

Appendix A

System Requirements and Operating Instructions for Personal Computers

System Requirements:

Computer

- Intel 80386-33 Mhz processor with 256K cache
- 80387-33 Math Coprocessor
- Hard disk with 4MB available space
- DOS 5.0 (or DOS 4.0 with minimum 610 K free memory)
- 1.44 Mbyte 3.5" floppy drive

Computer programs for the slurry reactor model have been developed in FORTRAN 77 using Microsoft Fortran compiler and Linker. The slurry reactor programs must be copied onto hard disk. Please follow these steps:

- 1) Create a new directory on your hard disk (say SLR)
Type: MD SLR
Type: CD SLR
- 2) Insert the program diskette, SLRD, into drive B.
- 3) Type: COPY B:*. * C:\SLR*. *

Executing Slurry Reactor Program for Methanol Synthesis:

- 1) Select input conditions by editing the input data file MTIN.
- 2) To run the methanol synthesis program
Type: MTR
- 3) At the end of the run print file MTR.OUT to look at input and output summary. A sample of MTR.OUT file is enclosed.

Type: PRINT MTR.OUT

Executing Slurry Reactor Program for Fischer-Tropsch Synthesis:

- 1) Select input conditions by editing the input data file FTIN
- 2) To run the Fischer Tropsch Synthesis program

Type: FTR

- 3) At the end of the run print file FTR.OUT to look at input and output summary. A sample of FTR.OUT file is enclosed.

Type: PRINT FTR.OUT

For any inquiry, please contact:

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Appendix B

Sample INPUT and OUTPUT Files for Methanol Synthesis Model

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***** Input Data File for Methanol Synthesis Slurry Reactor *****
*
*
*** Enter 1 for Gas Plug Flow; 2 for Gas Dispersion
*
2
*
*** Reactor Dimensions:
*
4.8          Diameter, m
12.5         Length, m
*
*** Operating Data:
*
513.         Reactor Temp., K
414.         Feed Gas Temp., K
423.         Slurry Inlet Temp., K
55.          Reactor Pressure, Atm
55.7         Feed Gas Pressure, Atm
0.155        Supf. Gas Velocity, m/s
0.00         Slurry Flow Rate, m**3/s
*
*** Feed Gas Composition; CO,CO2,H2,CH3OH,H2O
*
0.54         CO Mole Fraction
0.115        CO2 Mole Fraction
0.345        H2 Mole Fraction
0.000        CH3OH Mole Fraction
0.00         H2O Mole Fraction
0.00         N2 Mole Fraction
0.0          CH4 Mole Fraction
*
*** Liquid Phase Conc.; CO,CO2,H2,CH3OH,H2O
*
0.0,0.0,0.0,0.0,0.0,0.,0.
*
*** Catalyst Data:
*
0.34         Weight fraction of catalyst
5730.        Catalyst density, kg/m**3
0.000025     Particle diameter, m
0.49         Catalyst heat capacity
*
*** Selection of Kinetic Model for Methanol Synthesis:
*
*** Enter 1 for Graff et al. (1988); 2 for Wedel et al. (1988)
*
2
*
*** Selection of Gas Holdup Correlation:
*
*** Enter 1 for correlation by Hughmark (1967); 2 for correlation by
*** Hikita et al. (1980); 3 for correlation by Bukur et al. (1991);
*** 4 for experimental gas holdup
*
1
*
*** Enter experimental gas holdup; else 0.0
*
0.0

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*
*** Selection of Correlation for Vol. Mass Transfer Coeff.:
*
*** Enter 1 for correlation by Nguentien et al. (1985); 2 for
*** correlation by Akita and Yoshida (1972).
*
1
*
*** Selection of Correlation for Gas Dispersion:
*
*** Enter 1 for correlation by Towell and Ackerman (1972);
*** 2 for correlation from Air Products PDU data
*
2
*
*** Heat Exchanger Data:
*
*** Enter 1 for internal heat exchanger; 2 for external heat exchanger
*
1
*
*** Heat Exchanger Tubes Data:
*
.031           Inside diameter of tubes, m
.038           Outside diameter of tubes, m
12.           Tube length, m
.0187         Thermal conductivity of tube material
*
*** Temp. of saturated steam generated
*
488.
*
*** Fraction of head volume assumed effective (distributor region)
*
0.2
*

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 ISOTHERMAL BUBBLE-COLUMN SLURRY REACTOR SIMULATION
 FOR METHANOL SYNTHESIS

SUMMARY OF THE INPUT DATA

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

DIAMETER = 4.80000 m
 LENGTH = 12.50000 m

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

REACTOR TEMPERATURE = 513.00000 K
 PRESSURE = 55.00000 ATM
 GAS FLOW RATE = 82.15426 Nm³/s
 SLURRY FLOW RATE = .00000 m³/s
 SUPERFICIAL GAS VELOCITY = .15500 m/s
 SUPERFICIAL LIQUID VELOCITY = .00000 m/s
 FLOW RATE RATIO (slurry/gas) = .00000

***** FEED COMPOSITIONS *****

COMPONENT	GAS MOLE FRAC.	SLURRY MOLE FRAC.
*****	*****	*****
CO	.54000E+00	.00000E+00
CO2	.11500E+00	.00000E+00
H2	.34500E+00	.00000E+00
CH3OH	.10000E-04	.00000E+00
H2O	.00000E+00	.00000E+00

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

CATALYST LOADING = 34.00000 % Weight
 CATALYST DENSITY = 5730.00000 kg/m³
 PARTICLE DIAMETER = .25000E-04 m

OUTPUT SUMMARY

% HYDROGEN CONVERSION = .57286E+02
 % CO CONVERSION = .18242E+02
 % OVERALL CONVERSION = .33463E+02
 RATIO OF H2 CONSM/CO CONSM = .20063E+01
 SPACE VELOCITY = .13369E+04 Nm³/hr-m³
 GAS HOURLY SPACE VELOCITY = .52889E+01 Nm³/hr-kgcat
 SPACE TIME YIELD I = .48248E+04 Nm³ Syn Gas/hr-m³
 SPACE TIME YIELD II = .18838E+03 kg Methanol/hr-m³
 PRODUCTIVITY = .74523E+00 kg/hr-kgcat
 PRODUCTION RATE = .10001E+04 MTD
 HEAT TRANSFER AREA = .11333E+04 m²
 GAS HOLDUP = .30097E+00

LENGTH		GAS PHASE MOLE FRACTIONS				
ZZZ	XXX (M)	CO	CO2	H2	CH3OH	H2O

.00	.00	.54580E+00	.13397E+00	.23335E+00	.86687E-01	.19929E-01
.10	1.28	.54638E+00	.13571E+00	.22328E+00	.94422E-01	.21627E-01
.20	2.56	.54697E+00	.13722E+00	.21484E+00	.10075E+00	.22875E-01
.30	3.85	.54757E+00	.13854E+00	.20762E+00	.10605E+00	.23797E-01
.40	5.13	.54815E+00	.13968E+00	.20141E+00	.11052E+00	.24477E-01
.50	6.41	.54869E+00	.14067E+00	.19613E+00	.11427E+00	.24973E-01
.60	7.69	.54916E+00	.14149E+00	.19175E+00	.11736E+00	.25329E-01
.70	8.97	.54955E+00	.14215E+00	.18827E+00	.11978E+00	.25576E-01
.80	10.26	.54985E+00	.14263E+00	.18573E+00	.12155E+00	.25737E-01
.90	11.54	.55003E+00	.14293E+00	.18415E+00	.12264E+00	.25830E-01
1.00	12.82	.55010E+00	.14303E+00	.18361E+00	.12301E+00	.25860E-01

LENGTH		LIQUID PHASE CONCENTRATIONS (kmol/m**3)				
ZZZ	XXX (M)	CO	CO2	H2	CH3OH	H2O

.00	.00	.21504E+00	.63799E-01	.80023E-01	.74722E-01	.18865E-01
.10	1.28	.21511E+00	.63920E-01	.79280E-01	.75448E-01	.18979E-01
.20	2.56	.21528E+00	.64200E-01	.77684E-01	.77081E-01	.19188E-01
.30	3.85	.21552E+00	.64551E-01	.75813E-01	.79078E-01	.19387E-01
.40	5.13	.21578E+00	.64920E-01	.73958E-01	.81123E-01	.19545E-01
.50	6.41	.21605E+00	.65272E-01	.72265E-01	.83033E-01	.19655E-01
.60	7.69	.21629E+00	.65583E-01	.70813E-01	.84699E-01	.19727E-01
.70	8.97	.21650E+00	.65839E-01	.69645E-01	.86052E-01	.19770E-01
.80	10.26	.21665E+00	.66029E-01	.68791E-01	.87048E-01	.19793E-01
.90	11.54	.21675E+00	.66146E-01	.68270E-01	.87658E-01	.19804E-01
1.00	12.82	.21678E+00	.66186E-01	.68094E-01	.87863E-01	.19807E-01

LENGTH		CATALYST CONCENTRATION	
ZZZ	XXX (M)	DIM-LESS	ACTUAL (% WT)

.00	.00	1.00595	34.20234
.10	1.28	1.00476	34.16173
.20	2.56	1.00356	34.12118
.30	3.85	1.00237	34.08067
.40	5.13	1.00118	34.04021
.50	6.41	.99999	33.99980
.60	7.69	.99881	33.95944
.70	8.97	.99762	33.91912
.80	10.26	.99644	33.87885
.90	11.54	.99525	33.83863
1.00	12.82	.99407	33.79846

LENGTH		VELOCITY PROFILE	
ZZZ	XXX (M)	UG/UGO	ACTUAL (M/SEC)

.00	.00	1.000000	.15500E+00
.10	1.28	.981076	.15207E+00
.20	2.56	.961974	.14911E+00
.30	3.85	.942430	.14608E+00

.40	5.13	.922540	.14299E+00
.50	6.41	.902473	.13988E+00
.60	7.69	.882367	.13677E+00
.70	8.97	.862308	.13366E+00
.80	10.26	.842329	.13056E+00
.90	11.54	.822427	.12748E+00
1.00	12.82	.802571	.12440E+00

Appendix C

Sample INPUT and OUTPUT Files for FT Synthesis Model

```

***** Input Data for Fischer Tropsch Synthesis Slurry Reactor ****
*
*
*** Enter 1 for Gas Plug Flow; 2 for Gas Dispersion
*
2
*
*** Reactor Dimensions:
*
4.8          Diameter, m
11.5         Length, m
*
*** Operating Data:
*
528.0        Reactor Temp., K
420.0        Feed Gas Temp., K
423.         Slurry Inlet Temp., K
28.          Reactor Pressure, Atm
28.5         Feed Gas Pressure, Atm
0.155        Supf. Gas Velocity, m/s
0.000        Slurry Flow Rate, m**3/s
*
*** Feed Gas Composition; CO,CO2,H2,N2+CH4,H2O
*
0.55         CO Mole Fraction
0.04         CO2 Mole Fraction
0.35         H2 Mole Fraction
0.06         CH4+N2 Mole Fraction
0.0          H2O Mole Fraction
*
*** Liquid Phase Conc.; CO,CO2,H2,N2,H2O
*
0.0,0.0,0.0,0.0,0.0
*
*** Catalyst Data:
*
0.34         Weight fraction of catalyst
3011.        Catalyst density, kg/m**3
0.000025     Particle diameter, m
0.49         Catalyst heat capacity
*
*** Product Distribution:
*
0.85,0.85    Alpha1,Alpha2
1.           Fraction of type-1 site on catalyst
0.75         Fraction of paraffinic products
*
*** If Experimental Hydrogen to Carbon Ratio For Products is
*** Available Enter 2 ; otherwise enter 1
*
1
6.           Avg. carbon chain length of product molecules
2.2          Ratio of the average number of hydrocarbon
*            atoms to avg. carbon chain length of products
*
*** Selection of Kinetic Model:
*
*** Enter 1 for precipitated iron catalyst; 2 for cobalt catalyst
*
1

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*
*** Selection of Gas Holdup Correlation:
*
*** Enter 1 for correlation by Hughmark (1967); 2 for correlation by
*** Hikita et al. (1980); 3 for correlation by Bukur et al. (1991);
*** 4 for experimental gas holdup
*
1
*
*** Enter experimental gas holdup; else 0.0
*
0.
*
*** Selection of Correlation for Vol. Mass Transfer Coeff.:
*** Enter 1 for correlation by Nguentien et al. (1985); 2 for
*** correlation by Akita and Yoshida (1972).
*
1
*
*** Selection of Correlation for Gas Dispersion:
*** Enter 1 for correlation by Towell and Ackerman (1972);
*** 2 for correlation from Air Products PDU data
*
2
*
*** Heat Exchanger Data:
*** Enter 1 for internal heat exchanger; 2 for external heat exchanger
*
1
*
*** Heat Exchanger Tubes Data:
*
.031             Inside diameter of tubes, m
.038             Outside diameter of tubes, m
11.             Tube length, m
.0187           Thermal conductivity of tube material
*
*** Temp. of saturated steam generated
*
503.
*
*** Fraction of head volume assumed effective (distributor region)
*
0.2
*

```

 ISOTHERMAL BUBBLE-COLUMN SLURRY REACTOR SIMULATION
 FISCHER TROPSCH SYNTHESIS

SUMMARY OF THE INPUT DATA

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

DIAMETER = 4.80000 M
 LENGTH = 11.50000 M

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

INLET TEMPERATURE = 420.00000 K
 REACTOR TEMPERATURE = 528.00000 K
 PRESSURE = 28.00000 ATM
 GAS FLOW RATE = 32.41972 NM**3/SEC
 SLURRY FLOW RATE = .00000 M**3/SEC
 SUPERFICIAL GAS VELOCITY = .15500 M/SEC
 SUPERFICIAL LIQUID VELOCITY = .00000 M/SEC
 FLOW RATE RATIO (slurry/gas) = .00000

***** FEED COMPOSITIONS *****

COMPONENT	GAS MOLE FRAC.	SLURRY MOLE FRAC.
*****	*****	*****
CO	.55000E+00	.00000E+00
CO2	.40000E-01	.00000E+00
H2	.35000E+00	.00000E+00
CH4	.60000E-01	.00000E+00
H2O	.00000E+00	.00000E+00

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

CATALYST LOADING = 34.00000 % WEIGHT
 CATALYST DENSITY = 3011.00000 KG/M**3
 PARTICLE DIAMETER = .25000E-04 M

***** OUTPUT SUMMARY *****

% HYDROGEN CONVERSION = .71303E+02
 % CO CONVERSION = .74615E+02
 % OVERALL CONVERSION = .73327E+02
 RATIO OF H2 CONSM/CO CONSM = .60812E+00
 SPACE VELOCITY = .64336E+03 NM**3/hr-m**3
 GAS HOURLY SPACE VELOCITY = .24697E+01 NM**3/hr-kg
 SPACE TIME YIELD I = .42458E+03 NM**3 Syn Gas conv./hr-m**3
 SPACE TIME YIELD II = .10044E+03 kg HC/hr-m**3
 PRODUCTIVITY = .38557E+00 kg HC/hr-kg cat
 PROD. RATE TOTAL HC = .43729E+03 MTD
 PROD. RATE C3+ HC = .41198E+03 MTD
 HEAT TRANSFER AREA = .34190E+04 m**2
 GAS HOLDUP = .27259E+00

PREDICTION OF MULTICOMPONENT PHASE EQUILIBRIA USING
 PENG-ROBINSON EQUATION OF STATE FOR BOTH VAPOR AND LIQUID PHASES...

VAPOR-LIQUID EQUILIBRIA FOR FISCHER-TROPSCH SYNTHESIS

REACTOR TEMPERATURE = 528.00 K
 REACTOR PRESSURE = 28.000 ATMS.

TOTAL FLOW RATE =	.78520E+00 KMOLS/SEC,	.25495E+02 KG/SEC.
GAS FLOW RATE =	.78044E+00 KMOLS/SEC,	.23303E+02 KG/SEC
LIQUID FLOW RATE =	.47620E-02 KMOLS/SEC,	.21921E+01 KG/SEC

FEED COMPOSITION IS AS FOLLOWS...

MOLE FRACTION	WEIGHT FRACTION
Z(1)= .378714	AWZF(1)= .513310
Z(2)= .010803	AWZF(2)= .005994
Z(3)= .184977	AWZF(3)= .011485
Z(4)= .257128	AWZF(4)= .221809
Z(5)= .119183	AWZF(5)= .058887
Z(6)= .001845	AWZF(6)= .001594
Z(7)= .005535	AWZF(7)= .005125
Z(8)= .001568	AWZF(8)= .002032
Z(9)= .004704	AWZF(9)= .006389
Z(10)= .001333	AWZF(10)= .002303
Z(11)= .003999	AWZF(11)= .007158
Z(12)= .020527	AWZF(12)= .054480
Z(13)= .004630	AWZF(13)= .026287
Z(14)= .005056	AWZF(14)= .083147

LIQUID PHASE MOLE FRACTIONS.....

MOLE FRACTION	WEIGHT FRACTION
XC(1)= .042100	AWXC(1)= .004025
XC(2)= .001352	AWXC(2)= .000053
XC(3)= .011412	AWXC(3)= .000050
XC(4)= .017013	AWXC(4)= .001035
XC(5)= .011086	AWXC(5)= .000386
XC(6)= .000279	AWXC(6)= .000017
XC(7)= .000963	AWXC(7)= .000063
XC(8)= .000397	AWXC(8)= .000036
XC(9)= .001270	AWXC(9)= .000122
XC(10)= .000540	AWXC(10)= .000066
XC(11)= .001734	AWXC(11)= .000219
XC(12)= .020345	AWXC(12)= .003809
XC(13)= .058008	AWXC(13)= .023233
XC(14)= .833501	AWXC(14)= .966886

VAPOR PHASE MOLE FRACTIONS.....

MOLE FRACTION	WEIGHT FRACTION
YC(1)= .380768	AWYC(1)= .561217
YC(2)= .010861	AWYC(2)= .006553
YC(3)= .186036	AWYC(3)= .012560
YC(4)= .258593	AWYC(4)= .242577
YC(5)= .119842	AWYC(5)= .064390
YC(6)= .001854	AWYC(6)= .001742
YC(7)= .005562	AWYC(7)= .005602
YC(8)= .001575	AWYC(8)= .002220
YC(9)= .004725	AWYC(9)= .006978

YC(10)= .001338	AWYC(10)= .002514
YC(11)= .004013	AWYC(11)= .007811
YC(12)= .020528	AWYC(12)= .059246
YC(13)= .004304	AWYC(13)= .026574
YC(14)= .000001	AWYC(14)= .000016

LENGTH		GAS PHASE MOLE FRACTIONS				
ZZZ	XXX(M)	CO	CO2	H2	CH4	H2O

.00	.00	.39247E+00	.24559E+00	.26124E+00	.91961E-01	.87393E-
.10	1.20	.36946E+00	.27566E+00	.24839E+00	.96742E-01	.97513E-
.20	2.41	.34961E+00	.30159E+00	.23747E+00	.10102E+00	.10314E-
.30	3.61	.33224E+00	.32421E+00	.22802E+00	.10486E+00	.10666E-
.40	4.81	.31707E+00	.34392E+00	.21983E+00	.10827E+00	.10910E-
.50	6.01	.30400E+00	.36086E+00	.21281E+00	.11125E+00	.11090E-
.60	7.22	.29305E+00	.37501E+00	.20696E+00	.11376E+00	.11225E-
.70	8.42	.28430E+00	.38629E+00	.20231E+00	.11578E+00	.11325E-
.80	9.62	.27787E+00	.39457E+00	.19889E+00	.11727E+00	.11395E-
.90	10.83	.27391E+00	.39968E+00	.19679E+00	.11819E+00	.11437E-
1.00	12.03	.27255E+00	.40142E+00	.19607E+00	.11851E+00	.11451E-

LENGTH		LIQUID PHASE CONCENTRATIONS (kmol/m**3)				
ZZZ	XXX(M)	CO	CO2	H2	CH4	H2O

.00	.00	.36351E-01	.92822E-01	.20247E-01	.22995E-01	.15428E-
.10	1.20	.35913E-01	.94023E-01	.20036E-01	.23169E-01	.15569E-
.20	2.41	.34927E-01	.96798E-01	.19590E-01	.23573E-01	.15832E-
.30	3.61	.33726E-01	.10028E+00	.19072E-01	.24082E-01	.16105E-
.40	4.81	.32498E-01	.10392E+00	.18557E-01	.24618E-01	.16351E-
.50	6.01	.31351E-01	.10739E+00	.18084E-01	.25131E-01	.16560E-
.60	7.22	.30351E-01	.11045E+00	.17674E-01	.25588E-01	.16730E-
.70	8.42	.29538E-01	.11297E+00	.17343E-01	.25964E-01	.16862E-
.80	9.62	.28939E-01	.11484E+00	.17098E-01	.26245E-01	.16956E-
.90	10.83	.28573E-01	.11599E+00	.16948E-01	.26418E-01	.17013E-
1.00	12.03	.28449E-01	.11637E+00	.16898E-01	.26476E-01	.17032E-

LENGTH		CATALYST CONCENTRATION	
ZZZ	XXX(M)	DIM-LESS	ACTUAL(% WT)

.00	.00	1.00189	34.06423
.10	1.20	1.00151	34.05137
.20	2.41	1.00113	34.03852
.30	3.61	1.00075	34.02567
.40	4.81	1.00038	34.01282
.50	6.01	1.00000	33.99998
.60	7.22	.99962	33.98714
.70	8.42	.99924	33.97431
.80	9.62	.99887	33.96149
.90	10.83	.99849	33.94867
1.00	12.03	.99811	33.93585

LENGTH		VELOCITY PROFILE	
ZZZ	XXX(M)	UG/UGO	ACTUAL (M/SEC)

.00	.00	1.000000	.15500E+00
.10	1.20	.970320	.15040E+00
.20	2.41	.929025	.14400E+00
.30	3.61	.881493	.13663E+00
.40	4.81	.830719	.12876E+00
.50	6.01	.778370	.12065E+00
.60	7.22	.725348	.11243E+00
.70	8.42	.672102	.10418E+00
.80	9.62	.618818	.95917E-01
.90	10.83	.565541	.87659E-01
1.00	12.03	.512260	.79400E-01