

**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.

$$\dot{V}_{\text{internal recycle}} = (\text{meter gpm}/\text{ft}^2) \sqrt{0.85/\rho_{\text{actual}}} \times A \times 2.8 \times 10^{-3} \left( \frac{\text{ft}^3/\text{sec}}{\text{GPM}} \right)$$

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 <u>Period</u>	Catalyst <u>Density,</u> <u>gm/cc</u>	Slurry <u>Density,</u> <u>gm/cc</u>	Slurry <u>Viscosity,</u> <u>mPa.s</u>	Terminal <u>Velocity,</u> <u>m/s</u>	Terminal <u>Index</u> <u>n</u>
	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 ( $^{\circ}$ 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<sub>2</sub>) (-)

Total number of reactions (excluding H<sub>2</sub> 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 EBULLETTED 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 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('---'),/,,2BX,'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

C91

## SUBROUTINE HYDRO(UG,AKLA,PEL)

C .... THIS SUBROUTINE CALCULATES THE PECLET NUMBER AND THE VOLUMETRIC  
C MASS TRANSFER COEFFICIENT.  
C  
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+42.81\*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 /B8/ TEMP  
 COMMON /B10/ QSLUR,QRVCYC  
 COMMON /B13/ CATDEN,CATLEN,CATWT,SLUVOL  
 COMMON /B15/ ZKBAR,ERXN,DHS,HBAR,AKH2  
  
 GASENG=1.007                    IGAS CONSTANT IN CAL/GMOLE.DEG K  
 GASCON=82.057                 IGAS CONSTANT IN CC.ATM/GMOLE.DEG K  
  
 OPEN (UNIT=11,FILE='INPUT.DAT')  
 OPEN (UNIT=12,FILE='DATA.DAT')  
  
 READ(11,\*) RCVGAS,H2COM,H2FLOW,SLFEED,SLRCYC,PRES,TEMP  
 READ(11,\*) DIA,ALEN  
 READ(11,\*) ZKBAR,ERXN,DHS,HBAR,SLDEN,SLVVIS,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,H2COM,H2FLOW,SLFEED,SLRCYC,PRES,TEMP,DIA,ALEN  
  
 10 FORMAT (5X,'RECYCLE GAS FLOW IN SCFH ',T65,F12.5,/,
 \* 5X,'HYDROGEN CONCENTRATION IN RECYCLE GAS, vol % ',T65,F12.5,/,
 \* 5X,'MAKEUP H2 FLOW RATE SCFH ',T65,F12.5,/,
 \* 5X,'SLURRY FEED RATE, lb/hr ',T65,F12.5,/,
 \* 5X,'SLURRY RECYCLE RATE, GPM/ft\*\*2 ',T65,F12.5,/,
 \* 5X,'PRESSURE, psi ',T65,F12.5,/,
 \* 5X,'TEMPERATURE, deg. F ',T65,F12.5,/,
 \* 5X,'DIAMETER OF REACTOR, inches ',T65,F12.5,/,
 \* 5X,'LENGTH OF REACTOR, m ',T65,F12.5,/)  
 WRITE(12,31) SLDEN,SLVVIS,SLSURT  
 31 FORMAT(//5X,'SLURRY PHYSICAL PROPERTIES:',//,  
 \* 5X,'DENSITY OF SLURRY, gm/cc ',T65,F12.5,/,
 \* 5X,'VISCOSITY OF SLURRY, Pa.s ',T65,F12.5,/,
 \* 5X,'SURFACE TENSION OF SLURRY, dyne/cm ',T65,F12.5,/)  
  
 WRITE(12,40) UT,AN,UTB,EMF,HMF  
 40 FORMAT(//5X,'RICHARDSON-ZAIKI PARAMETERS:',//,  
 \* 5X,'TERMINAL VELOCITY OF PARTICLE, ft/s ',T65,F12.5,/,
 \* 5X,'RICHARDSON-ZAIKI INDEX [-] ',T65,F12.5,/,
 \* 5X,'BUBLING VELOCITY, ft/s ',T65,F12.5,/,
 \* 5X,'VOIDAGE AT MINIMUM FLUIDIZATION [-] ',T65,F12.5,/,
 \* 5X,'HEIGHT OF BED AT MINIMUM FLUIDIZATION, m  
 \* ',T65,F12.5,/)  
 WRITE(12,77) CATDEN,CATLEN,CATDIA,CATWT  
 77 FORMAT(//5X,'CATALYST PROPERTIES:',//,  
 \* 5X,'CATALYST DENSITY, gm/cc ',T65,F12.5,/,
 \* 5X,'CATALYST LENGTH, inches ',T65,F12.5,/,
 \* 5X,'CATALYST DIAMETER, inches ',T65,F12.5,/,
 \* 5X,'WEIGHT OF CATALYST LOADED, gm ',T65,F12.5,/)  
 CATLEN=CATLEN/2.84  
 CATDIA=CATDIA/2.84  
 CATWT=CATWT/1000.  
 UT=UT\*0.3048  
 UTB=UTB\*0.3048  
 CLOSE (UNIT=11)  
 CLOSE (UNIT=12)  
  
 SLDEN=SLDEN\*82.4

DIA=DIA/12.0  
TEMP=TEMP+460.

```
AREA=DATAN(1.0D0)*DIA**2
QSLUR=SLFEED/3800./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/3800./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 PECKLET 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
```

C SUBROUTINE REATEM  
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,NCVCL
COMMON /B14/ NAME
```

NCOMP=2+NSP

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

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

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

```
ALPHA=0.2
AK2S=AK(2)+AK(5)
AK3G=AK(3)+AK(6)
AK2PM=AK(2)+AK(5)*(1.-EPSN)
HENCON=1.0/HENCON
```

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

222 CONTINUE
DO 21 ITER=1,ITMAX

MH=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
```

```

11      WRITE(23,84) X,X*EFFLEN,Z(3),Z(4),Z(5),Z(6),Z(7)
10      CONTINUE
      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 18
      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
      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(22,600)
WRITE(23,601)
CLOSE(UNIT=21)
CLOSE(UNIT=22)
CLOSE(UNIT=23)
50 FORMAT(T21,'HYDROGEN PROFILE IN REACTOR',//,T50,'(GAS PHASE)',/
*,70('''),/,T7,'DISTANCE ALONG REACTOR',12X,
*, 'HYDROGEN CONCENTRATION',//,T8,'DIMENSIONLESS',4X,
*, 'CENTIMETERS',8X,
*, 'DIMENSIONLESS',4X,'MOLE/CC',//,70('''),/)
51 FORMAT(T21,'HYDROGEN PROFILE IN REACTOR',//,T28,'(LIQUID PHASE)',/
*,70('''),/,T7,'DISTANCE ALONG REACTOR',12X,
*, 'HYDROGEN CONCENTRATION',//,T8,'DIMENSIONLESS',4X,
*, 'CENTIMETERS',8X,
*, 'DIMENSIONLESS',4X,'MOLE/CC',//,70('''),/)
52 FORMAT(T50,'CONCENTRATION PROFILE IN REACTOR',//,
*, T16,100('''),/,,T22,'DISTANCE ALONG REACTOR',20X,
*, 'CHEMICAL SPECIES',/,,10X,'DIMENSIONLESS',4X,'CENTIMETERS',5X,
*, '1',11X,'2',11X,'3',11X,'4',11X,'5',/,,T16,100('''))
53 FORMAT(8X,F5.2,8X,F8.1,12X,F8.4,8X,E11.4)
54 FORMAT(28X,F5.2,8X,6X,F8.1,10X,F7.4,4(3X,F7.4))
500 FORMAT(/,70('''))
501 FORMAT(/,T16,100('''))
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/ GAYDEN,CATLEN,CATWT,SLRVOL
COMMON /B14/ NAME
COMMON /B16/ ZKBAR,ERIN,DHS,HBAR,AKH2

OPEN (UNIT=12,FILE='KIN.DAT')
OPEN (UNIT=15,FILE='KINDAT.DAT')
DIFFP=1.738E-03    !CM**3/SEC
DIFFA=2.18E-05    !"

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

51 WRITE (15,61)
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)/80.
20 CONTINUE

63 WRITE (15,63) AK(1),AK(2),AK(3),AK(4)
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

64 WRITE (15,64) DIFFP,DIFFA,EFF1,EFF2,AK(5),AK(6)
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,//)

65 WRITE (15,65)
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 C .... THE GAS AND LIQUID HOLDUPS ARE CALCULATED USING DARTON AND  
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=EL0

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

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

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

C 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),Y(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)=Y(J)

PHI(J)=F(J)

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

**APPENDIX IV**

**INPUT PROGRAM LISTING**

C  
C  
C  
C  
C

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---

PROGRAM TO INPUT DATA TO MAIN SIMULATION ROUTINE

---

```
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION CINIT(10)
CHARACTER*20 NAME(10)
OPEN (UNIT=11,FILE='INPUT.DAT')
OPEN (UNIT=8,FILE='CHECK.DAT')
WRITE(8,11)
11 FORMAT(//5X,'THREE PHASE FLUIDIZED BED REACTOR SIMULATION',///)
WRITE(8,10)
10 WRITE(8,10)
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 RECYLE RATE, GPM/ft**2',//,
      *      5X,'PRESSURE, psf',//,
      *      5X,'TEMPERATURE, deg. F',//)
READ(5,*) RCGAS,H2CON,H2FLOW,SLFEED,SLRCYC,PRES,TEMP
WRITE(11,*) RCGAS,H2CON,H2FLOW,SLFEED,SLRCYC,PRES,TEMP
WRITE(8,*) RCGAS,H2CON,H2FLOW,SLFEED,SLRCYC,PRES,TEMP
WRITE(8,20)
20 WRITE(8,20)
FORMAT(//5X,'ENTER VALUES OF VARIABLES LISTED BELOW:',//)
WRITE(8,30)
30 WRITE(8,30)
FORMAT(5X,'DIAMETER OF REACTOR, inches',//,
      *      5X,'LENGTH OF REACTOR, m',//)
READ(5,*) DIA,ALEN
WRITE(11,*) DIA,ALEN
WRITE(8,*) DIA,ALEN
WRITE(8,31)
31 WRITE(8,31)
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>1iq/<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(8,*) ZKBAR,ERXN,DHS,HBAR,SLDEN,SLVIS,SLSURT
WRITE(8,40)
40 WRITE(8,40)
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,*) UY,AN,UTB,ECMF,HMF
WRITE(11,*) UT,AN,UTB,ECMF,HMF
WRITE(8,*) UY,AN,UTB,ECMF,HMF
WRITE(8,77)
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(8,77)
READ(5,*) CATDEN,CATLEN,CATDIA,WTGAT
WRITE(11,*) CATDEN,CATLEN,CATDIA,WTGAT
WRITE(8,*) CATDEN,CATLEN,CATDIA,WTGAT

CLOSE (UNIT=11)
OPEN (UNIT=12,FILE='KIN.DAT')
WRITE(8,80)
WRITE(8,80)
60 * FORMAT(//5X,'REACTION NETWORK DATA',
*      //,5X,'ENTER NUMBER OF REACTING SPECIES ',\$)
READ(5,*) NSP
WRITE(12,*) NSP
WRITE(8,*) NSP

DO 2 I=1,NSP
WRITE(8,81) I
WRITE(8,81) I
51 FORMAT(5X,'ENTER NAME OF SPECIES NUMBER',I2,3X,\$)
READ(8,82) NAME(I)
WRITE(8,82) NAME(Y)
WRITE(12,82) NAME(I)
FORMAT(A20)
52 CONTINUE
2
CONTINUE
53 WRITE(8,53)
FORMAT(/5X,'THE SPECIES HAVE BEEN CODED AS: ',//)

DO 3 I=1,NSP
WRITE(8,81) I,NAME(I)
FORMAT(5X,I2,2X,'=',2X,A20)
3
CONTINUE

WRITE(8,80)
WRITE(8,80)
50 FORMAT(//5X,'ENTER TOTAL NUMBER OF REACTIONS ',\$)
READ(5,*) NR
WRITE(12,*) NR
WRITE(8,*) NR

DO 41 J=1,NR
WRITE(8,82) J
WRITE(8,82) J
82 * FORMAT(//5X,'FOR REACTION NO. ',I2,/5X,'ENTER ARRHENIUS FACTOR',
*      ' ACTIVATION ENERGY'//)
READ(5,*) AK,ACTVEN
WRITE(12,*) AK,ACTVEN
WRITE(8,*) AK,ACTVEN
41 CONTINUE

WRITE(8,70)

```

```
    WRITE(6,70)
70  * FORMAT(//5X,'ENTER INITIAL CONCENTRATION OF EACH SPECIES',
      '(gm/gm)')
      DO 5 I=1,NSP
      WRITE(9,71)
      WRITE(9,71) I
      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

2200.000000000000, 100.0000000000000, 2830.000000000000,  
628.000000000000, 19.1000000000000, 2972.000000000000,  
815.000000000000

ENTER VALUES OF VARIABLES LISTED BELOW:

DIAMETER OF REACTOR, inches

LENGTH OF REACTOR, m

8.50000000000000, 4.00000000000000

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

3213.000000000000, 21000.000000000000, 770.000000000000,  
1.20000000000000, 0.89400000000000, 1.80000000000000E-02,  
30.00000000000000

L/T

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

0.48400000000000, 2.80000000000000, 0.0350000000000000,  
0.42000000000000, 1.98000000000000

INPUT CATALYST PROPERTIES:

CATALYST DENSITY, gm/cc

CATALYST LENGTH, inches

CATALYST DIAMETER, inches

WEIGHT OF CATALYST LOADED, gm

1.677000000000000, 0.274000000000000, 8.2000000000000E-02,  
33485.0000000000

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 8

FOR REACTION NO. 1  
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

0.180000000000000, 0.000000000000000E+00

FOR REACTION NO. 2  
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

0.800000000000000E-02, 0.000000000000000E+00

FOR REACTION NO. 3  
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

0.400000000000000E-03, 0.000000000000000E+00

FOR REACTION NO. 4  
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

1.050000000000000E-02, 0.000000000000000E+00

FOR REACTION NO. 5  
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

1.080000000000000, 0.000000000000000E+00

FOR REACTION NO. 6  
ENTER ARRHENIUS FACTOR ACTIVATION ENERGY

0.187700000000000, 0.000000000000000E+00

081

ENTER INITIAL CONCENTRATION OF EACH SPECIES(gm/gm)

SPECIE NUMBER

0.33000000000000000000

SPECIE NUMBER

0.53000000000000000000

SPECIE NUMBER

6.000000000000000E-02

SPECIE NUMBER

8.000000000000000E-02

SPECIE NUMBER

0.000000000000000E+00

**INPUT DATA FOR FLUIDIZED BED REACTOR SIMULATION**

RECYCLE GAS FLOW IN SCFH	2200.00000
HYDROGEN CONCENTRATION IN RECYCLE GAS, vol %	100.00000
MAKEUP H <sub>2</sub> FLOW RATE SCFH	2830.00000
SLURRY FEED RATE, lb/hr	0.000.00000
SLURRY RECYCLE RATE, GPM/ft <sup>2</sup>	10.10000
PRESSURE, psi	2072.00000
TEMPERATURE, deg. F	818.00000
DIAMETER OF REACTOR, inches	0.80000
LENGTH OF REACTOR, in	4.00000

**SLURRY PHYSICAL PROPERTIES:**

DENSITY OF SLURRY, gm/cc	0.80400
VISCOOSITY OF SLURRY, Pa.s	0.01800
SURFACE TENSION OF SLURRY, dyne/cm	20.00000

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**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, in	1.08000

**CATALYST PROPERTIES:**

CATALYST DENSITY, gm/cc	1.67700
CATALYST LENGTH, Inches	0.27400
CATALYST DIAMETER, inches	0.03200
WEIGHT OF CATALYST LOADED, gm	33485.00000

## KINETIC AND THERMODYNAMIC DATA

ARRHENIUS FACTOR FOR H <sub>2</sub> REACTION, 1/s	0.32130E+04
ACTIVATION ENERGY FOR H <sub>2</sub> REACTION, cal/gmole	0.21000E+05
RATE CONSTANT FOR H <sub>2</sub> REACTION, 1/s	0.10801E-02
SOLUBILITY COEFFICIENT FOR H <sub>2</sub>	0.12000E+01
HEAT OF DISSOLUTION, cal/gmole	0.77000E+03

## SPECIES PRESENT

- 1 - COAL
- 2 - OIL
- 3 - PREASPHALTENE
- 4 - ASPHALTENE
- 5 - GAS

[8]

## 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	0.15887E-03
REACTION 4 C --- G	0.32500E-03

## CATALYTIC REACTION DATA

DIFFUSIVITY OF PREASPHALTENES, cm**2/s	0.17380E-05
DIFFUSIVITY OF ASPHALTENES, cm**2/s	0.21800E-04
EFFECTIVENESS FACTOR FOR P --- A	0.91038E-01
EFFECTIVENESS FACTOR FOR A --- O	0.88777E+00
RATE CONSTANT FOR RXN 5 P --- A (1/s)	0.71938E-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	0.3906
GAS PHASE HOLDUP	0.2484
EFFECTIVE REACTOR LENGTH, m	3.1810
STANTON NUMBER	8.0162
SLURRY RESIDENCE TIME, s	82.4676
RECYCLE RATIO	5.2200
HENRY'S CONSTANT	0.8943

**HYDROGEN PROFILE IN REACTOR**  
**(GAS PHASE)**

DISTANCE ALONG REACTOR DIMENSIONLESS	CENTIMETERS	HYDROGEN CONCENTRATION DIMENSIONLESS	QMOLE/CC
0.00	0.0	1.0000	0.3479E-02
0.01	3.2	0.0480	0.3208E-02
0.02	6.4	0.0025	0.3140E-02
0.03	9.6	0.8820	0.3002E-02
0.04	12.7	0.8282	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	0.7488	0.2605E-02
0.08	25.4	0.7285	0.2538E-02
0.09	28.6	0.7100	0.2474E-02
0.10	31.8	0.6958	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	0.2207E-02
0.14	44.6	0.6514	0.2287E-02
0.15	47.7	0.6437	0.2230E-02
0.16	50.9	0.6360	0.2210E-02
0.17	54.1	0.6300	0.2195E-02
0.18	57.3	0.6258	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	0.2138E-02
0.22	70.0	0.6108	0.2128E-02
0.23	73.2	0.6083	0.2118E-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	0.5956	0.2072E-02
0.33	105.0	0.5949	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	0.5920	0.2063E-02
0.38	120.9	0.5918	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	0.2060E-02
0.42	133.6	0.5918	0.2058E-02
0.43	136.8	0.5914	0.2050E-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	0.2058E-02
0.47	149.5	0.5909	0.2058E-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	0.5908	0.2055E-02
0.52	165.4	0.5908	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	208.9	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	0.5902	0.2054E-02

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

DISTANCE ALONG REACTOR DIMENSIONLESS CENTIMETERS		HYDROGEN CONCENTRATION DIMENSIONLESS	MOLE/CC
0.00	0.0	0.0000	0.0000E+00
0.01	3.2	0.0920	0.1811E-03
0.02	6.4	0.0875	0.3301E-03
0.03	9.6	0.1371	0.4771E-03
0.04	12.7	0.1718	0.5078E-03
0.05	15.9	0.2020	0.7028E-03
0.06	19.1	0.2264	0.7939E-03
0.07	22.3	0.2514	0.8747E-03
0.08	25.4	0.2718	0.9447E-03
0.09	28.6	0.2891	0.1003E-02
0.10	31.8	0.3044	0.1050E-02
0.11	35.0	0.3178	0.1103E-02
0.12	38.2	0.3295	0.1148E-02
0.13	41.4	0.3397	0.1182E-02
0.14	44.6	0.3488	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	0.3743	0.1302E-02
0.19	60.4	0.3797	0.1318E-02
0.20	63.6	0.3847	0.1331E-02
0.21	66.8	0.3881	0.1343E-02
0.22	70.0	0.3901	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	0.1383E-02
0.27	85.9	0.3988	0.1388E-02
0.28	89.1	0.4008	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	0.1403E-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	0.1418E-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	0.4088	0.1422E-02
0.44	140.0	0.4087	0.1422E-02
0.45	143.1	0.4088	0.1423E-02
0.46	146.3	0.4089	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	190.8	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 DIMENSIONLESS CENTIMETERS	1	CHEMICAL SPECIES				
		2	3	4	5	6
0.00	0.0	0.1865	0.5543	0.1156	0.1190	0.0237
0.01	3.2	0.1862	0.5543	0.1157	0.1200	0.0238
0.02	6.4	0.1858	0.5543	0.1159	0.1200	0.0238
0.03	9.5	0.1853	0.5544	0.1160	0.1201	0.0238
0.04	12.7	0.1853	0.5545	0.1161	0.1202	0.0238
0.05	15.9	0.1850	0.5545	0.1162	0.1203	0.0240
0.06	19.1	0.1847	0.5546	0.1164	0.1203	0.0240
0.07	22.3	0.1843	0.5546	0.1165	0.1204	0.0241
0.08	25.4	0.1841	0.5547	0.1165	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	0.0242
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	44.6	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	0.1178	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	0.5555	0.1185	0.1217	0.0249
0.25	79.5	0.1790	0.5556	0.1188	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	0.5559	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	0.1195	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	0.0256
0.39	124.1	0.1750	0.5564	0.1202	0.1228	0.0256
0.40	127.3	0.1747	0.5565	0.1203	0.1228	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	0.1208	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	162.3	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	203.5	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	0.5598	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 1965**

**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 oxygen 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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**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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