas/mol MeOH feed)',T60,F9.5,/,
     *  5X,'FEED RATE OF METHANOL (kg/sec)',T60,F9.5,/,
     *  5X,'FEED RATE OF WATER (kg/sec)',T60,F9.5,/,
     *  5X,'LENGTH OF REACTOR (m)',T60,F9.5,/,
     *  5X,'DIAMETER OF REACTOR (m)',T60,F9.5,///)
 82     FORMAT(5X,'COMPOSITION OF RECYCLE GAS IN MOLE FRACTION',//,
     *  5X,'METHANE',T50,F5.2,/,
     *  5X,'HYDROGEN',T50,F5.2,/,
     *  5X,'CARBON MONOXIDE',T50,F5.2,/,
     *  5X,'PROPYLENE',T50,F5.2,/,
     *  5X,'PROPANE',T50,F5.2,/,
     *  5X,'ETHYLENE',T50,F5.2,/,
     *  5X,'ETHANE',T50,F5.2,/)
        CLOSE (UNIT=24)
        AREA=DATAN(1.0D0)*DT*DT

        OPEN (UNIT=20,FILE='MIH.DAT')
        OPEN(UNIT=21,FILE='NAM.DAT')
        OPEN(UNIT=22,FILE='PROP.DAT')
```

```
      READ(20,*) NR,NSP

      DO 21 I=1,NSP
      READ(21,8) NAME(I),NAM1(I)
8     FORMAT(A7,A30)
21    CONTINUE
      IF(IPRINT.EQ.0) GO TO 78
      OPEN (UNIT=15,FILE='PARAM.DAT')
      WRITE(15,33)
33    FORMAT(//10X,'SPECIES ID',10X,'FORMULA',10X,'NAME',//)
      DO 22 I=1,NSP
22    WRITE(15,85) I,NAME(I),NAM1(I)
85    FORMAT(/15X,I3,13X,A7,10X,A30)
78    CONTINUE
      CLOSE(UNIT=21)

      DO 31 I=1,NSP
      READ(22,*) XMW(I),CPA(I),CPB(I),CPC(I),CPD(I),DELHG(I)
      DELHG(I)=DELHG(I)*1000.
31    CONTINUE
      FMEOH=FMEOH/XMW(1)
      FH2O=FH2O/XMW(5)
      RCYCL=RCYCL*FMEOH
      FC1=C1*RCYCL
      FC2=C2*RCYCL
      FC3=C3*RCYCL
      FC4=C4*RCYCL
      FC5=C5*RCYCL
      FC6=C6*RCYCL
      FC7=C7*RCYCL

      IF(IPRINT.EQ.0) GO TO 67
      WRITE(15,432)
432   FORMAT('1',3X,'SPECIES ID',2X,'MOLECULAR WT.',8X,'CPA',8X,'CPB'
     *       ,10X,'CPC',8X,'CPD',8X,'HEAT OF FORMATION',/,
     *       82X,'    kcal/kmol  ',///)
      DO 35 I=1,NSP
35    WRITE(15,199) I,XMW(I),CPA(I),CPB(I),CPC(I),CPD(I),DELHG(I)
199   FORMAT(/5X,I3,5X,6(3X,E12.5))

67    CONTINUE
      DO 10 J=1,NSP
      DO 10 I=1,NR
      IOR(I,J)=0
      IA(I,J)=0
10    A(I,J)=0.0

      IF(IPRINT.EQ.0) GO TO 63
      WRITE(15,73)
73    FORMAT('1',5X,'REACTION NO.',5X,'COMPONENTS',//)

63    DO 20 J=1,NR
      READ(20,*) AK(J),E(J)
      AK(J)=DEXP(AK(J))
      E(J)=E(J)/4.187
      READ(20,*) NSPR
      DO 30 I=1,NSPR
      READ(20,*) II(I)
      READ(20,*) A(J,II(I))
      IA(J,II(I))=INT(A(J,II(I)))
```

```
      IF(A(J,II(I)).LT.0.0) IOR(J,II(I))=ABS(IA(J,II(I)))
30    CONTINUE

      IF(IPRINT.EQ.0) GO TO 20
      IF(NSPR.EQ.2) WRITE(15,77) J,(NAME(II(I)),I=1,NSPR),
     *                           (IA(J,II(I)),I=1,NSPR)
      IF(NSPR.EQ.3) WRITE(15,79) J,(NAME(II(I)),I=1,NSPR),
     *                           (IA(J,II(I)),I=1,NSPR)
      IF(NSPR.EQ.4) WRITE(15,80) J,(NAME(II(I)),I=1,NSPR),
     *                           (IA(J,II(I)),I=1,NSPR)
77    FORMAT(/5X,I3,10X,2(A10),/,22X,I2,8X,I2)
79    FORMAT(/5X,I3,10X,3(A10),/,22X,I2,8X,I2,8X,I2)
80    FORMAT(/5X,I3,10X,4(A10),/,22X,I2,8X,I2,8X,I2,8X,I2)

20    CONTINUE
      IF(IPRINT.EQ.0) GO TO 89
      WRITE(15,100)
100   FORMAT('1',5X,'REACTION NO.',5X,'ARRHENIUS FREQENCY',5X,
     *  'ACTIVATION ENERGY',/,25X,'FACTOR',15X,'   kcal/kmol',//)

      DO 44 J=1,NR
      WRITE(15,88) J,AK(J),E(J)
88    FORMAT(/9X,I3,10X,E12.5,11X,E12.5)
44    CONTINUE
      CLOSE (UNIT=15)
89    WRITE(6,45)
45    FORMAT('1')
      CLOSE (UNIT=22)
      CLOSE (UNIT=20)
      RETURN
      END
```

I-A-9 Sample Output from Fixed Bed Reactor Simulation

```
SIMULATION OF FIXED BED COMPLETE
OUTPUT CAN BE FOUND IN THE FOLLOWING FILES:

DEHYDRATION REACTOR RESULTS      : DHYDN.DAT
MTG REACTOR RESULTS              : OUTPT1.DAT
INPUT DATA                       : DATA.DAT
PHYSICO-CHEMICAL & KINETIC DATA  : PARAM.DAT
```

SPECIES ID	FORMULA	NAME
1	CH3OH	Methanol
2	CO	Carbon Monoxide
3	H2	Hydrogen
4	CH3OCH3	Dimethylether
5	H2O	Water
6	:CH2	Carbene ion
7	C2H4	Ethylene
8	C3H6	Propylene
9	C4H8	1-Butene
10	C5H10	1-Pentene
11	C6H12	1-Hexene
12	C7H14	1-Heptene
13	CH4	Methane
14	C2H5+	Carbenium ion
15	C3H7+	Carbenium ion
16	C4H9+	Carbenium ion
17	C5H11+	Carbenium ion
18	C6H10	1,5-Hexadiene
19	C2H6	Ethane
20	C7H12	1,6-Heptadiene
21	C3H8	Propane
22	C4H10	n-Butane
23	C5H12	n-Pentane
24	C6H8	1,3-cyclohexadiene
25	C7H10	1,3-cycloheptadiene
26	C7H8	Toluene
27	C6H6	Benzene

28	C10H8	Naphthalene
29	C9H8	Aromatic compound
30	C	carbon
31	C8H10	o-xylene
32	C9H12	1,2,4-trimethylbenzene
33	C10H14	1,2,4,5-tetramethylbenzene
34	C11H16	1,2,4,5,6-pentamethylbenzene
35	C12H18	1,2,3,4,5,6-hexamethylbenzene
36	C11H10	1-methylnaphthalene
37	C12H12	1,2-dimethylnaphthalene

REACTION NO.	COMPONENTS			
1	CH3OH	CO	H2	
	-1	1	2	
2	CH3OH	CH3OCH3	H2O	
	-2	1	1	
3	CH3OCH3	:CH2	H2O	
	-1	2	1	
4	:CH2	CH3OH	C2H4	H2O
	-1	-1	1	1
5	:CH2	CH3OCH3	C2H4	CH3OH
	-1	-1	1	1
6	:CH2	CH3OCH3	C3H6	H2O
	-1	-1	1	1
7	:CH2	C2H4	C3H6	
	-1	-1	1	
8	:CH2	C3H6	C4H8	
	-1	-1	1	
9	:CH2	C4H8	C5H10	
	-1	-1	1	
10	:CH2	C5H10	C6H12	
	-1	-1	1	
11	:CH2	C6H12	C7H14	
	-1	-1	1	
12	:CH2	H2	CH4	
	-1	-1	1	
13	C2H4	C2H5+		
	-1	1		
14	C3H6	C3H7+		
	-1	1		
15	C4H8	C4H9+		
	-1	1		
16	C5H10	C5H11+		
	-1	1		
17	C3H7+	C3H6	C6H12	
	-1	-1	1	
18	C4H9+	C2H4	C6H12	
	-1	-1	1	
19	C4H9+	C3H6	C7H14	
	-1	-1	1	

20	C5H11+	C2H4	C7H14	
	-1	-1	1	
21	C2H5+	C6H12	C2H6	C6H10
	-1	-1	1	1
22	C2H5+	C7H14	C2H6	C7H12
	-1	-1	1	1
23	C3H7+	C6H12	C3H8	C6H10
	-1	-1	1	1
24	C3H7+	C7H14	C3H8	C7H12
	-1	-1	1	1
25	C4H9+	C6H12	C4H10	C6H10
	-1	-1	1	1
26	C4H9+	C7H14	C4H10	C7H12
	-1	-1	1	1
27	C5H11+	C6H12	C5H12	C6H10
	-1	-1	1	1
28	C5H11+	C7H14	C5H12	C7H12
	-1	-1	1	1
29	C3H7+	C6H10	C6H8	C3H8
	-1	-1	1	1
30	C3H7+	C7H12	C7H10	C3H8
	-1	-1	1	1
31	C4H9+	C6H10	C6H8	C4H10
	-1	-1	1	1
32	C4H9+	C7H12	C7H10	C4H10
	-1	-1	1	1
33	C5H11+	C6H10	C6H8	C5H12
	-1	-1	1	1
34	C5H11+	C7H12	C7H10	C5H12
	-1	-1	1	1
35	C3H7+	C6H8	C6H6	C3H8
	-1	-1	1	1
36	C3H7+	C7H10	C7H8	C3H8
	-1	-1	1	1
37	C4H9+	C6H8	C6H6	C4H10
	-1	-1	1	1
38	C4H9+	C7H10	C7H8	C4H10
	-1	-1	1	1
39	C5H11+	C6H8	C6H6	C5H12
	-1	-1	1	1

40	C5H11+	C7H10	C7H8	C5H12
	-1	-1	1	1
41	C6H6	C10H8	C2H4	
	-2	1	1	
42	C6H6	C9H8	C2H4	C
	-2	1	1	1
43	CH3OH	C6H6	C7H8	H2O
	-1	-1	1	1
44	CH3OH	C7H8	C8H10	H2O
	-1	-1	1	1
45	CH3OH	C8H10	C9H12	H2O
	-1	-1	1	1
46	CH3OH	C9H12	C10H14	H2O
	-1	-1	1	1
47	CH3OH	C10H14	C11H16	H2O
	-1	-1	1	1
48	CH3OH	C11H16	C12H18	H2O
	-1	-1	1	1
49	CH3OH	C10H8	C11H10	H2O
	-1	-1	1	1
50	CH3OH	C11H10	C12H12	H2O
	-1	-1	1	1
51	C5H12	C4H8	CH4	
	-1	1	1	
52	C4H10	C3H6	CH4	
	-1	1	1	
53	C3H8	C2H4	CH4	
	-1	1	1	
54	CH3OH	CH3OCH3	H2O	
	2	-1	-1	
55	C2H4	C2H5+		
	1	-1		
56	C3H6	C3H7+		
	1	-1		
57	C4H8	C4H9+		
	1	-1		
58	C5H10	C5H11+		
	1	-1		

REACTION NO.	ARRHENIUS FREQENCY FACTOR	ACTIVATION ENERGY kcal/kmol
1	0.11077E+04	0.99952E+04
2	0.79426E+04	0.39981E+03
3	0.35874E+02	0.21989E+04
4	0.57935E+10	0.00000E+00
5	0.11667E+11	0.00000E+00
6	0.51384E+10	0.00000E+00
7	0.19821E+11	0.00000E+00
8	0.33339E+11	0.00000E+00
9	0.38735E+11	0.00000E+00
10	0.11637E+12	0.00000E+00
11	0.70579E+11	0.00000E+00
12	0.12860E+12	0.00000E+00
13	0.55023E-01	0.49976E+03
14	0.80252E+00	0.29986E+03
15	0.18221E+01	0.19967E+03
16	0.25857E+01	0.19967E+03
17	0.53104E+05	0.00000E+00
18	0.53104E+05	0.00000E+00
19	0.53104E+05	0.00000E+00
20	0.53104E+05	0.00000E+00
21	0.39239E+06	0.00000E+00
22	0.17585E+07	0.00000E+00
23	0.39239E+06	0.00000E+00
24	0.17585E+07	0.00000E+00
25	0.39239E+06	0.00000E+00
26	0.17585E+07	0.00000E+00
27	0.39239E+06	0.00000E+00
28	0.17585E+07	0.00000E+00

29	0.35321E+08	0.00000E+00
30	0.35321E+08	0.00000E+00
31	0.35321E+08	0.00000E+00
32	0.35321E+08	0.00000E+00
33	0.35321E+08	0.00000E+00
34	0.35321E+08	0.00000E+00
35	0.31795E+10	0.00000E+00
36	0.31795E+10	0.00000E+00
37	0.31795E+10	0.00000E+00
38	0.31795E+10	0.00000E+00
39	0.31795E+10	0.00000E+00
40	0.31795E+10	0.00000E+00
41	0.83226E+13	0.19967E+05
42	0.28547E+13	0.29986E+05
43	0.18535E+06	0.40980E+04
44	0.44686E+06	0.36982E+04
45	0.32775E+06	0.32984E+04
46	0.29954E+06	0.31985E+04
47	0.22866E+06	0.30985E+04
48	0.14952E+04	0.36982E+04
49	0.44686E+06	0.39531E+04
50	0.11242E+06	0.38481E+04
51	0.25393E+08	0.22989E+05
52	0.19529E+09	0.26187E+05
53	0.26825E+10	0.29486E+05
54	0.26704E+04	0.59971E+03
55	0.36693E+01	0.00000E+00
56	0.36693E+01	0.00000E+00
57	0.36693E+01	0.00000E+00
58	0.36693E+01	0.00000E+00

SPECIES ID	MOLECULAR WT.	CPA	CPB	CPC	CPD	HEAT OF FORMATION kcal/kmol
1	0.32000E+02	0.50520E+01	0.16940E-01	0.81790E-05	-0.68110E-08	-0.48080E+05
2	0.28000E+02	0.73730E+01	-0.30700E-02	0.66820E-05	-0.30370E-08	-0.26420E+05
3	0.20000E+01	0.64830E+01	0.22150E-02	-0.32980E-05	0.18260E-08	0.00000E+00
4	0.46000E+02	0.40640E+01	0.42770E-01	-0.12500E-04	-0.45800E-09	-0.43990E+05
5	0.18000E+02	0.77010E+01	0.45950E-03	0.25210E-05	-0.85900E-09	-0.57800E+05
6	0.14000E+02	0.52660E+00	0.18357E-01	-0.95400E-05	0.19500E-07	0.61900E+04
7	0.28000E+02	0.90900E+00	0.37400E-01	-0.19940E-04	0.41920E-08	0.12500E+05
8	0.42000E+02	0.88600E+00	0.56020E-01	-0.27710E-04	0.52660E-08	0.48800E+04
9	0.56000E+02	-0.71500E+00	0.84360E-01	-0.47540E-04	0.10660E-07	-0.30000E+02
10	0.70000E+02	-0.32000E-01	0.10340E+00	-0.55340E-04	0.11180E-07	-0.50000E+04
11	0.84000E+02	-0.41700E+00	0.12680E+00	-0.64900E-04	0.11530E-07	-0.12510E+05
12	0.98000E+02	-0.78900E+00	0.15040E+00	-0.83880E-04	0.18170E-07	-0.14890E+05
13	0.16000E+02	0.45980E+01	0.12450E-01	0.28600E-05	-0.27030E-08	-0.17890E+05
14	0.29000E+02	0.11353E+01	0.39790E-01	-0.18060E-05	0.13300E-07	-0.40600E+04
15	0.43000E+02	0.15298E+01	0.61153E-01	-0.30030E-04	0.15896E-07	-0.90000E+04
16	0.57000E+02	0.19243E+01	0.82520E-01	-0.42000E-04	0.18492E-07	-0.13940E+05
17	0.71000E+02	0.23188E+01	0.10388E+00	-0.53975E-04	0.21088E-07	-0.18880E+05
18	0.82000E+02	0.13436E+01	0.11189E+00	-0.62300E-04	0.13452E-07	0.20000E+05
19	0.30000E+02	0.12920E+01	0.42540E-01	-0.16570E-04	0.20810E-08	-0.20240E+05
20	0.98000E+02	0.17381E+01	0.13325E+00	-0.74270E-04	0.16050E-07	0.15220E+05
21	0.44000E+02	-0.10090E+01	0.73150E-01	-0.37890E-04	0.76780E-08	-0.24820E+05
22	0.58000E+02	0.22660E+01	0.79130E-01	-0.26470E-04	-0.67400E-09	-0.30150E+05
23	0.72000E+02	-0.86600E+00	0.11640E+00	-0.61630E-04	0.12670E-07	-0.35000E+05
24	0.80000E+02	-0.13655E+02	0.14108E+00	-0.90270E-04	0.21673E-07	0.25280E+05
25	0.94000E+02	-0.11218E+02	0.15830E+00	-0.98910E-04	0.33582E-07	0.22870E+05
26	0.92000E+02	-0.58170E+01	0.12240E+00	-0.66050E-04	0.11730E-07	0.11950E+05
27	0.78000E+02	-0.81010E+01	0.11330E+00	-0.72060E-04	0.17030E-07	0.19820E+05
28	0.12800E+03	-0.16433E+02	0.20300E+00	-0.15540E-03	0.47310E-07	0.36080E+05

29	0.11600E+03	-0.16433E+02	0.20300E+00	-0.15540E-03	0.47310E-07	0.36080E+05
30	0.12000E+02	0.46440E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
31	0.10600E+03	-0.37860E+01	0.14240E+00	-0.82240E-04	0.17980E-07	0.45400E+04
32	0.12000E+03	-0.11150E+01	0.14900E+00	-0.77930E-04	0.15230E-07	-0.33300E+04
33	0.13400E+03	0.39460E+01	0.15570E+00	-0.68760E-04	0.77790E-08	-0.10820E+05
34	0.14800E+03	-0.53552E+01	0.20211E+00	-0.10838E-03	0.73030E-07	-0.20230E+05
35	0.16200E+03	-0.48776E+01	0.21955E+00	-0.11526E-03	0.84054E-07	-0.28200E+05
36	0.14200E+03	-0.15482E+02	0.22420E+00	-0.16580E-03	0.48140E-07	0.27930E+05
37	0.15600E+03	-0.10059E+02	0.21241E+00	-0.12050E-03	0.50172E-07	0.19180E+05

LIST OF INPUT DATA:

INLET TEMPERATURE TO DEHYDRATION REACTOR (K)	603.15000
INLET TEMPERATURE TO MTG REACTOR (K)	615.37222
OPERATING PRESSURE (atm)	19.02721
RECYCLE RATIO (mol recycle gas/mol MeOH feed)	3.30000
FEED RATE OF METHANOL (kg/sec)	0.00012
FEED RATE OF WATER (kg/sec)	0.00002
LENGTH OF REACTOR (m)	0.23950
DIAMETER OF REACTOR (m)	0.03300

COMPOSITION OF RECYCLE GAS IN MOLE FRACTION

METHANE	0.40
HYDROGEN	0.10
CARBON MONOXIDE	0.10
PROPYLENE	0.10
PROPANE	0.10
ETHYLENE	0.10
ETHANE	0.10

CONDITIONS AT EXIT OF DEHYDRATION REACTOR:

EXIT TEMPERATURE FROM DEHYDRATION REACTOR (K)	696.04395
EQUILIBRIUM METHANOL CONVERSION IN DEHYDRATION REACTOR (%)	76.46770
FLOW RATE OF METHANOL (kmol/s)	.8918374E-06
FLOW RATE OF DME (kmol/s)	.1449003E-05
FLOW RATE OF WATER (kmol/s)	.2829003E-05

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.000 TEMPERATURE = 615.37222 K

SPECIES NAME	WEIGHT PERCENT
Methanol	6.43100
Carbon Monoxide	7.89107
Hydrogen	0.56365
Dimethylether	15.02000
Water	11.47489
Ethylene	7.89107
Propylene	11.83661
1-Butene	0.00000
1-Pentene	0.00000
1-Hexene	0.00000
1-Heptene	0.00000
Methane	18.03674
1,5-Hexadiene	0.00000
Ethane	8.45472
1,6-Heptadiene	0.00000
Propane	12.40026
n-Butane	0.00000
n-Pentane	0.00000
1,3-cyclohexadiene	0.00000
1,3-cycloheptadiene	0.00000
Toluene	0.00000
Benzene	0.00000
Naphthalene	0.00000
Aromatic compound	0.00000
carbon	0.00000
o-xylene	0.00000
1,2,4-trimethylbenzene	0.00000
1,2,4,5-tetramethylbenzene	0.00000
1,2,4,5,6-pentamethylbenzene	0.00000
1,2,3,4,5,6-hexamethylbenzene	0.00000
1-methylnaphthalene	0.00000
1,2-dimethylnaphthalene	0.00000

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	22.28484
WT. PERCENT PARAFFINS	43.93297
WT. PERCENT AROMATICS	0.00000

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.100 TEMPERATURE = 704.73718 K

SPECIES NAME	WEIGHT PERCENT
Methanol	5.95009
Carbon Monoxide	8.26504
Hydrogen	0.27249
Dimethylether	6.59213
Water	14.80284
Ethylene	8.10305
Propylene	10.07161
1-Butene	2.66401
1-Pentene	0.34828
1-Hexene	0.70105
1-Heptene	0.22541
Methane	21.15327
1,5-Hexadiene	0.00938
Ethane	8.48784
1,6-Heptadiene	0.01319
Propane	11.75799
n-Butane	0.09121
n-Pentane	0.01755
1,3-cyclohexadiene	0.00010
1,3-cycloheptadiene	0.00014
Toluene	0.00813
Benzene	0.00775
Naphthalene	0.00133
Aromatic compound	0.00001
carbon	0.00000
o-xylene	0.00947
1,2,4-trimethylbenzene	0.01078
1,2,4,5-tetramethylbenzene	0.01443
1,2,4,5,6-pentamethylbenzene	0.35817
1,2,3,4,5,6-hexamethylbenzene	0.02443
1-methylnaphthalene	0.00499
1,2-dimethylnaphthalene	0.02989

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	25.98236
WT. PERCENT PARAFFINS	48.71977
WT. PERCENT AROMATICS	0.55092

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.200 TEMPERATURE = 730.46444 K

SPECIES NAME	WEIGHT PERCENT
Methanol	4.35988
Carbon Monoxide	8.71097
Hydrogen	0.20774
Dimethylether	3.11258
Water	16.77223
Ethylene	9.52376
Propylene	9.10728
1-Butene	3.48747
1-Pentene	0.63552
1-Hexene	1.04343
1-Heptene	0.40272
Methane	23.33448
1,5-Hexadiene	0.01385
Ethane	8.52298
1,6-Heptadiene	0.02406
Propane	9.09177
n-Butane	0.31864
n-Pentane	0.08179
1,3-cyclohexadiene	0.00015
1,3-cycloheptadiene	0.00026
Toluene	0.01268
Benzene	0.00803
Naphthalene	0.00293
Aromatic compound	0.00003
carbon	0.00000
o-xylene	0.01496
1,2,4-trimethylbenzene	0.01712
1,2,4,5-tetramethylbenzene	0.02307
1,2,4,5,6-pentamethylbenzene	0.92859
1,2,3,4,5,6-hexamethylbenzene	0.11849
1-methylnaphthalene	0.01106
1,2-dimethylnaphthalene	0.10822

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	29.12309
WT. PERCENT PARAFFINS	49.68254
WT. PERCENT AROMATICS	1.49610

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.300 TEMPERATURE = 735.91673 K

SPECIES NAME	WEIGHT PERCENT
Methanol	3.12931
Carbon Monoxide	9.06266
Hydrogen	0.20259
Dimethylether	1.50736
Water	17.86647
Ethylene	11.07319
Propylene	8.54527
1-Butene	3.53741
1-Pentene	0.69190
1-Hexene	1.26257
1-Heptene	0.43643
Methane	24.96464
1,5-Hexadiene	0.01749
Ethane	8.56283
1,6-Heptadiene	0.02755
Propane	6.39341
n-Butane	0.52043
n-Pentane	0.14515
1,3-cyclohexadiene	0.00019
1,3-cycloheptadiene	0.00030
Toluene	0.01682
Benzene	0.00894
Naphthalene	0.00545
Aromatic compound	0.00006
carbon	0.00001
o-xylene	0.01989
1,2,4-trimethylbenzene	0.02277
1,2,4,5-tetramethylbenzene	0.03071
1,2,4,5,6-pentamethylbenzene	1.46668
1,2,3,4,5,6-hexamethylbenzene	0.24277
1-methylnaphthalene	0.02026
1,2-dimethylnaphthalene	0.21550

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	31.15938
WT. PERCENT PARAFFINS	49.41522
WT. PERCENT AROMATICS	2.49576

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.400 TEMPERATURE = 737.25428 K

SPECIES NAME	WEIGHT PERCENT
Methanol	2.21006
Carbon Monoxide	9.31422
Hydrogen	0.21195
Dimethylether	0.72739
Water	18.52703
Ethylene	12.25055
Propylene	8.12156
1-Butene	3.32542
1-Pentene	0.64354
1-Hexene	1.40491
1-Heptene	0.39518
Methane	26.08731
1,5-Hexadiene	0.02046
Ethane	8.60695
1,6-Heptadiene	0.02641
Propane	4.48797
n-Butane	0.65288
n-Pentane	0.18501
1,3-cyclohexadiene	0.00022
1,3-cycloheptadiene	0.00029
Toluene	0.02071
Benzene	0.00986
Naphthalene	0.00950
Aromatic compound	0.00010
carbon	0.00001
o-xylene	0.02447
1,2,4-trimethylbenzene	0.02798
1,2,4,5-tetramethylbenzene	0.03768
1,2,4,5,6-pentamethylbenzene	1.92438
1,2,3,4,5,6-hexamethylbenzene	0.36419
1-methylnaphthalene	0.03431
1,2-dimethylnaphthalene	0.34462

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	32.14384
WT. PERCENT PARAFFINS	49.12073
WT. PERCENT AROMATICS	3.43402

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.500 TEMPERATURE = 737.88206 K

SPECIES NAME	WEIGHT PERCENT
Methanol	1.52168
Carbon Monoxide	9.48878
Hydrogen	0.22393
Dimethylether	0.33887
Water	18.95406
Ethylene	13.10991
Propylene	7.74659
1-Butene	3.03387
1-Pentene	0.56121
1-Hexene	1.50346
1-Heptene	0.33128
Methane	26.87060
1,5-Hexadiene	0.02307
Ethane	8.65418
1,6-Heptadiene	0.02342
Propane	3.22350
n-Butane	0.72229
n-Pentane	0.20155
1,3-cyclohexadiene	0.00025
1,3-cycloheptadiene	0.00025
Toluene	0.02474
Benzene	0.01064
Naphthalene	0.01596
Aromatic compound	0.00015
carbon	0.00002
o-xylene	0.02912
1,2,4-trimethylbenzene	0.03317
1,2,4,5-tetramethylbenzene	0.04449
1,2,4,5,6-pentamethylbenzene	2.29446
1,2,3,4,5,6-hexamethylbenzene	0.46708
1-methylnaphthalene	0.05529
1,2-dimethylnaphthalene	0.48931

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	32.49183
WT. PERCENT PARAFFINS	48.95017
WT. PERCENT AROMATICS	4.27463

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.600 TEMPERATURE = 738.52277 K

SPECIES NAME	WEIGHT PERCENT
Methanol	1.00517
Carbon Monoxide	9.60628
Hydrogen	0.23467
Dimethylether	0.14687
Water	19.24419
Ethylene	13.74935
Propylene	7.39683
1-Butene	2.73092
1-Pentene	0.47455
1-Hexene	1.57148
1-Heptene	0.26913
Methane	27.44086
1,5-Hexadiene	0.02544
Ethane	8.70366
1,6-Heptadiene	0.02011
Propane	2.38439
n-Butane	0.74364
n-Pentane	0.20077
1,3-cyclohexadiene	0.00028
1,3-cycloheptadiene	0.00022
Toluene	0.02964
Benzene	0.01122
Naphthalene	0.02641
Aromatic compound	0.00020
carbon	0.00002
o-xylene	0.03454
1,2,4-trimethylbenzene	0.03900
1,2,4,5-tetramethylbenzene	0.05184
1,2,4,5,6-pentamethylbenzene	2.58278
1,2,3,4,5,6-hexamethylbenzene	0.54609
1-methylnaphthalene	0.08580
1,2-dimethylnaphthalene	0.64086

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	32.49091
WT. PERCENT PARAFFINS	48.87986
WT. PERCENT AROMATICS	5.01314

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.700 TEMPERATURE = 739.32211 K

SPECIES NAME	WEIGHT PERCENT
Methanol	0.62022
Carbon Monoxide	9.68158
Hydrogen	0.24286
Dimethylether	0.05617
Water	19.44780
Ethylene	14.23913
Propylene	7.06683
1-Butene	2.44314
1-Pentene	0.39507
1-Hexene	1.61352
1-Heptene	0.21708
Methane	27.87690
1,5-Hexadiene	0.02759
Ethane	8.75479
1,6-Heptadiene	0.01713
Propane	1.82051
n-Butane	0.73114
n-Pentane	0.18883
1,3-cyclohexadiene	0.00030
1,3-cycloheptadiene	0.00019
Toluene	0.03673
Benzene	0.01160
Naphthalene	0.04387
Aromatic compound	0.00026
carbon	0.00003
o-xylene	0.04186
1,2,4-trimethylbenzene	0.04638
1,2,4,5-tetramethylbenzene	0.06052
1,2,4,5,6-pentamethylbenzene	2.79798
1,2,3,4,5,6-hexamethylbenzene	0.60131
1-methylnaphthalene	0.12889
1,2-dimethylnaphthalene	0.78707

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	32.30200
WT. PERCENT PARAFFINS	48.87783
WT. PERCENT AROMATICS	5.65653

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.800 TEMPERATURE = 740.24221 K

SPECIES NAME	WEIGHT PERCENT
Methanol	0.34230
Carbon Monoxide	9.72601
Hydrogen	0.24829
Dimethylether	0.01739
Water	19.59075
Ethylene	14.62580
Propylene	6.75449
1-Butene	2.18006
1-Pentene	0.32651
1-Hexene	1.63235
1-Heptene	0.17600
Methane	28.22622
1,5-Hexadiene	0.02951
Ethane	8.80718
1,6-Heptadiene	0.01467
Propane	1.43582
n-Butane	0.69635
n-Pentane	0.17069
1,3-cyclohexadiene	0.00032
1,3-cycloheptadiene	0.00016
Toluene	0.04859
Benzene	0.01179
Naphthalene	0.07462
Aromatic compound	0.00032
carbon	0.00003
o-xylene	0.05253
1,2,4-trimethylbenzene	0.05597
1,2,4,5-tetramethylbenzene	0.07066
1,2,4,5,6-pentamethylbenzene	2.94731
1,2,3,4,5,6-hexamethylbenzene	0.63572
1-methylnaphthalene	0.18639
1,2-dimethylnaphthalene	0.91251

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	32.01108
WT. PERCENT PARAFFINS	48.92008
WT. PERCENT AROMATICS	6.21372

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 0.900 TEMPERATURE = 741.17266 K

SPECIES NAME	WEIGHT PERCENT
Methanol	0.15799
Carbon Monoxide	9.74888
Hydrogen	0.25130
Dimethylether	0.00383
Water	19.68503
Ethylene	14.93961
Propylene	6.45864
1-Butene	1.94351
1-Pentene	0.26907
1-Hexene	1.63020
1-Heptene	0.14428
Methane	28.51759
1,5-Hexadiene	0.03120
Ethane	8.86057
1,6-Heptadiene	0.01271
Propane	1.16952
n-Butane	0.64826
n-Pentane	0.14995
1,3-cyclohexadiene	0.00034
1,3-cycloheptadiene	0.00014
Toluene	0.06946
Benzene	0.01183
Naphthalene	0.13014
Aromatic compound	0.00039
carbon	0.00004
o-xylene	0.06735
1,2,4-trimethylbenzene	0.06712
1,2,4,5-tetramethylbenzene	0.08079
1,2,4,5,6-pentamethylbenzene	3.03711
1,2,3,4,5,6-hexamethylbenzene	0.65398
1-methylnaphthalene	0.25431
1,2-dimethylnaphthalene	1.00223

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	31.66247
WT. PERCENT PARAFFINS	48.98948
WT. PERCENT AROMATICS	6.69203

TEMPERATURE AND WEIGHT PERCENT OF SPECIES ALONG REACTOR LENGTH

X = 1.000 TEMPERATURE = 741.99935 K

SPECIES NAME	WEIGHT PERCENT
Methanol	0.05594
Carbon Monoxide	9.75841
Hydrogen	0.25261
Dimethylether	0.00051
Water	19.73760
Ethylene	15.20095
Propylene	6.17718
1-Butene	1.73209
1-Pentene	0.22161
1-Hexene	1.60976
1-Heptene	0.11958
Methane	28.76809
1,5-Hexadiene	0.03269
Ethane	8.91475
1,6-Heptadiene	0.01116
Propane	0.98274
n-Butane	0.59372
n-Pentane	0.12904
1,3-cyclohexadiene	0.00035
1,3-cycloheptadiene	0.00012
Toluene	0.10425
Benzene	0.01177
Naphthalene	0.22542
Aromatic compound	0.00046
carbon	0.00005
o-xylene	0.08371
1,2,4-trimethylbenzene	0.07657
1,2,4,5-tetramethylbenzene	0.08791
1,2,4,5,6-pentamethylbenzene	3.07921
1,2,3,4,5,6-hexamethylbenzene	0.66169
1-methylnaphthalene	0.31685
1,2-dimethylnaphthalene	1.05062

HYDROCARBON DISTRIBUTION ON WATER FREE BASIS

WT. PERCENT OLEFINS	31.27927
WT. PERCENT PARAFFINS	49.07446
WT. PERCENT AROMATICS	7.09977