# APPENDIX I

## DATA REDUCTION

DATA REDUCTION

Schaefer et al. (1983) have used the following methods to calculate linear gas and slurry velocities from the metered values of the HRI PDU runs.

a. Gas Velocity

The gas velocity is calculated assuming ideal gas behavior. Gas velocities were calculated at the PDU reactor inlet and outlet and these typically were within 10% of each other. This implies that contraction or expansion effects were negligible.

b. Slurry Velocity

The superficial liquid velocity is computed by summing its two components, slurry feed and slurry recycle:

$$U_L = \frac{\dot{V}_{\text{slurry feed}} + \dot{V}_{\text{internal recycle}}}{A}$$

where $\dot{V}$ = volumetric flow rate

$U_L$ = slurry superficial velocity

$A$ = PDU cross-sectional area

The fresh slurry feed was assumed to have the same density as the recycle slurry at reactor conditions. This assumption was based on comparisons of the density of the slurry in the mix tank with that of the recycle slurry, both at room temperature. The densities were found to be comparable. The internal

recycle rate was measured by a Venturi meter, which was first calibrated with water and then adjusted to an assumed density of 0.85.

$$\dot{V}_{\text{internal recycle}} = (\text{meter gpm/ft}^2)\ \sqrt{0.85/\rho_{\text{actual}}} \times A \times 2.8\times10^{-3}\ \left(\frac{\text{ft}^3/\text{sec}}{\text{GPM}}\right)$$

c. Catalyst Bed Expansion: was calculated using the formula

$$\%\ \text{bed expansion} = \frac{(\text{expanded bed height} - \text{initial bed height})}{(\text{initial bed height} - 8")}$$

The 8" offset accounts for the height taken up by the plenum chamber and distributor plate. The settled initial bed height for all the fluid dynamic tests was determined to be 78" and this was also taken to be height at minimum fluidization.

Physical Properties of Slurry

Slurry densities and viscosities determined for the PDU runs as well as the Richardson-Zaki parameters are shown in Table A-1.

Table A-1. Physical Properties of Slurries and Richardson-Zaki Parameters

| HRI Period | Catalyst Density, gm/cc | Slurry Density, gm/cc | Slurry Viscosity, mPa.s | Terminal Velocity, m/s | Index n |
|---|---|---|---|---|---|
| 04B | 1.55 | 0.837 | 6.83 | 0.117 | 3.29 |
| 10A | 1.55 | 0.947 | 13.68 | 0.082 | 3.62 |
| 27B | 1.62 | 0.941 | 6.76 | 0.108 | 3.28 |
| 34B | 1.64 | 0.987 | 10.76 | 0.092 | 3.47 |
| 41B | 1.67 | 0.880 | 8.44 | 0.116 | 3.35 |
| 42A | 1.67 | 0.902 | 9.99 | 0.108 | 3.42 |
| 42B | 1.67 | 0.888 | 9.08 | 0.113 | 3.38 |
| 43A | 1.68 | 0.900 | 15.2 | 0.095 | 3.62 |
| 43B | 1.68 | 0.894 | 7.19 | 0.119 | 3.28 |
| 44A | 1.68 | 0.880 | 8.43 | 0.117 | 3.35 |
| 44B | 1.68 | 0.914 | 3.64 | 0.134 | 3.03 |
| 45A | 1.68 | 0.954 | 14.24 | 0.091 | 3.58 |
| 45B | 1.68 | 0.947 | 10.96 | 0.100 | 3.46 |
| 46A | 1.69 | 0.938 | 10.40 | 0.103 | 3.43 |

# APPENDIX II

## USER MANUAL

Use of Simulator

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

- Design parameters and operating conditions

  Length of reactor (m)

  Diameter of reactor (inches)

  Reactor pressure (psi)

  Reactor temperature ($^{o}F$)

  Recycle gas flow (SCFH)

  Hydrogen concentration in recycle gas (vol %)

  Makeup hydrogen flow rate (SCFH)

  Slurry feed rate (lb/hr)

  Slurry recycle rate ($GPM/ft^2$)

- Richardson-Zaki and related parameters

  Terminal velocity of particle (ft/s)

  Richardson-Zaki index, n (-)

  Rise velocity of single bubble (ft/s)

  Voidage at minimum fluidization (-)

  Height of bed at minimum fluidization conditions (m)

- Catalyst properties

  Catalyst density (gm/cc)

  Catalyst length (inches)

  Catalyst diameter (inches)

  Weight of catalyst loaded (gm)

- Physico-Chemical Data

  Density of slurry (gm/cc)

  Viscosity of slurry (Pa.s)

  Surface Tension of slurry (dyne/cm)

  Heat of dissolution (cal/gmole)

  Solubility constant (-)

- Kinetic Parameters

  Arrhenius frequency factor for hydrogen consumption kinetics (1/sec)

  Activation energy for hydrogen consumption kinetics (cal/gmole)

  Number of reacting species (excluding $H_2$) (-)

  Total number of reactions (excluding $H_2$ consumption) (-)

  For each reaction:

  Arrhenius frequency factor (1/min)

  Activation energy (cal/gmole)

The above input data are entered via an interactive program, INPUT.FOR. A file called INPUT.DAT and another called KIN.DAT are created on executing this program, as well as a file called CHECK.DAT which contains the user's responses to the input entry program. The files INPUT.DAT and KIN.DAT provides the data to the main program, ITSL2.FOR.

The following subroutines are used in the simulator.

| SUBROUTINE NAME | PURPOSE |
|---|---|
| HYDRO | Calculates mass transfer coefficient and Peclet number |
| HOLDUP | Calculates gas and slurry holdups |
| INPUT | Reads input data on design, parameters, operating conditions etc. |
| INPUT1 | Reads input data on coal liquefaction kinetics |
| REATEM | Defines the differential equations for the mass balances |
| RUNGE | Integrates system of simultaneous first-order differential equations using Runge-Kutta method. |

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

| | | |
|---|---|---|
| DATA.DAT | - | Input data |
| KIN.DAT | - | Kinetic data |
| OUTPUT.DAT | - | Output summary |
| H2GAS.DAT | - | Hydrogen gas profile |
| H2LIQ.DAT | - | Hydrogen liquid profile |
| SPCONC.DAT | - | Species concentration profile |

# APPENDIX III

## MAIN PROGRAM LISTING

```
C       ------------------------------------------------------------------

C       PROGRAM TO SIMULATE THREE PHASE EBULLATED BED REACTOR, WHICH
C       CONSTITUTES THE SECOND STAGE IN THE WILSONVILLE INTEGRATED
C       TWO-STAGE LIQUEFACTION (ITSL) PROCESS.

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

        IMPLICIT REAL*8(A-H,O-Z)
        IFLAG=1
        CALL INPUT(IFLAG)
        IF (IFLAG.EQ.0) GO TO 10
        CALL INPUT1
        CALL REATEM
        WRITE(6,200)
        GO TO 11
 10     WRITE(6,100)
 100    FORMAT(5X,'CONVERGENCE WAS NOT OBTAINED IN SUBROUTINE HOLDUP',/,
     *         5X,'PROGRAM TERMINATED',//)
 200    FORMAT(70('-'),/,25X,'SIMULATION COMPLETE',/,70('-'),/,
     *  10X,'OUTPUT IS CONTAINED IN THE FOLLOWING FILES',/,
     *  10X,'INPUT DATA',T50,'DATA.DAT',/,
     *  10X,'KINETIC DATA ',T50,'KINDAT.DAT',/,
     *  10X,'OUTPUT SUMMARY',T50,'OUTPUT.DAT',/,
     *  10X,'HYDROGEN PROFILE (GAS PHASE)',T50,'H2GAS.DAT',/,
     *  10X,'HYDROGEN PROFILE (LIQUID PHASE)',T50,'H2LIQ.DAT',/,
     *  10X,'SPECIES CONCENTRATION PROFILE',T50,'SPECIE.DAT',/,70('-'))
 11     CONTINUE
        STOP
        END


        SUBROUTINE HYDRO(UG,AKLA,PEL)

C       ....THIS SUBROUTINE CALCULATES THE PECLET NUMBER AND THE VOLUMETRIC
C       MASS TRANSFER COEFFICIENT.

C       UG - GAS VELOCITY, m/s
C       UG1 - GAS VELOCITY, cm/s
C       UG2 - GAS VELOCITY, ft/s
C       AKLA - MASS TRANSFER COEFFICIENT, 1/s
C       PEL - PECLET NUMBER [-]

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

        UG1=UG*100.
        UG2=UG/0.3048
        PEL=5.05+42.91*DEXP(-35.48*UG2)
        AKLA=0.0252*UG1

        RETURN
        END

        SUBROUTINE INPUT(IFLAG)

C            THIS SUBROUTINE READS THE INPUT DATA ON THE PHYSICAL DIMENSIONS
C       OF THE UNITS, PHYSICAL AND THERMAL PROPERTIES AND HYDROGEN CONSUMPTION
C       KINETICS.

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

```
      COMMON /B1/ ST,HENCON,DAH2,H2CON,EFFLEN
      COMMON /B4/ TERM,UR
      COMMON /B6/ TEMP
      COMMON /B10/ QSLUR,QRCYC
      COMMON /B13/ CATDEN,CATLEN,CATWT,SLUVOL
      COMMON /B15/ ZKBAR,ERXN,DHS,HBAR,AKH2

      GASENG=1.987          !GAS CONSTANT IN CAL/GMOLE.DEG K
      GASCON=82.057         !GAS CONSTANT IN CC.ATM/GMOLE.DEG K

      OPEN (UNIT=11,FILE='INPUT.DAT')
      OPEN (UNIT=12,FILE='DATA.DAT')

      READ(11,*) RCVGAS,H2CON,H2FLOW,SLFEED,SLRCYC,PRES,TEMP
      READ(11,*) DIA,ALEN
      READ(11,*) ZKBAR,ERXN,DHS,HBAR,SLDEN,SLVIS,SLSURT
      READ(11,*) UT,AN,UTB,EMF,HMF
      READ(11,*) CATDEN,CATLEN,CATDIA,CATWT
      WRITE(12,11)
11    FORMAT(//5X,'INPUT DATA FOR FLUIDIZED BED REACTOR SIMULATION',///)
      WRITE(12,10) RCVGAS,H2CON,H2FLOW,SLFEED,SLRCYC,PRES,TEMP,DIA,ALEN

10    FORMAT (5X,'RECYCLE GAS FLOW IN SCFH    ',T55,F12.5,/,
     *  5X,'HYDROGEN CONCENTRATION IN RECYCLE GAS, vol % ',T55,F12.5,/,
     *                 5X,'MAKEUP H2 FLOW RATE SCFH    ',T55,F12.5,/,
     *                  5X,'SLURRY FEED RATE, lb/hr   ',T55,F12.5,/,
     *              5X,'SLURRY RECYCLE RATE, GPM/ft**2   ',T55,F12.5,/,
     *                  5X,'PRESSURE, psi ',T55,F12.5,/,
     *                  5X,'TEMPERATURE, deg. F ',T55,F12.5,/,
     *         5X,'DIAMETER OF REACTOR, inches',T55,F12.5,/,
     *          5X,'LENGTH OF REACTOR, m ',T55,F12.5,//)
      WRITE(12,31) SLDEN,SLVIS,SLSURT
31    FORMAT(//5X,'SLURRY PHYSICAL PROPERTIES:',//,
     *  5X,'DENSITY OF SLURRY, gm/cc ',T55,F12.5,/,
     *  5X,'VISCOSITY OF SLURRY, Pa.s ',T55,F12.5,/,
     *  5X,'SURFACE TENSION OF SLURRY, dyne/cm ',T55,F12.5,//)

      WRITE(12,40) UT,AN,UTB,EMF,HMF
40    FORMAT(///5X,'RICHARDSON-ZAKI PARAMETERS:',//,
     *  5X,'TERMINAL VELOCITY OF PARTICLE, ft/s ',T55,F12.5,/,
     *  5X,'RICHARDSON-ZAKI INDEX [-] ',T55,F12.5,/,
     *  5X,'BUBBLING VELOCITY, ft/s',T55,F12.5,/,
     *  5X,'VOIDAGE AT MINIMUM FLUIDIZATION [-] ',T55,F12.5,/,
     *  5X,'HEIGHT OF BED AT MINIMUM FLUIDIZATION, m '
     *  ,T55,F12.5,//)
      WRITE(12,77) CATDEN,CATLEN,CATDIA,CATWT
77    FORMAT(//5X,'CATALYST PROPERTIES:',//,
     *  5X,'CATALYST DENSITY, gm/cc ',T55,F12.5,/,
     *  5X,'CATALYST LENGTH,  inches ',T55,F12.5,/,
     *  5X,'CATALYST DIAMETER, inches ',T55,F12.5,/,
     *  5X,'WEIGHT OF CATALYST LOADED, gm ',T55,F12.5,//)
      CATLEN=CATLEN/2.54
      CATDIA=CATDIA/2.54
      CATWT=CATWT/1000.
      UT=UT*0.3048
      UTB=UTB*0.3048
      CLOSE (UNIT=11)
      CLOSE (UNIT=12)

      SLDEN=SLDEN*62.4
```

```
      DIA=DIA/12.0
      TEMP=TEMP+460.

      AREA=DATAN(1.0D0)*DIA**2
      QSLUR=SLFEED/3600./SLDEN
      SLDEN=SLDEN/62.4
      QRCYC=SLRCYC*AREA*2.228D-03*(0.85/SLDEN)**0.5
      UL=(QSLUR+QRCYC)/AREA
      RRATIO=QRCYC/QSLUR
      CFH=(RCYGAS+H2FLOW)*14.7*TEMP/520./PRES
      UG=CFH/3600./AREA

      TEMP=(TEMP-492.)*5./9.+273.15
      DIA=DIA*0.3048
      UL=UL*0.3048
      UG=UG*0.3048
      PRES=PRES/14.7

      H2CON=(RCYGAS*H2CON*.01+H2FLOW)/(RCYGAS+H2FLOW)
      H2CON=H2CON*PRES/(GASCON*TEMP)
      HENCON=HBAR*DEXP(-DHS/(GASENG*TEMP))

      CALL HYDRO (UG,AKLA,PEL)
      CALL HOLDUP (UG,UL,UT,AN,UTB,EPSL,EPSG,IFLAG)
      IF(IFLAG.EQ.0) RETURN
      EFFLEN=HMF*(1.-EMF)/(1.-EPSL-EPSG)
      ST=EFFLEN*AKLA/UG
      AKH2=ZKBAR*DEXP(-ERXN/(GASENG*TEMP))
      UR=UL/UG
      TERM=EFFLEN*EPSL/UL
      DAH2=TERM*AKH2
      DAH2=0.0
      AREA=AREA*0.0929       !SQ. FT TO SQ. M
      SLUVOL=AREA*EFFLEN*EPSL
      OPEN (UNIT=14,FILE='OUTPUT.DAT')
      WRITE(14,100) UG,UL,AKLA,PEL,EPSL,EPSG,EFFLEN,ST,TERM,RRATIO
     *                          ,HENCON
  100 FORMAT(//,5X,'CALCULATED HYDRODYNAMIC AND MASS TRANSFER',
     *  ' PARAMETERS',///,
     *  5X,'SUPERFICIAL GAS VELOCITY, m/s',T55,F8.4,//,
     *  5X,'SUPERFICIAL LIQUID VELOCITY, m/s',T55,F8.4,//,
     *  5X,'LIQUID-SIDE MASS TRANSFER COEFFICIENT, 1/s',T55,F8.4,//,
     *  5X,'LIQUID PHASE PECLET NUMBER',T55,F8.4,//,
     *  5X,'LIQUID PHASE HOLDUP',T55,F8.4,//,
     *  5X,'GAS PHASE HOLDUP',T55,F8.4,//,
     *  5X,'EFFECTIVE REACTOR LENGTH, m',T55,F8.4,//,
     *  5X,'STANTON NUMBER',T55,F8.4,//,
     *  5X,'SLURRY RESIDENCE TIME, s',T55,F8.4,//,
     *  5X,'RECYCLE RATIO ',T55,F8.4,//,
     *  5X,'HENRY''S CONSTANT',T55,F8.4,///)
      CLOSE (UNIT=14)
      RETURN
      END


      SUBROUTINE REATEM
C        THIS SUBROUTINE SIMULATES THE THERMAL BEHAVIOR OF THE REACTOR.

      IMPLICIT REAL*8(A-H,O-Z)
      CHARACTER*20 NAME(10)
```

```
      INTEGER RUNGE
      EXTERNAL RUNGE

      DIMENSION F(7),Z(7),CASS(10),CCAL(10)
      COMMON /B1/ ST,HENCON,DAH2,H2CON,EFFLEN
      COMMON /B3/ AK(10),EPSN
      COMMON /B4/ TERM,UR
      COMMON /B5/ NSP,NR
      COMMON /B7/ CSLR(10)
      COMMON /B8/ CINIT(10)
      COMMON /B10/ SLFEED,NCYCL
      COMMON /B14/ NAME

      NCOMP=2+NSP

      ITMAX=20
      IFLAG=0
      EFFLEN=EFFLEN*100.

C     .....TRIAL AND ERROR CALCULATIONS HAVE TO BE PERFORMED SINCE
C     RECYCLE SLURRY COMPOSITION IS NOT KNOWN. THE CALCULATIONS ARE
C     INITIATED BY ASSUMING THAT THE RECYCLE SLURRY HAS THE SAME
C     COMPOSITION AS THE FRESH FEED.

      DO 22 I=1,NSP
      CSLR(I)=CINIT(I)
   22 CASS(I)=CINIT(I)

      ALPHA=0.2
      AK25=AK(2)+AK(5)
      AK36=AK(3)+AK(6)
      AK2PN=AK(2)+AK(5)*(1.-EPSN)
      HENCON=1.0/HENCON

      OPEN (UNIT=21,FILE='H2GAS.DAT')
      OPEN (UNIT=22,FILE='H2LIQ.DAT')
      OPEN (UNIT=23,FILE='SPECIE.DAT')
      WRITE(21,80)
      WRITE(22,81)
      WRITE(23,82)

  222 CONTINUE
      DO 21 ITER=1,ITMAX

      HH=0.01

C     ....SUPPLY INITIAL CONDITIONS FOR RUNGE-KUTTA INTEGRATION.

      X=0.0
      Z(1)=1.0
      Z(2)=0.0
      Z(3)=CSLR(1)
      Z(4)=CSLR(2)
      Z(5)=CSLR(3)
      Z(6)=CSLR(4)
      Z(7)=CSLR(5)

      IF(IFLAG.EQ.0) GO TO 11
      WRITE(21,83) X,X*EFFLEN,Z(1),Z(1)*H2CON
      WRITE(22,83) X,X*EFFLEN,Z(2),Z(2)*H2CON
```

```
      WRITE(23,84) X,X*EFFLEN,Z(3),Z(4),Z(5),Z(6),Z(7)
11    CONTINUE
10    K=RUNGE(NCOMP,Z,F,X,HH)
      IF(K.NE.1) GO TO 15

      F(1)=-ST*(Z(1)-HENCON*Z(2))/HENCON
      F(2)=ST*(Z(1)-HENCON*Z(2))/HENCON-DAH2*Z(2)

      T1=AK(1)*Z(3)*Z(4)
      F(3)=-(T1+AK(4)*Z(3))*TERM
      F(4)=-(T1*ALPHA-AK36*Z(6)-
     *                          AK(5)*EPSN*Z(5))*TERM
      F(5)=-(AK25*Z(5)-T1*(1.+ALPHA))*TERM
      F(6)=-(AK36*Z(6)-AK2PM*Z(5))*TERM
      F(7)=AK(4)*Z(3)*TERM
      GO TO 10

15    CONTINUE
      IF (IFLAG.EQ.0) GO TO 223

      WRITE(21,83) X,X*EFFLEN,Z(1),Z(1)*H2CON
      WRITE(22,83) X,X*EFFLEN,Z(2),Z(2)*H2CON
      WRITE(23,84) X,X*EFFLEN,Z(3),Z(4),Z(5),Z(6),Z(7)

223   IF(X.GE.1.0) GO TO 16
      GO TO 10
16    CONTINUE
      CRYC1=Z(3)
      CRYC2=Z(4)
      CRYC3=Z(5)
      CRYC4=Z(6)
      CRYC5=Z(7)

      IF(IFLAG.EQ.1) GO TO 224

      DO 33 I=1,NSP
      IND1=I+2
33    CCAL(I)=Z(IND1)

      SUM=0.D0
      DO 31 I=1,NSP
      ERR=(CASS(I)-CCAL(I))/CCAL(I)
      ERR=ERR*ERR
      SUM=SUM+ERR
31    CONTINUE
      IF(SUM.LE.1.0D-4) GO TO 42

      DO 52 I=1,NSP
      CASS(I)=CCAL(I)
      CSLR(I)=(CINIT(I)*SLFEED+CASS(I)*RCYCL)/(SLFEED+RCYCL)
52    CONTINUE

21    CONTINUE

      IF(ITER.EQ.ITMAX) WRITE(6,101)
101   FORMAT(//5X,'NO. OF ITERATIONS REQUIRED FOR CONVERGENCE EXCEEDED')
      RETURN

42    CONTINUE
      WRITE(6,333) ITER,SUM
```

```
333     FORMAT(//5X,'NUMBER OF ITERATIONS REQUIRED FOR CONVERGENCE IN',
     *  ' SUBROUTINE REATEM = ',T75,I3,//,5X,
     *  'ERROR CRITERION SUM = ',T50,E12.5)

        IFLAG=1
        GO TO 222
224     CONTINUE
        WRITE(21,500)
        WRITE(22,500)
        WRITE(23,501)
        CLOSE(UNIT=21)
        CLOSE(UNIT=22)
        CLOSE(UNIT=23)
80      FORMAT(T21,'HYDROGEN PROFILE IN REACTOR',/,T30,'(GAS PHASE)',
     *  /,70('-'),/,T7,'DISTANCE ALONG REACTOR',12X,
     *  'HYDROGEN CONCENTRATION',/,T5,'DIMENSIONLESS',4X,
     *  'CENTIMETERS',8X,
     *  'DIMENSIONLESS',4X,'G-MOLE/CC',/,70('-'),/)
81      FORMAT(T21,'HYDROGEN PROFILE IN REACTOR',/,T28,'(LIQUID PHASE)',
     *  /,70('-'),/,T7,'DISTANCE ALONG REACTOR',12X,
     *  'HYDROGEN CONCENTRATION',/,T5,'DIMENSIONLESS',4X,
     *  'CENTIMETERS',8X,
     *  'DIMENSIONLESS',4X,'G-MOLE/CC',/,70('-'),/)
82      FORMAT(T30,'CONCENTRATION PROFILE IN REACTOR',/,
     *  T15,100('-'),/,T22,'DISTANCE ALONG REACTOR',20X,
     *  'CHEMICAL SPECIES',/,10X,'DIMENSIONLESS',4X,'CENTIMETERS',5X,
     *  '1',11X,'2',11X,'3',11X,'4',11X,'5',/,T15,100('-'))

83      FORMAT(6X,F5.2,8X,F8.1,12X,F8.4,6X,E11.4)
84      FORMAT(23X,F5.2,8X,6X,F8.1,10X,F7.4,4(3X,F7.4))
500     FORMAT(/,70('-'))
501     FORMAT(/,T15,100('-'))
        RETURN
        END

        SUBROUTINE INPUT1

C           THIS SUBROUTINE READS THE INPUT DATA ON COAL CONVERSION KINETICS.

        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION ACTVEN(10)
        CHARACTER*20 NAME(10)
        COMMON /B3/ AK(10),EPSN
        COMMON /B5/ NSP,NR
        COMMON /B6/ TEMP
        COMMON /B8/ CINIT(10)
        COMMON /B13/ CAYDEN,CATLEN,CATWT,SLRVOL
        COMMON /B14/ NAME
        COMMON /B16/ ZKBAR,ERXN,DHS,HBAR,AKH2

        OPEN (UNIT=12,FILE='KIN.DAT')
        OPEN (UNIT=15,FILE='KINDAT.DAT')
        DIFFP=1.73E-03      !CM**2/SEC
        DIFFA=2.18E-05      !  "

        WRITE (15,60) ZKBAR,ERXN,AKH2,HBAR,DHS
60      FORMAT(///,5X,'KINETIC AND THERMODYNAMIC DATA',///,
     *  5X,'ARRHENIUS FACTOR FOR H2 REACTION, 1/s',T55,E12.5,/,
     *  5X,'ACTIVATION ENERGY FOR H2 REACTION, cal/gmole',T55,E12.5,/,
     *  5X,'RATE CONSTANT FOR H2 REACTION, 1/s ',T55,E12.5,/,
```

```
     *   5X,'SOLUBILITY COEFFICIENT FOR H2 ',T55,E12.5,/,
     *   5X,'HEAT OF DISSOLUTION, cal/gmole ',T55,E12.5,//)

         WRITE (15,61)
61       FORMAT(//5X,'SPECIES PRESENT',//)
         READ(12,*) NSP
         DO 21 I=1,NSP
         READ(12,8) NAME(I)
21       WRITE (15,62) I,NAME(I)
8        FORMAT(A20)
62       FORMAT(5X,I3,' - ',A20,/)
         READ(12,*) NR

         DO 20 J=1,NR
         READ(12,*) AK(J),ACTVEN(J)
         AK(J)=AK(J)*DEXP(-ACTVEN(J)/1.987/TEMP)
         AK(J)=AK(J)/60.
20       CONTINUE

         WRITE (15,63) AK(1),AK(2),AK(3),AK(4)
63       FORMAT(//5X,'THERMAL REACTION RATE CONSTANTS (1/s):',//,
     *   5X,'REACTION 1 C + O --- P ',T55,E12.5,/,
     *   5X,'REACTION 2       P --- A ',T55,E12.5,/,
     *   5X,'REACTION 3       A --- O ',T55,E12.5,/,
     *   5X,'REACTION 4       C --- G ',T55,E12.5,//)

         GAMMA=(AK(5)/DIFFP)**0.5
         BETA=(AK(6)/DIFFA)**0.5
         EFF1=DTANH(GAMMA*CATLEN)/(GAMMA*CATLEN)
         EFF2=DTANH(BETA*CATLEN)/(BETA*CATLEN)
         EPSN=(1.0-EFF2/EFF1)/(1.0-(GAMMA/BETA)**2)

         CATLDG=CATWT/SLRVOL
         CATLDG=CATLDG*1.0D-03
         AK(5)=AK(5)*CATLDG*EFF1/CATDEN
         AK(6)=AK(6)*CATLDG*EFF2/CATDEN

         WRITE (15,64) DIFFP,DIFFA,EFF1,EFF2,AK(5),AK(6)
64       FORMAT(//5X,'CATALYTIC REACTION DATA ',//,
     *   5X,'DIFFUSIVITY OF PREASPHALTENES, cm**2/s ',T55,E12.5,/,
     *   5X,'DIFFUSIVITY OF ASPHALTENES, cm**2/S ',T55,E12.5,/,
     *   5X,'EFFECTIVENESS FACTOR FOR P --- A ',T55,E12.5,/,
     *   5X,'EFFECTIVENESS FACTOR FOR A --- O ',T55,E12.5,/,
     *   5X,'RATE CONSTANT FOR RXN 5  P --- A (1/s)',T55,E12.5,/,
     *   5X,'RATE CONSTANT FOR RXN 6  A --- O (1/s)',T55,E12.5,//)

         WRITE (15,65)
65       FORMAT(//5X,'INITIAL WEIGHT FRACTIONS OF SPECIES IN FEED:',//)
         DO 5 I=1,NSP
         READ(12,*) CINIT(I)
         WRITE(15,66) NAME(I),CINIT(I)
5        CONTINUE
66       FORMAT(5X,A20,5X,F12.5,/)

         CLOSE (UNIT=12)
         CLOSE (UNIT=15)
         RETURN
         END
```

```
      SUBROUTINE HOLDUP(UG,UL,UT,AN,UTB,EPSL,EPSG,IFLAG)

C     .....THE GAS AND LIQUID HOLDUPS ARE CALCULATED USING DARTON AND
C     HARRISON'S WAKE-FREE MODEL.

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

      AK=1.4*(UL/UG)**.33-1.0
      ELO=(UL/UT)**(1./AN)
      EL=ELO

      DO 30 ITER=1,20
      T1=(UG*EL+UL+EL*UTB)/UL
      EPSG=(T1-SQRT(T1*T1-4.*UG*EL/UL))/2.
      ELN=(UL/UT-AK*UG/UT)**(1./AN)*(1.-EPSG-AK*EPSG)**(1.-1./AN)+
     *          AK*EPSG
      IF(ABS((ELN-EL)/EL).LE.1.0E-4) GO TO 40
      EL=ELN
30    CONTINUE
      IFLAG=0
      RETURN
40    T1=(UG*EL+UL+EL*UTB)/UL
      EPSG=(T1-SQRT(T1*T1-4.*UG*EL/UL))/2.
      ELN=(UL/UT-AK*UG/UT)**(1./AN)*(1.-EPSG-AK*EPSG)**(1.-1./AN)+
     *          AK*EPSG
      EPSL=ELN
      IFLAG=1
      RETURN
      END


      FUNCTION RUNGE(N,V,F,X,H)

C          THE FUNCTION RUNGE EMPLOYS THE FOURTH ORDER RUNGE-KUTTA METHOD
C     WITH GILL'S COEFFICIENTS TO INTEGRATE A SYSTEM OF N SIMULTANEOUS
C     FIRST ORDER DIFFERENTIAL EQUATIONS ACROSS ONE STEP OF LENGTH H IN
C     THE INDEPENDENT VARIABLE X, SUBJECT TO THE INITIAL CONDITIONS.

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

      DIMENSION PHI(50),SAVEY(50),V(20),F(20)

      DATA M /0/

      M=M+1
      GO TO (1,2,3,4,5),M
1     RUNGE=1
      RETURN
2     DO 22 J=1,N
      SAVEY(J)=V(J)
      PHI(J)=F(J)
22    V(J)=SAVEY(J)+0.5*H*F(J)
      X=X+0.5*H
      RUNGE=1
      RETURN
3     DO 33 J=1,N
      PHI(J)=PHI(J)+2.0*F(J)
33    V(J)=SAVEY(J)+0.5*H*F(J)
```

```
      RUNGE=1
      RETURN
4     DO 44 J=1,N
      PHI(J)=PHI(J)+2.0*F(J)
44    Y(J)=SAVEY(J)+H*F(J)
      X=X+0.5*H
      RUNGE=1
      RETURN
5     DO 55 J=1,N
55    Y(J)=SAVEY(J)+(PHI(J)+F(J))*H/6.0
      M=0
      RUNGE=0
      RETURN
      END
```

# APPENDIX IV

## INPUT PROGRAM LISTING

```
C     ------------------------------------------------------------------
CCC
CCC   PROGRAM TO INPUT DATA TO MAIN SIMULATION ROUTINE
CCC
C     ------------------------------------------------------------------


      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION CINIT(10)
      CHARACTER*20 NAME(10)
      OPEN (UNIT=11,FILE='INPUT.DAT')
      OPEN (UNIT=9,FILE='CHECK.DAT')
      WRITE(6,11)
 11   FORMAT(//5X,'THREE PHASE FLUIDIZED BED REACTOR SIMULATION',///)
      WRITE(6,10)
      WRITE(9,10)
 10   FORMAT(5X,'INPUT INLET CONDITIONS IN FREE FORMAT',//,
     *                  5X,'RECYCLE GAS FLOW IN SCFH   '/,
     *          5X,'HYDROGEN CONCENTRATION IN RECYCLE GAS, vol % ',/,
     *                5X,'MAKEUP H2 FLOW RATE SCFH    '/,
     *                     5X,'SLURRY FEED RATE, lb/hr  '/,
     *                   5X,'SLURRY RECYCLE RATE, GPM/ft**2  ',/,
     *                   5X,'PRESSURE, psi ',/,
     *                   5X,'TEMPERATURE, deg. F ',/)
      READ(5,*) RCYGAS,H2CON,H2FLOW,SLFEED,SLRCYC,PRES,TEMP
      WRITE(11,*) RCYGAS,H2CON,H2FLOW,SLFEED,SLRCYC,PRES,TEMP
      WRITE(9,*) RCYGAS,H2CON,H2FLOW,SLFEED,SLRCYC,PRES,TEMP
      WRITE(6,20)
      WRITE(9,20)
 20   FORMAT(//5X,'ENTER VALUES OF VARIABLES LISTED BELOW:',//)
      WRITE(9,30)
      WRITE(6,30)
 30   FORMAT(5X,'DIAMETER OF REACTOR, inches',/,
     *          5X,'LENGTH OF REACTOR, m ',/)
      READ(5,*) DIA,ALEN
      WRITE(11,*) DIA,ALEN
      WRITE(9,*) DIA,ALEN
      WRITE(9,31)
      WRITE(6,31)
 31   FORMAT(//5X,'PHYSICO-CHEMICAL DATA INPUT:',//,
     *  5X,'ARRHENIUS FREQUENCY FACTOR FOR H2 CONSUMPTION KINETICS',
     *  ' (1/sec) ',/,
     *  5X,'ACTIVATION ENERGY FOR H2 CONSUMPTION KINETICS',
     *  ' (cal/gmole) ',/,
     *  5X,'HEAT OF DISSOLUTION (cal/gmole) ',/,
     *  5X,'SOLUBILITY CONSTANT, (<gm/cc>liq/<gm/cc>gas)',/,
     *  5X,'DENSITY OF SLURRY, gm/cc ',/,
     *  5X,'VISCOSITY OF SLURRY, Pa.s ',/,
     *  5X,'SURFACE TENSION OF SLURRY, dyne/cm ',/)
      READ(5,*) ZKBAR,ERXN,DHS,HBAR,SLDEN,SLVIS,SLSURT
      WRITE(11,*) ZKBAR,ERXN,DHS,HBAR,SLDEN,SLVIS,SLSURT
      WRITE(9,*) ZKBAR,ERXN,DHS,HBAR,SLDEN,SLVIS,SLSURT
      WRITE(9,40)

      WRITE(6,40)
 40   FORMAT(///5X,'INPUT RICHARDSON-ZAKI PARAMETERS',//,
     *  5X,'TERMINAL VELOCITY OF PARTICLE, ft/s ',/,
     *  5X,'RICHARDSON-ZAKI INDEX [-] ',/,
     *  5X,'BUBBLING VELOCITY, ft/s',/,
     *  5X,'VOIDAGE AT MINIMUM FLUIDIZATION [-] ',/,
```

```
     *   5X,'HEIGHT OF BED AT MINIMUM FLUIDIZATION CONDITIONS, m ',/)
         READ(5,*) UT,AN,UTB,EMF,HMF
         WRITE(11,*) UT,AN,UTB,EMF,HMF
         WRITE(9,*) UT,AN,UTB,EMF,HMF
         WRITE(6,77)
77       FORMAT(//5X,'INPUT CATALYST PROPERTIES:',/,
     *   5X,'CATALYST DENSITY, gm/cc ',/,
     *   5X,'CATALYST LENGTH,  inches ',/,
     *   5X,'CATALYST DIAMETER, inches ',/,
     *   5X,'WEIGHT OF CATALYST LOADED, gm ',//)
         WRITE(9,77)
         READ(5,*) CATDEN,CATLEN,CATDIA,WTCAT
         WRITE(11,*) CATDEN,CATLEN,CATDIA,WTCAT
         WRITE(9,*) CATDEN,CATLEN,CATDIA,WTCAT

         CLOSE (UNIT=11)
         OPEN (UNIT=12,FILE='KIN.DAT')
         WRITE(9,60)
         WRITE(6,60)
60       FORMAT(///5X,'REACTION NETWORK DATA',
     *         //,5X,'ENTER NUMBER OF REACTING SPECIES ',$)
         READ(5,*) NSP
         WRITE(12,*) NSP
         WRITE(9,*) NSP

         DO 2 I=1,NSP
         WRITE(9,51) I
         WRITE(6,51) I
51       FORMAT(5X,'ENTER NAME OF SPECIES NUMBER',I2,3X,$)
         READ(5,52) NAME(I)
         WRITE(9,52) NAME(I)
         WRITE(12,52) NAME(I)
52       FORMAT(A20)
2        CONTINUE
         WRITE(6,53)
53       FORMAT(/5X,'THE SPECIES HAVE BEEN CODED AS:',//)

         DO 3 I=1,NSP
         WRITE(6,61) I,NAME(I)
61       FORMAT(5X,I2,2X,'=',2X,A20)
3        CONTINUE

         WRITE(9,50)
         WRITE(6,50)
50       FORMAT(//5X,'ENTER TOTAL NUMBER OF REACTIONS ',$)
         READ(5,*) NR
         WRITE(12,*) NR
         WRITE(9,*) NR

         DO 41 J=1,NR
         WRITE(9,62) J
         WRITE(6,62) J
62       FORMAT(//5X,'FOR REACTION NO. ',I2,/5X,'ENTER ARRHENIUS FACTOR',
     *   ' ACTIVATION ENERGY'//)
         READ(5,*) AK,ACTVEN
         WRITE(12,*) AK,ACTVEN
         WRITE(9,*) AK,ACTVEN
41       CONTINUE

         WRITE(9,70)
```

```
      WRITE(6,70)
70    FORMAT(///5X,'ENTER INITIAL CONCENTRATION OF EACH SPECIES',
     *  '(gm/gm)')
      DO 5 I=1,NSP
      WRITE(9,71)
      WRITE(6,71) I
71    FORMAT(5X,'SPECIE NUMBER',2X,I2,3X,$)
      READ(5,*) CINIT(I)
      WRITE(12,*) CINIT(I)
      WRITE(9,*) CINIT(I)
5     CONTINUE

      CLOSE (UNIT=12)
      CLOSE (UNIT=9)
      WRITE(6,99)
99    FORMAT(//5X,'DATA HAVE BEEN ENTERED IN INPUT.DAT',/,
     *  5X,'DATA CAN BE CHECKED BY EXAMINING FILE CHECK.DAT',/,
     *  5X,'MAIN SIMULATION ROUTINE CAN BE RUN NOW',//)
      STOP
      END
```

# APPENDIX V

## SAMPLE DATA INPUT

```
     INPUT INLET CONDITIONS IN FREE FORMAT

     RECYCLE GAS FLOW IN SCFH
     HYDROGEN CONCENTRATION IN RECYCLE GAS, vol %
     MAKEUP H2 FLOW RATE SCFH
     SLURRY FEED RATE, lb/hr
     SLURRY RECYCLE RATE, GPM/ft**2
     PRESSURE, psi
     TEMPERATURE, deg. F

2200.0000000000000, 100.00000000000000, 2830.0000000000000,
628.00000000000000, 19.100000000000000, 2972.0000000000000,
815.00000000000000

     ENTER VALUES OF VARIABLES LISTED BELOW:


     DIAMETER OF REACTOR, inches
     LENGTH OF REACTOR, m

8.5000000000000000, 4.0000000000000000

     PHYSICO-CHEMICAL DATA INPUT:

     ARRHENIUS FREQUENCY FACTOR FOR H2 CONSUMPTION KINETICS (1/sec)
     ACTIVATION ENERGY FOR H2 CONSUMPTION KINETICS (cal/gmole)
     HEAT OF DISSOLUTION (cal/gmole)
     SOLUBILITY CONSTANT, (<gm/cc>liq/<gm/cc>gas)
     DENSITY OF SLURRY, gm/cc
     VISCOSITY OF SLURRY, Pa.s
     SURFACE TENSION OF SLURRY, dyne/cm

3213.0000000000000, 21000.000000000000, 770.00000000000000,
1.2000000000000000, 0.89400000000000000, 1.8000000000000000E-02,
30.000000000000000


     INPUT RICHARDSON-ZAKI PARAMETERS

     TERMINAL VELOCITY OF PARTICLE, ft/s
     RICHARDSON-ZAKI INDEX [-]
     BUBBLING VELOCITY, ft/s
     VOIDAGE AT MINIMUM FLUIDIZATION [-]
     HEIGHT OF BED AT MINIMUM FLUIDIZATION CONDITIONS, m

0.48400000000000000, 2.8000000000000000, 0.03500000000000000,
0.42000000000000000, 1.8800000000000000


     INPUT CATALYST PROPERTIES:
     CATALYST DENSITY, gm/cc
     CATALYST LENGTH, inches
     CATALYST DIAMETER, inches
     WEIGHT OF CATALYST LOADED, gm
```

1.6770000000000000, 0.2740000000000000, 8.2000000000000000E-02,
33485.000000000000

REACTION NETWORK DATA

ENTER NUMBER OF REACTING SPECIES 5
ENTER NAME OF SPECIES NUMBER 1 COAL
ENTER NAME OF SPECIES NUMBER 2 OIL
ENTER NAME OF SPECIES NUMBER 3 PREASPHALTENE
ENTER NAME OF SPECIES NUMBER 4 ASPHALTENE
ENTER NAME OF SPECIES NUMBER 5 GAS

ENTER TOTAL NUMBER OF REACTIONS 6

FOR REACTION NO. 1
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

0.1800000000000000, 0.0000000000000000E+00

FOR REACTION NO. 2
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

8.8000000000000000E-02, 0.0000000000000000E+00

FOR REACTION NO. 3
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

8.4000000000000000E-03, 0.0000000000000000E+00

FOR REACTION NO. 4
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

1.9500000000000000E-02, 0.0000000000000000E+00

FOR REACTION NO. 5
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

1.0800000000000000, 0.0000000000000000E+00

FOR REACTION NO. 6
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

0.1677000000000000, 0.0000000000000000E+00

```
    ENTER INITIAL CONCENTRATION OF EACH SPECIES(gm/gm)
    SPECIE NUMBER
0.33000000000000000
    SPECIE NUMBER
0.53000000000000000
    SPECIE NUMBER
8.0000000000000000E-02
    SPECIE NUMBER
8.0000000000000000E-02
    SPECIE NUMBER
0.0000000000000000E+00
```

INPUT DATA FOR FLUIDIZED BED REACTOR SIMULATION

| | |
|---|---|
| RECYCLE GAS FLOW IN SCFH | 2200.00000 |
| HYDROGEN CONCENTRATION IN RECYCLE GAS, vol % | 100.00000 |
| MAKEUP H2 FLOW RATE SCFH | 2830.00000 |
| SLURRY FEED RATE, lb/hr | 838.00000 |
| SLURRY RECYCLE RATE, GPM/ft**2 | 10.10000 |
| PRESSURE, psi | 2972.00000 |
| TEMPERATURE, deg. F | 815.00000 |
| DIAMETER OF REACTOR, inches | 8.50000 |
| LENGTH OF REACTOR, m | 4.00000 |

SLURRY PHYSICAL PROPERTIES:

| | |
|---|---|
| DENSITY OF SLURRY, gm/cc | 0.89400 |
| VISCOSITY OF SLURRY, Pa.s | 0.01800 |
| SURFACE TENSION OF SLURRY, dyne/cm | 30.00000 |

RICHARDSON-ZAKI PARAMETERS:

| | |
|---|---|
| TERMINAL VELOCITY OF PARTICLE, ft/s | 0.48400 |
| RICHARDSON-ZAKI INDEX [-] | 2.80000 |
| BUBBLING VELOCITY, ft/s | 0.03500 |
| VOIDAGE AT MINIMUM FLUIDIZATION [-] | 0.42000 |
| HEIGHT OF BED AT MINIMUM FLUIDIZATION, m | 1.00000 |

CATALYST PROPERTIES:

| | |
|---|---|
| CATALYST DENSITY, gm/cc | 1.67700 |
| CATALYST LENGTH, inches | 0.27400 |
| CATALYST DIAMETER, inches | 0.08200 |
| WEIGHT OF CATALYST LOADED, gm | 33485.00000 |

KINETIC AND THERMODYNAMIC DATA

| | |
|---|---|
| ARRHENIUS FACTOR FOR H2 REACTION, 1/s | 0.32130E+04 |
| ACTIVATION ENERGY FOR H2 REACTION, cal/gmole | 0.21000E+05 |
| RATE CONSTANT FOR H2 REACTION, 1/s | 0.10601E-02 |
| SOLUBILITY COEFFICIENT FOR H2 | 0.12000E+01 |
| HEAT OF DISSOLUTION, cal/gmole | 0.77000E+03 |

SPECIES PRESENT

1 - COAL

2 - OIL

3 - PREASPHALTENE

4 - ASPHALTENE

5 - GAS



THERMAL REACTION RATE CONSTANTS (1/s):

| | |
|---|---|
| REACTION 1 C + O --- P | 0.30000E-02 |
| REACTION 2 P --- A | 0.11333E-02 |
| REACTION 3 A --- O | 0.15867E-03 |
| REACTION 4 C --- G | 0.32500E-03 |

CATALYTIC REACTION DATA

| | |
|---|---|
| DIFFUSIVITY OF PREASPHALTENES, cm**2/s | 0.17360E-05 |
| DIFFUSIVITY OF ASPHALTENES, cm**2/S | 0.21800E-04 |
| EFFECTIVENESS FACTOR FOR P --- A | 0.91038E-01 |
| EFFECTIVENESS FACTOR FOR A --- O | 0.68777E+00 |
| RATE CONSTANT FOR RXN 5 P --- A (1/s) | 0.71936E-03 |
| RATE CONSTANT FOR RXN 6 A --- O (1/s) | 0.84387E-03 |

INITIAL WEIGHT FRACTIONS OF SPECIES IN FEED:

| | |
|---|---|
| COAL | 0.33000 |
| OIL | 0.53000 |

| | |
|---|---|
| PREASPHALTENE | 0.08000 |
| ASPHALTENE | 0.08000 |
| GAS | 0.00000 |

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# APPENDIX VI

## SAMPLE OUTPUT

CALCULATED HYDRODYNAMIC AND MASS TRANSFER PARAMETERS

| | |
|---|---|
| SUPERFICIAL GAS VELOCITY, m/s | 0.0131 |
| SUPERFICIAL LIQUID VELOCITY, m/s | 0.0151 |
| LIQUID-SIDE MASS TRANSFER COEFFICIENT, 1/s | 0.0330 |
| LIQUID PHASE PECLET NUMBER | 14.3810 |
| LIQUID PHASE HOLDUP | 0.3006 |
| GAS PHASE HOLDUP | 0.2484 |
| EFFECTIVE REACTOR LENGTH, m | 3.1810 |
| STANTON NUMBER | 0.0162 |
| SLURRY RESIDENCE TIME, s | 82.4676 |
| RECYCLE RATIO | 5.2200 |
| HENRY'S CONSTANT | 0.8043 |

HYDROGEN PROFILE IN REACTOR
(GAS PHASE)

| DISTANCE ALONG REACTOR | | HYDROGEN CONCENTRATION | |
|---|---|---|---|
| DIMENSIONLESS | CENTIMETERS | DIMENSIONLESS | GMOLE/CC |
| 0.00 | 0.0 | 1.0000 | 0.3470E-02 |
| 0.01 | 3.2 | 0.9480 | 0.3290E-02 |
| 0.02 | 6.4 | 0.9025 | 0.3140E-02 |
| 0.03 | 9.5 | 0.8620 | 0.3002E-02 |
| 0.04 | 12.7 | 0.8263 | 0.2882E-02 |
| 0.05 | 15.9 | 0.7980 | 0.2777E-02 |
| 0.06 | 19.1 | 0.7716 | 0.2685E-02 |
| 0.07 | 22.3 | 0.7486 | 0.2605E-02 |
| 0.08 | 25.4 | 0.7285 | 0.2535E-02 |
| 0.09 | 28.6 | 0.7109 | 0.2474E-02 |
| 0.10 | 31.8 | 0.6956 | 0.2420E-02 |
| 0.11 | 35.0 | 0.6822 | 0.2374E-02 |
| 0.12 | 38.2 | 0.6705 | 0.2333E-02 |
| 0.13 | 41.4 | 0.6603 | 0.2297E-02 |
| 0.14 | 44.5 | 0.6514 | 0.2267E-02 |
| 0.15 | 47.7 | 0.6437 | 0.2230E-02 |
| 0.16 | 50.9 | 0.6369 | 0.2216E-02 |
| 0.17 | 54.1 | 0.6309 | 0.2195E-02 |
| 0.18 | 57.3 | 0.6256 | 0.2177E-02 |
| 0.19 | 60.4 | 0.6213 | 0.2162E-02 |
| 0.20 | 63.6 | 0.6173 | 0.2148E-02 |
| 0.21 | 66.8 | 0.6139 | 0.2136E-02 |
| 0.22 | 70.0 | 0.6109 | 0.2125E-02 |
| 0.23 | 73.2 | 0.6083 | 0.2116E-02 |
| 0.24 | 76.3 | 0.6060 | 0.2108E-02 |
| 0.25 | 79.5 | 0.6040 | 0.2101E-02 |
| 0.26 | 82.7 | 0.6022 | 0.2095E-02 |
| 0.27 | 85.9 | 0.6007 | 0.2090E-02 |
| 0.28 | 89.1 | 0.5994 | 0.2085E-02 |
| 0.29 | 92.3 | 0.5982 | 0.2081E-02 |
| 0.30 | 95.4 | 0.5972 | 0.2078E-02 |
| 0.31 | 98.6 | 0.5963 | 0.2075E-02 |
| 0.32 | 101.8 | 0.5955 | 0.2072E-02 |
| 0.33 | 105.0 | 0.5948 | 0.2070E-02 |
| 0.34 | 108.2 | 0.5943 | 0.2068E-02 |
| 0.35 | 111.3 | 0.5938 | 0.2066E-02 |
| 0.36 | 114.5 | 0.5933 | 0.2064E-02 |
| 0.37 | 117.7 | 0.5929 | 0.2063E-02 |
| 0.38 | 120.9 | 0.5926 | 0.2062E-02 |
| 0.39 | 124.1 | 0.5923 | 0.2061E-02 |
| 0.40 | 127.2 | 0.5920 | 0.2060E-02 |
| 0.41 | 130.4 | 0.5918 | 0.2059E-02 |
| 0.42 | 133.6 | 0.5916 | 0.2058E-02 |
| 0.43 | 136.8 | 0.5914 | 0.2058E-02 |
| 0.44 | 140.0 | 0.5913 | 0.2057E-02 |
| 0.45 | 143.1 | 0.5911 | 0.2057E-02 |
| 0.46 | 146.3 | 0.5910 | 0.2056E-02 |
| 0.47 | 149.5 | 0.5909 | 0.2056E-02 |

| | | | |
|---|---|---|---|
| 0.48 | 152.7 | 0.5908 | 0.2056E-02 |
| 0.49 | 155.9 | 0.5908 | 0.2055E-02 |
| 0.50 | 159.1 | 0.5907 | 0.2055E-02 |
| 0.51 | 162.2 | 0.5906 | 0.2055E-02 |
| 0.52 | 165.4 | 0.5906 | 0.2055E-02 |
| 0.53 | 168.6 | 0.5905 | 0.2055E-02 |
| 0.54 | 171.8 | 0.5905 | 0.2055E-02 |
| 0.55 | 175.0 | 0.5905 | 0.2054E-02 |
| 0.56 | 178.1 | 0.5904 | 0.2054E-02 |
| 0.57 | 181.3 | 0.5904 | 0.2054E-02 |
| 0.58 | 184.5 | 0.5904 | 0.2054E-02 |
| 0.59 | 187.7 | 0.5904 | 0.2054E-02 |
| 0.60 | 190.9 | 0.5903 | 0.2054E-02 |
| 0.61 | 194.0 | 0.5903 | 0.2054E-02 |
| 0.62 | 197.2 | 0.5903 | 0.2054E-02 |
| 0.63 | 200.4 | 0.5903 | 0.2054E-02 |
| 0.64 | 203.6 | 0.5903 | 0.2054E-02 |
| 0.65 | 206.8 | 0.5903 | 0.2054E-02 |
| 0.66 | 209.9 | 0.5903 | 0.2054E-02 |
| 0.67 | 213.1 | 0.5903 | 0.2054E-02 |
| 0.68 | 216.3 | 0.5903 | 0.2054E-02 |
| 0.69 | 219.5 | 0.5903 | 0.2054E-02 |
| 0.70 | 222.7 | 0.5903 | 0.2054E-02 |
| 0.71 | 225.9 | 0.5903 | 0.2054E-02 |
| 0.72 | 229.0 | 0.5903 | 0.2054E-02 |
| 0.73 | 232.2 | 0.5902 | 0.2054E-02 |
| 0.74 | 235.4 | 0.5902 | 0.2054E-02 |
| 0.75 | 238.6 | 0.5902 | 0.2054E-02 |
| 0.76 | 241.8 | 0.5902 | 0.2054E-02 |
| 0.77 | 244.9 | 0.5902 | 0.2054E-02 |
| 0.78 | 248.1 | 0.5902 | 0.2054E-02 |
| 0.79 | 251.3 | 0.5902 | 0.2054E-02 |
| 0.80 | 254.5 | 0.5902 | 0.2054E-02 |
| 0.81 | 257.7 | 0.5902 | 0.2054E-02 |
| 0.82 | 260.8 | 0.5902 | 0.2054E-02 |
| 0.83 | 264.0 | 0.5902 | 0.2054E-02 |
| 0.84 | 267.2 | 0.5902 | 0.2054E-02 |
| 0.85 | 270.4 | 0.5902 | 0.2054E-02 |
| 0.86 | 273.6 | 0.5902 | 0.2054E-02 |
| 0.87 | 276.8 | 0.5902 | 0.2054E-02 |
| 0.88 | 279.9 | 0.5902 | 0.2054E-02 |
| 0.89 | 283.1 | 0.5902 | 0.2054E-02 |
| 0.90 | 286.3 | 0.5902 | 0.2054E-02 |
| 0.91 | 289.5 | 0.5902 | 0.2054E-02 |
| 0.92 | 292.7 | 0.5902 | 0.2054E-02 |
| 0.93 | 295.8 | 0.5902 | 0.2054E-02 |
| 0.94 | 299.0 | 0.5902 | 0.2054E-02 |
| 0.95 | 302.2 | 0.5902 | 0.2054E-02 |
| 0.96 | 305.4 | 0.5902 | 0.2054E-02 |
| 0.97 | 308.6 | 0.5902 | 0.2054E-02 |
| 0.98 | 311.7 | 0.5902 | 0.2054E-02 |
| 0.99 | 314.9 | 0.5902 | 0.2054E-02 |
| 1.00 | 318.1 | | |

---

## HYDROGEN PROFILE IN REACTOR
## (LIQUID PHASE)

| DISTANCE ALONG REACTOR | | HYDROGEN CONCENTRATION | |
|---|---|---|---|
| DIMENSIONLESS | CENTIMETERS | DIMENSIONLESS | G-MOLE/CC |
| 0.00 | 0.0 | 0.0000 | 0.0000E+00 |
| 0.01 | 3.2 | 0.0520 | 0.1811E-03 |
| 0.02 | 6.4 | 0.0975 | 0.3381E-03 |
| 0.03 | 9.5 | 0.1371 | 0.4771E-03 |
| 0.04 | 12.7 | 0.1716 | 0.5976E-03 |
| 0.05 | 15.9 | 0.2020 | 0.7028E-03 |
| 0.06 | 19.1 | 0.2284 | 0.7948E-03 |
| 0.07 | 22.3 | 0.2514 | 0.8747E-03 |
| 0.08 | 25.4 | 0.2715 | 0.9447E-03 |
| 0.09 | 28.6 | 0.2891 | 0.1003E-02 |
| 0.10 | 31.8 | 0.3044 | 0.1059E-02 |
| 0.11 | 35.0 | 0.3178 | 0.1106E-02 |
| 0.12 | 38.2 | 0.3295 | 0.1146E-02 |
| 0.13 | 41.4 | 0.3397 | 0.1182E-02 |
| 0.14 | 44.5 | 0.3486 | 0.1213E-02 |
| 0.15 | 47.7 | 0.3563 | 0.1240E-02 |
| 0.16 | 50.9 | 0.3631 | 0.1263E-02 |
| 0.17 | 54.1 | 0.3691 | 0.1284E-02 |
| 0.18 | 57.3 | 0.3742 | 0.1302E-02 |
| 0.19 | 60.4 | 0.3787 | 0.1318E-02 |
| 0.20 | 63.6 | 0.3827 | 0.1331E-02 |
| 0.21 | 66.8 | 0.3861 | 0.1343E-02 |
| 0.22 | 70.0 | 0.3891 | 0.1354E-02 |
| 0.23 | 73.2 | 0.3917 | 0.1363E-02 |
| 0.24 | 76.3 | 0.3940 | 0.1371E-02 |
| 0.25 | 79.5 | 0.3960 | 0.1378E-02 |
| 0.26 | 82.7 | 0.3978 | 0.1384E-02 |
| 0.27 | 85.9 | 0.3993 | 0.1389E-02 |
| 0.28 | 89.1 | 0.4006 | 0.1394E-02 |
| 0.29 | 92.3 | 0.4018 | 0.1398E-02 |
| 0.30 | 95.4 | 0.4028 | 0.1401E-02 |
| 0.31 | 98.6 | 0.4037 | 0.1405E-02 |
| 0.32 | 101.8 | 0.4045 | 0.1407E-02 |
| 0.33 | 105.0 | 0.4051 | 0.1410E-02 |
| 0.34 | 108.2 | 0.4057 | 0.1412E-02 |
| 0.35 | 111.3 | 0.4062 | 0.1413E-02 |
| 0.36 | 114.5 | 0.4067 | 0.1415E-02 |
| 0.37 | 117.7 | 0.4071 | 0.1416E-02 |
| 0.38 | 120.9 | 0.4074 | 0.1418E-02 |
| 0.39 | 124.1 | 0.4077 | 0.1419E-02 |
| 0.40 | 127.2 | 0.4080 | 0.1419E-02 |
| 0.41 | 130.4 | 0.4082 | 0.1420E-02 |
| 0.42 | 133.6 | 0.4084 | 0.1421E-02 |
| 0.43 | 136.8 | 0.4086 | 0.1422E-02 |
| 0.44 | 140.0 | 0.4087 | 0.1422E-02 |
| 0.45 | 143.1 | 0.4089 | 0.1423E-02 |
| 0.46 | 146.3 | 0.4090 | 0.1423E-02 |
| 0.47 | 149.5 | 0.4091 | 0.1423E-02 |

| | | | |
|---|---|---|---|
| 0.48 | 152.7 | 0.4092 | 0.1424E-02 |
| 0.49 | 155.9 | 0.4092 | 0.1424E-02 |
| 0.50 | 159.1 | 0.4093 | 0.1424E-02 |
| 0.51 | 162.2 | 0.4094 | 0.1424E-02 |
| 0.52 | 165.4 | 0.4094 | 0.1424E-02 |
| 0.53 | 168.6 | 0.4095 | 0.1425E-02 |
| 0.54 | 171.8 | 0.4095 | 0.1425E-02 |
| 0.55 | 175.0 | 0.4095 | 0.1425E-02 |
| 0.56 | 178.1 | 0.4096 | 0.1425E-02 |
| 0.57 | 181.3 | 0.4096 | 0.1425E-02 |
| 0.58 | 184.5 | 0.4096 | 0.1425E-02 |
| 0.59 | 187.7 | 0.4096 | 0.1425E-02 |
| 0.60 | 190.9 | 0.4097 | 0.1425E-02 |
| 0.61 | 194.0 | 0.4097 | 0.1425E-02 |
| 0.62 | 197.2 | 0.4097 | 0.1425E-02 |
| 0.63 | 200.4 | 0.4097 | 0.1425E-02 |
| 0.64 | 203.6 | 0.4097 | 0.1425E-02 |
| 0.65 | 206.8 | 0.4097 | 0.1426E-02 |
| 0.66 | 209.9 | 0.4097 | 0.1426E-02 |
| 0.67 | 213.1 | 0.4097 | 0.1426E-02 |
| 0.68 | 216.3 | 0.4097 | 0.1426E-02 |
| 0.69 | 219.5 | 0.4097 | 0.1426E-02 |
| 0.70 | 222.7 | 0.4097 | 0.1426E-02 |
| 0.71 | 225.9 | 0.4097 | 0.1426E-02 |
| 0.72 | 229.0 | 0.4097 | 0.1426E-02 |
| 0.73 | 232.2 | 0.4098 | 0.1426E-02 |
| 0.74 | 235.4 | 0.4098 | 0.1426E-02 |
| 0.75 | 238.6 | 0.4098 | 0.1426E-02 |
| 0.76 | 241.8 | 0.4098 | 0.1426E-02 |
| 0.77 | 244.9 | 0.4098 | 0.1426E-02 |
| 0.78 | 248.1 | 0.4098 | 0.1426E-02 |
| 0.79 | 251.3 | 0.4098 | 0.1426E-02 |
| 0.80 | 254.5 | 0.4098 | 0.1426E-02 |
| 0.81 | 257.7 | 0.4098 | 0.1426E-02 |
| 0.82 | 260.8 | 0.4098 | 0.1426E-02 |
| 0.83 | 264.0 | 0.4098 | 0.1426E-02 |
| 0.84 | 267.2 | 0.4098 | 0.1426E-02 |
| 0.85 | 270.4 | 0.4098 | 0.1426E-02 |
| 0.86 | 273.6 | 0.4098 | 0.1426E-02 |
| 0.87 | 276.8 | 0.4098 | 0.1426E-02 |
| 0.88 | 279.9 | 0.4098 | 0.1426E-02 |
| 0.89 | 283.1 | 0.4098 | 0.1426E-02 |
| 0.90 | 286.3 | 0.4098 | 0.1426E-02 |
| 0.91 | 289.5 | 0.4098 | 0.1426E-02 |
| 0.92 | 292.7 | 0.4098 | 0.1426E-02 |
| 0.93 | 295.8 | 0.4098 | 0.1426E-02 |
| 0.94 | 299.0 | 0.4098 | 0.1426E-02 |
| 0.95 | 302.2 | 0.4098 | 0.1426E-02 |
| 0.96 | 305.4 | 0.4098 | 0.1426E-02 |
| 0.97 | 308.6 | 0.4098 | 0.1426E-02 |
| 0.98 | 311.7 | 0.4098 | 0.1426E-02 |
| 0.99 | 314.9 | 0.4098 | 0.1426E-02 |
| 1.00 | 318.1 | 0.4098 | 0.1426E-02 |

CONCENTRATION PROFILE IN REACTOR

| DISTANCE ALONG REACTOR | | CHEMICAL SPECIES | | | | |
|---|---|---|---|---|---|---|
| DIMENSIONLESS | CENTIMETERS | 1 | 2 | 3 | 4 | 5 |
| 0.00 | 0.0 | 0.1865 | 0.5543 | 0.1156 | 0.1198 | 0.0237 |
| 0.01 | 3.2 | 0.1862 | 0.5543 | 0.1157 | 0.1200 | 0.0236 |
| 0.02 | 6.4 | 0.1859 | 0.5544 | 0.1158 | 0.1200 | 0.0236 |
| 0.03 | 9.5 | 0.1856 | 0.5544 | 0.1160 | 0.1201 | 0.0236 |
| 0.04 | 12.7 | 0.1853 | 0.5545 | 0.1161 | 0.1202 | 0.0237 |
| 0.05 | 15.9 | 0.1850 | 0.5545 | 0.1162 | 0.1203 | 0.0238 |
| 0.06 | 19.1 | 0.1847 | 0.5546 | 0.1164 | 0.1203 | 0.0238 |
| 0.07 | 22.3 | 0.1844 | 0.5546 | 0.1165 | 0.1204 | 0.0239 |
| 0.08 | 25.4 | 0.1841 | 0.5547 | 0.1166 | 0.1205 | 0.0241 |
| 0.09 | 28.6 | 0.1838 | 0.5547 | 0.1167 | 0.1205 | 0.0242 |
| 0.10 | 31.8 | 0.1835 | 0.5548 | 0.1168 | 0.1203 | 0.0243 |
| 0.11 | 35.0 | 0.1832 | 0.5548 | 0.1170 | 0.1207 | 0.0243 |
| 0.12 | 38.2 | 0.1829 | 0.5549 | 0.1171 | 0.1208 | 0.0243 |
| 0.13 | 41.4 | 0.1826 | 0.5550 | 0.1172 | 0.1208 | 0.0244 |
| 0.14 | 44.5 | 0.1823 | 0.5550 | 0.1173 | 0.1209 | 0.0244 |
| 0.15 | 47.7 | 0.1820 | 0.5551 | 0.1175 | 0.1210 | 0.0245 |
| 0.16 | 50.9 | 0.1817 | 0.5551 | 0.1176 | 0.1211 | 0.0245 |
| 0.17 | 54.1 | 0.1814 | 0.5552 | 0.1177 | 0.1211 | 0.0245 |
| 0.18 | 57.3 | 0.1811 | 0.5552 | 0.1178 | 0.1212 | 0.0246 |
| 0.19 | 60.4 | 0.1808 | 0.5553 | 0.1179 | 0.1213 | 0.0247 |
| 0.20 | 63.6 | 0.1805 | 0.5553 | 0.1181 | 0.1214 | 0.0247 |
| 0.21 | 66.8 | 0.1802 | 0.5554 | 0.1182 | 0.1214 | 0.0248 |
| 0.22 | 70.0 | 0.1799 | 0.5555 | 0.1183 | 0.1215 | 0.0248 |
| 0.23 | 73.2 | 0.1796 | 0.5555 | 0.1184 | 0.1216 | 0.0249 |
| 0.24 | 76.3 | 0.1793 | 0.5556 | 0.1185 | 0.1217 | 0.0249 |
| 0.25 | 79.5 | 0.1790 | 0.5556 | 0.1186 | 0.1217 | 0.0250 |
| 0.26 | 82.7 | 0.1787 | 0.5557 | 0.1188 | 0.1218 | 0.0250 |
| 0.27 | 85.9 | 0.1784 | 0.5557 | 0.1189 | 0.1219 | 0.0251 |
| 0.28 | 89.1 | 0.1782 | 0.5558 | 0.1190 | 0.1220 | 0.0251 |
| 0.29 | 92.3 | 0.1779 | 0.5558 | 0.1191 | 0.1220 | 0.0252 |
| 0.30 | 95.4 | 0.1776 | 0.5559 | 0.1192 | 0.1221 | 0.0252 |
| 0.31 | 98.6 | 0.1773 | 0.5560 | 0.1193 | 0.1222 | 0.0253 |
| 0.32 | 101.8 | 0.1770 | 0.5560 | 0.1194 | 0.1223 | 0.0253 |
| 0.33 | 105.0 | 0.1767 | 0.5561 | 0.1195 | 0.1223 | 0.0253 |
| 0.34 | 108.2 | 0.1764 | 0.5561 | 0.1196 | 0.1224 | 0.0254 |
| 0.35 | 111.3 | 0.1761 | 0.5562 | 0.1197 | 0.1225 | 0.0254 |
| 0.36 | 114.5 | 0.1758 | 0.5563 | 0.1199 | 0.1226 | 0.0255 |
| 0.37 | 117.7 | 0.1755 | 0.5563 | 0.1200 | 0.1226 | 0.0255 |
| 0.38 | 120.9 | 0.1752 | 0.5564 | 0.1201 | 0.1227 | 0.0255 |
| 0.39 | 124.1 | 0.1750 | 0.5564 | 0.1202 | 0.1228 | 0.0256 |
| 0.40 | 127.2 | 0.1747 | 0.5565 | 0.1203 | 0.1229 | 0.0257 |
| 0.41 | 130.4 | 0.1744 | 0.5566 | 0.1204 | 0.1229 | 0.0257 |
| 0.42 | 133.6 | 0.1741 | 0.5566 | 0.1205 | 0.1230 | 0.0258 |
| 0.43 | 136.8 | 0.1738 | 0.5567 | 0.1206 | 0.1231 | 0.0258 |
| 0.44 | 140.0 | 0.1735 | 0.5567 | 0.1207 | 0.1232 | 0.0259 |
| 0.45 | 143.1 | 0.1732 | 0.5568 | 0.1208 | 0.1233 | 0.0259 |
| 0.46 | 146.3 | 0.1730 | 0.5568 | 0.1209 | 0.1233 | 0.0260 |
| 0.47 | 149.5 | 0.1727 | 0.5569 | 0.1210 | 0.1234 | 0.0260 |
| 0.48 | 152.7 | 0.1724 | 0.5570 | 0.1211 | 0.1235 | 0.0260 |
| 0.49 | 155.9 | 0.1721 | 0.5570 | 0.1212 | 0.1236 | 0.0261 |
| 0.50 | 159.1 | 0.1718 | 0.5571 | 0.1213 | 0.1236 | 0.0261 |
| 0.51 | 162.2 | 0.1715 | 0.5572 | 0.1214 | 0.1237 | 0.0262 |
| 0.52 | 165.4 | 0.1713 | 0.5572 | 0.1215 | 0.1238 | 0.0262 |
| 0.53 | 168.6 | 0.1710 | 0.5573 | 0.1216 | 0.1239 | 0.0263 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.54 | 171.8 | 0.1707 | 0.5573 | 0.1217 | 0.1240 | 0.0263 |
| 0.55 | 175.0 | 0.1704 | 0.5574 | 0.1218 | 0.1240 | 0.0264 |
| 0.56 | 178.1 | 0.1701 | 0.5575 | 0.1219 | 0.1241 | 0.0264 |
| 0.57 | 181.3 | 0.1699 | 0.5575 | 0.1220 | 0.1242 | 0.0265 |
| 0.58 | 184.5 | 0.1696 | 0.5576 | 0.1221 | 0.1243 | 0.0265 |
| 0.59 | 187.7 | 0.1693 | 0.5577 | 0.1222 | 0.1243 | 0.0266 |
| 0.60 | 190.8 | 0.1690 | 0.5577 | 0.1223 | 0.1244 | 0.0266 |
| 0.61 | 194.0 | 0.1687 | 0.5578 | 0.1223 | 0.1245 | 0.0266 |
| 0.62 | 197.2 | 0.1685 | 0.5578 | 0.1224 | 0.1246 | 0.0267 |
| 0.63 | 200.4 | 0.1682 | 0.5579 | 0.1225 | 0.1247 | 0.0267 |
| 0.64 | 203.6 | 0.1679 | 0.5580 | 0.1226 | 0.1247 | 0.0268 |
| 0.65 | 206.8 | 0.1676 | 0.5580 | 0.1227 | 0.1248 | 0.0268 |
| 0.66 | 209.9 | 0.1674 | 0.5581 | 0.1228 | 0.1249 | 0.0269 |
| 0.67 | 213.1 | 0.1671 | 0.5582 | 0.1229 | 0.1250 | 0.0269 |
| 0.68 | 216.3 | 0.1668 | 0.5582 | 0.1230 | 0.1250 | 0.0270 |
| 0.69 | 219.5 | 0.1665 | 0.5583 | 0.1231 | 0.1251 | 0.0270 |
| 0.70 | 222.7 | 0.1662 | 0.5583 | 0.1232 | 0.1252 | 0.0270 |
| 0.71 | 225.9 | 0.1660 | 0.5584 | 0.1232 | 0.1253 | 0.0271 |
| 0.72 | 229.0 | 0.1657 | 0.5585 | 0.1233 | 0.1254 | 0.0271 |
| 0.73 | 232.2 | 0.1654 | 0.5585 | 0.1234 | 0.1254 | 0.0272 |
| 0.74 | 235.4 | 0.1652 | 0.5586 | 0.1235 | 0.1255 | 0.0272 |
| 0.75 | 238.6 | 0.1649 | 0.5587 | 0.1236 | 0.1256 | 0.0273 |
| 0.76 | 241.8 | 0.1646 | 0.5587 | 0.1237 | 0.1257 | 0.0273 |
| 0.77 | 244.9 | 0.1643 | 0.5588 | 0.1238 | 0.1258 | 0.0274 |
| 0.78 | 248.1 | 0.1641 | 0.5589 | 0.1238 | 0.1258 | 0.0274 |
| 0.79 | 251.3 | 0.1638 | 0.5589 | 0.1239 | 0.1259 | 0.0274 |
| 0.80 | 254.5 | 0.1635 | 0.5590 | 0.1240 | 0.1260 | 0.0275 |
| 0.81 | 257.7 | 0.1633 | 0.5590 | 0.1241 | 0.1261 | 0.0275 |
| 0.82 | 260.8 | 0.1630 | 0.5591 | 0.1242 | 0.1262 | 0.0276 |
| 0.83 | 264.0 | 0.1627 | 0.5592 | 0.1242 | 0.1262 | 0.0276 |
| 0.84 | 267.2 | 0.1625 | 0.5592 | 0.1243 | 0.1263 | 0.0277 |
| 0.85 | 270.4 | 0.1622 | 0.5593 | 0.1244 | 0.1264 | 0.0277 |
| 0.86 | 273.6 | 0.1619 | 0.5594 | 0.1245 | 0.1265 | 0.0277 |
| 0.87 | 276.8 | 0.1616 | 0.5594 | 0.1246 | 0.1266 | 0.0278 |
| 0.88 | 279.9 | 0.1614 | 0.5595 | 0.1246 | 0.1266 | 0.0278 |
| 0.89 | 283.1 | 0.1611 | 0.5596 | 0.1247 | 0.1267 | 0.0279 |
| 0.90 | 286.3 | 0.1609 | 0.5596 | 0.1248 | 0.1268 | 0.0279 |
| 0.91 | 289.5 | 0.1606 | 0.5597 | 0.1249 | 0.1269 | 0.0280 |
| 0.92 | 292.7 | 0.1603 | 0.5598 | 0.1249 | 0.1270 | 0.0280 |
| 0.93 | 295.8 | 0.1601 | 0.5598 | 0.1250 | 0.1270 | 0.0281 |
| 0.94 | 299.0 | 0.1598 | 0.5599 | 0.1251 | 0.1271 | 0.0281 |
| 0.95 | 302.2 | 0.1595 | 0.5600 | 0.1252 | 0.1272 | 0.0281 |
| 0.96 | 305.4 | 0.1593 | 0.5600 | 0.1252 | 0.1273 | 0.0282 |
| 0.97 | 308.6 | 0.1590 | 0.5601 | 0.1253 | 0.1274 | 0.0282 |
| 0.98 | 311.7 | 0.1587 | 0.5602 | 0.1254 | 0.1274 | 0.0283 |
| 0.99 | 314.9 | 0.1585 | 0.5602 | 0.1255 | 0.1275 | 0.0283 |
| 1.00 | 318.1 | 0.1582 | 0.5603 | 0.1255 | 0.1276 | 0.0284 |

APPENDIX VII

TECHNICAL REPORT NO. 1

NOVEMBER 1985

SUMMARY

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SUMMARY

This report presents the findings of a research effort directed to three tasks as summarized below.

Task 1: To develop a computer simulator for a direct coal liquefaction reactor.

A computer simulator, written in modular form in FORTRAN, has been developed on a DECsystem 1099 computer. The design parameters, operating conditions, physico-chemical and kinetic parameters are the input to the program. They are entered via an interactive program. The simulator provides detailed information on the performance of each process unit, the characteristics of each flow stream, and an overall summary of the products leaving each unit. The simulator is versatile in the sense that kinetics for the liquefaction of any type and rank of coal can be handled so long as the reactions follow first-order kinetics. The simulator can also provide graphical output of the results using a PDP-11/70 computer by means of a program developed by Schneider Consulting Engineers who served as subcontractors for this task.

The model development, descriptions of the mathematical procedures used to predict the performance of the units, a source code of the program, instructions for its use and a sample problem showing both the input data and the resulting output are included in the report on this task.

Task 2: To conduct a comprehensive review of indirect liquefaction for the production of fuels and, to a lesser extent, of chemicals.

This portion of the report provides an overview of the various routes for converting synthesis gas (a mixture of hydrogen and carbon monoxide) to liquid fuels and to chemicals. The catalytic species and the possible mechanisms involved in carrying out these reactions are discussed. Processes

which are now in commercial use and others that will become commercial in the near future are detailed. Among the subjects covered are:

- The commercial production of gasoline, diesel oil and other products via the Fischer-Tropsch and related reactions.
- The commercial production of methanol in high purity with different catalysts under varying conditions.
- The production of high octane gasoline from methanol using shape selective catalysts.
- The production and use of methanol, ethanol, higher alcohols and ethers as gasoline extenders or as substitutes for gasoline.
- The production of chemicals from synthesis gas. All the known petrochemical feedstocks can be made from synthesis gas. The commercial production of acetic acid and acetic anhydride from coal-derived synthesis gas has already been realized.
- The point is made that essentially all fuels and chemicals can be manufactured from synthesis gas in what may be termed a petroleum-less refinery.
- It is quite likely that in a decade or so this "refinery" will be based on synthesis gas made mainly from coal.

Task 3: To conduct a literature review and analysis of the physical, chemical, and thermodynamic properties (PCT) of the products from direct coal liquefaction processes.

Experimental values for viscosities, thermal conductivities, heats of reaction, vapor pressures, surface tension and convective heat transfer coefficients for cuts of coal liquids derived from the SRC-II process are

presented. The data are fitted to various correlations and an analysis of how well the correlations fit the data is given. Following the completion of this task two points were very evident:

1. The number of experimental measurements made at actual liquefaction conditions for the properties studied is very limited.
2. Correlations which have proven to be satisfactory when applied to petroleum products should be utilized for coal liquids with great caution.

Viscosity data for coal liquids derived from the Exxon Donor Solvent process and from fractions of liquids derived from the SRC-II process are treated. The two sets of data are comparable. The empirical correlation developed by Gray and Holder (1982) seems to be the most satisfactory one to represent coal liquid viscosities at the present time.

Thermal conductivity data for cuts of liquids derived from the SRC-II process are fitted to empirical expressions relating the thermal conductivity to the reduced temperature. One equation includes a term to account for the oxgyen content in the coal liquid cut. An alternative correlation utilizes the normal boiling point as an independent variable for those cases where the oxygen content is unknown.

Vapor pressure measurements of coal liquids derived from the SRC-II process are presented. Five correlations representing these data are tested. The Starling correlation is the best, followed by the Mobil, Riedel, and Wilson correlations, which are of approximately equal value. The Linear correlation is the least satisfactory.

Heat of reaction data for coal derived liquids are very limited. The data that are available have been correlated by an empirical expression with hydrogen consumption as the independent variable. Attempts to estimate the

heat of reaction from heat of combustion data were not successful as only order of magnitude values resulted.

Empirical correlations representing the surface tension of coal liquids from both the Exxon Donor Solvent and SRC-II processes are presented. These correlations represent the data with an average deviation of 16%.

Prandtl numbers and convective heat transfer coefficients for cuts of coal liquids derived from the SRC-II process are calculated. Actual measurements of the convective heat transfer coefficient are compared with the values predicted by the correlations of Hausen, Dittus-Boelter, and Petukhov. The Dittus-Boelter equation best represents the data for both the transition and the turbulent flow regimes.

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# COMPUTER SIMULATION OF PREHEATER AND REACTOR IN DIRECT COAL LIQUEFACTION

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Prepared By:

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APPENDIX VIII

TECHNICAL PROGRESS REPORT NO. 2

OCTOBER 1985

SUMMARY

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SUMMARY

The report is divided into two sections plus an appendix. The first section reports on computer simulations which were developed for three important coal liquefaction processes -- the Mobil Methanol to Gasoline (MTG) process, the Fischer-Tropsch (F-T) process, and the synthesis of methanol. The models are designed to be general and information such as new kinetic equations or new physical property information can be readily added. Each of the models also provides for alternate reactor configurations. For the MTG process either a fixed bed or a fluidized bed can be used. The F-T model provides for a bubble column slurry reactor, a fluidized bed reactor or a fixed bed reactor. Either a fixed bed or a slurry bed can be used in the methanol synthesis model. A comparison of results obtained using the models and results reported in the literature is included to verify the model. Comparisons of alternate processing methods are also included to provide guidance in the selection of a reactor configuration for a specific process. Complete program listings are given in the Appendix, and sample problems with inputs and outputs are provided for the user. The programs are written in the FORTRAN language. It is ultimately desirable to make these models available in a form which can be used in ASPEN, the process simulator developed for DOE. As a first step, the use of ASPEN PLUS to predict thermodynamic and transport properties of systems of interest to coal liquefaction was studied.

In the second section, five areas of potential importance to indirect and direct coal liquefaction are reviewed. They are the synthesis of methanol via methyl formate, the role of carbon dioxide in methanol synthesis, the

synthesis of methanol using noble metal catalysts, the catalytic synthesis of higher alcohols from a new, high-yield sulfur-tolerant catalyst, and the direct liquefaction of coal mixed with heavy oils -- so-called coprocessing. Some unexpected but desirable synergistic effects are found when these two forms of fossil fuels, coal and heavy oil, are processed together. For each of these topics, a careful review of the literature was made and the reported findings evaluated. In certain cases, notably the role of carbon dioxide in methanol synthesis, conflicting experimental results and theories have been reported, although it does appear that the commercial synthesis of methanol proceeds through a carbon dioxide intermediate.

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