

APPENDIX I-C
SAMPLE OUTPUT

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USE OF SIMDAT.FOR

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EX SIMDAT.FOR
FORTRAN 7(1716): SIMDAT.FOR
MAIN,   OCTAL PROG SIZE=12434
LINK:   Loading
[LNKXCT SIMDAT execution]

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IF THE USER WISHES TO TEST DIFFERENT REACTION NETWORKS FOR THE SAME SET OF INPUT CONDITIONS , THEN AFTER "SIM1.DAT" HAS BEEN CREATED , THE USER SHOULD SPECIFY "IDUM = 1" IN SUBSEQUENT RUNS TO SKIP READING THE SAME INPUT CONDITIONS. OTHERWISE SET IDUM = 2 WHAT IS THE VALUE OF IDUM ? >2

SIMULATION OF DIRECT COAL LIQUEFACTION

IF ONE REACTOR : ENTER 1
 IF TWO REACTORS IN SERIES : ENTER 2, AND SO ON (MAXIMUM OF 4) >1

ENTER INLET CONDITIONS:

Flowrate of gas to preheater (cm**3/sec)
 Flowrate of slurry to preheater (cm**3/sec)
 Length of preheater coil (cm)
 Length of reactor/reactors (cm)
 Diameter of preheater coil (cm)
 Diameter of reactor/reactors (cm)
 Inlet temperature of the slurry to preheater (degrees C)
 Operating pressure (atm)
 Mole fraction of hydrogen in inlet gas to preheater
 Temperature of furnace (degrees C)
 ALL ENTRIES TO BE MADE IN FREE FORMAT

>1172. 243. 4000. 700. 3.81 30.48 127. 150. .5 407.

ENTER VALUES OF VARIABLES LISTED BELOW:

Heat capacity of gas (cal/sm C)
 Heat capacity of slurry (cal/sm C)
 Arrhenius frequency factor for hydrogen consumption kinetics (1/sec)
 Activation energy for hydrogen consumption kinetics (cal/smole)
 Heat of reaction (cal/sm)
 Heat of dissolution (cal/sm)
 Solubility constant (<sm/cm**3>)/(<sm/cm**3>gas)
 Diffusivity of the gas (cm**2/sec)
 Surface tension of the slurry (dynes/cm)
 Density of the slurry (sm/cm**3)
 ALL ENTRIES TO BE MADE IN FREE FORMAT

>.89 .45 3213. 21000. 5850. 770. 1.2 .0000513 20. 1.3

Enter total number of species present in preheater >3

Enter Name of Species Number 1 >SP1

Enter Name of Species Number 2 >SP2

Enter Name of Species Number 3 >SP3

The Species have been Coded as:

1 = SP1

2 = SP2

3 = SP3

Enter Total Number of Non-Zero Rate Constants
for reaction network in preheater >2

Enter the Following Data for Each Rate Constant

For Rate Constant Number 1 Enter

Code of Reacting Species >1

Code of Product Species >2

Arrhenius Factor for Rate Constant (1/sec) >24.

Activation Energy (cal/mol) >12200.

For Rate Constant Number 2 Enter

Code of Reacting Species >2

Code of Product Species >3

Arrhenius Factor for Rate Constant (1/sec) >24.

Activation Energy (cal/mol) >12200.

Enter total number of species present in reactor >3

Enter Name of Species Number 1 >SP1

Enter Name of Species Number 2 >SP2

Enter Name of Species Number 3 >SP3

The Species have been Coded as:

1 = SP1

2 = SP2

3 = SP3

Enter total number of non-zero rate constants
for reaction network in reactor >2

Enter the Following Data for Each Rate Constant

For Rate Constant Number 1 Enter
Code of Reacting Species >1
Code of Product Species >2
Arrhenius Factor for Rate Constant (1/sec) >24.
Activation Energy (cal/mol) >12200.

For Rate Constant Number 2 Enter
Code of Reacting Species >2
Code of Product Species >3
Arrhenius Factor for Rate Constant (1/sec) >24.
Activation Energy (cal/mol) >12200.

Enter Initial Concentration of Each Species(gm/gm)
Species Number 1 >1.
Species Number 2 >0.
Species Number 3 >0.

DATA FILES HAVE BEEN CREATED
THE INPUT DATA ARE LISTED IN THE FILE "INPUT.DAT"
THE SIMULATOR CAN NOW BE RUN IN BATCH OR TIME SHARING MODE

End of execution FOROT7 7(3256)
CPU time 1.51 Elapsed time 5:29.08

EXIT

USE OF FITDAT.FOR

EX FITDAT.FOR
FORTRAN 7(1716): FITDAT.FOR
MAIN. OCTAL PROG SIZE=10756
LINK: Loading
[LNKXCT FITDAT execution]

IF ISOTHERMAL REACTOR SPECIFY IND=1
FOR NON-ISOTHERMAL REACTOR SPECIFY IND=2
WHAT IS THE VALUE OF IND ? >2

ENTER EQUIPMENT SIZES

Length of preheater (cm)
Length of reactor (cm)
Diameter of preheater (cm)
Diameter of reactor (cm)
ALL ENTRIES TO BE MADE IN FREE FORMAT

>7000. 400. 3.81 30.48

ENTER PHYSICO-CHEMICAL PARAMETERS

Heat capacity of gas (cal/sm C)
Heat capacity of slurry (cal/sm C)
Arrhenius frequency factor for hydrogen consumption kinetics (1/sec)
Activation energy for hydrogen consumption kinetics (cal/smole)
Heat of reaction (cal/sm)
Heat of dissolution (cal/sm)
Solubility constant ($\frac{\text{sm/cm}^3}{\text{sm/cm}^3}$)
Diffusivity of the gas (cm^2/sec)
Surface tension of the slurry (dynes/cm)
Density of the slurry (sm/cm^3)
ALL ENTRIES TO BE MADE IN FREE FORMAT

>.89 .45 3213. 21000. 5850. 770. 1.2 .0000513 20. 1.3

Enter Total Number of Species>3

Enter Name of Species Number 1>SP1

Enter Name of Species Number 2>SP2

Enter Name of Species Number 3>SP3

1 = SP1
2 = SP2
3 = SP3

Enter Total Number of Non-Zero Rate Constants>2

Enter the Following Data for Each Rate Constant

For Rate Constant Number 1 Enter

Code of Reacting Species>1

Code of Product Species>2

Lower & Upper bounds on Arrhenius Factor for Rate Constant (1/sec)

>15. 30.

Lower & Upper Bounds on Activation Energy (cal/smol)

>10000. 15000.

For Rate Constant Number 2 Enter

Code of Reacting Species>2

Code of Product Species>3

Lower & Upper bounds on Arrhenius Factor for Rate Constant (1/sec)

>15. 30.

Lower & Upper Bounds on Activation Energy (cal/smol)

>10000. 15000.

Enter no. of data points>1

FOR EACH DATA POINT, ENTER THE FOLLOWING

FOR DATA PT NO 1

Gas flowrate (cm³/sec)

Slurry flowrate (cm³/sec)

Inlet temp of slurry to preheater (deg C)

Operating pressure (atm)

Mole frac of hydrogen in inlet to preheater

Temp of heating medium

ENTER IN FREE FORMAT

>1172. 243. 127. 150. .5 407.

ENTER INLET CONC OF EACH SPECIES, GM/GM
Species Number 1>1.
Species Number 2>0.
Species Number 3>0.

ENTER OUTLET CONC OF EACH SPECIES, GM/GM
Species Number 1>.002475
Species Number 2>.006843
Species Number 3>.9907

ENTER DATA FOR TEMPERATURE PROFILE IN REACTOR

ENTER NUMBER OF POSITIONS AT WHICH TEMPERATURE WAS MEASURED >11
ENTER PAIRS OF POSITION-TEMPERATURE DATA
POSITION IN CM, TEMPERATURE IN DEG. C

>0. 605.9
>70. 614.9
>140. 621.6
>210. 626.6
>280. 630.1
>350. 632.7
>420. 634.4
>490. 635.6
>560. 636.3
>630. 636.8
>700. 636.9

DATA FILES "FIT01.DAT" & "FIT02.DAT" HAVE
EEN CREATED. THE SIMULATOR MAY NOW BE RUN IN BATCH MODE

End of execution FOROT7 7(3256)
CPU time 1.25 Elapsed time 6:09.95

EXIT

LIST OF INPUT DATA :

Flowrate of gas to preheater (cm**3/sec)	0.1172E+04
Flowrate of slurry to preheater (cm**3/sec)	0.2430E+03
Length of preheater coil (cm)	0.4000E+04
Length of reactor/reactors (cm)	0.7000E+03
Diameter of preheater coil (cm)	0.3810E+01
Diameter of reactor/reactors (cm)	0.3048E+02
Inlet temperature of slurry to preheater (deg. C)	0.1270E+03
Operating pressure (atm)	0.1500E+03
Mole fraction of hydrogen in inlet gas to preheater	0.5000E+00
Temperature of furnace (deg. C)	0.4070E+03
Heat capacity of gas (cal/gm C)	0.8900E+00
Heat capacity of slurry (cal/gm C)	0.4500E+00
Arrhenius frequency factor for H ₂ kinetics (1/s)	0.3213E+04
Activation energy for H ₂ kinetics (cal/gmole)	0.2100E+05
Heat of reaction (cal/gm)	0.5850E+04
Heat of dissolution (cal/gm)	0.7700E+03
Solubility constant (<gm/cm**3>liq/<gm/cm**3>gas)	0.1200E+01
Diffusivity of the gas (cm**2/sec)	0.5130E-04
Surface tension of the slurry (dynes/cm)	0.2000E+02
Density of the slurry (gm/cm**3)	0.1300E+01

Total number of species present in preheater = 3

Total Number of Non-Zero Rate Constants for reaction = 2
network in preheater

The Reaction Pathways for preheater are:

For the reaction path 1 to 2
 $k_0 = 0.2400E+02$ $E = 0.1220E+05$

For the reaction path 2 to 3
 $k_0 = 0.2400E+02$ $E = 0.1220E+05$

Total number of species present in reactor = 3

Total number of non-zero rate constants for reaction = 2
network in reactor

The Reaction pathways for reactor are:

For the reaction path 1 to 2
 $k_0 = 0.2400E+02$ $E = 0.1220E+05$

For the reaction path 2 to 3
 $k_0 = 0.2400E+02$ $E = 0.1220E+05$

Initial Concentration of Each Species (gm/gm)

Concentration of species # 1 = $0.1000E+01$

Concentration of species # 2 = $0.0000E+00$

Concentration of species # 3 = $0.0000E+00$

OUTPUT SUMMARY

Number of Species in Preheater	3
Number of Species in Reactor	3
Flow Rate of Slurry <kg/hr>	0.1137E+04
Flow Rate of Gas <kg/hr>	0.1928E+02

Conditions at Preheater Inlet

Temperature <Degrees C>	0.1270E+03
Hydrogen Concentration (Gas Phase) <gm/cm**3>	0.4570E-02
Hydrogen Concentration (Liquid Phase) <gm/cm**3>	0.0000E+00

Concentration of Species 1 <gm/gm>	0.1000E+01
Concentration of Species 2 <gm/gm>	0.0000E+00
Concentration of Species 3 <gm/gm>	0.0000E+00

Conditions at Preheater Outlet (Reactor Inlet)

Temperature <Degrees C>	0.4071E+03
Hydrogen Concentration (Gas Phase) <gm/cm**3>	0.3985E-02
Hydrogen Concentration (Liquid Phase) <gm/cm**3>	0.2697E-02

Concentration of Species 1 <gm/gm>	0.9995E+00
Concentration of Species 2 <gm/gm>	0.5464E-03
Concentration of Species 3 <gm/gm>	0.1486E-06

Conditions at Outlet of Reactor # 1

Temperature <Degrees C>	0.6369E+03
Hydrogen Concentration (Gas Phase) <gm/cm**3>	0.1214E-03
Hydrogen Concentration (Liquid Phase) <gm/cm**3>	0.8495E-04

Concentration of Species 1 <gm/gm>	0.2198E-02
Concentration of Species 2 <gm/gm>	0.6190E-02
Concentration of Species 3 <gm/gm>	0.9916E+00

COST ESTIMATES

PREHEATER

Capital Cost <\$>	0.6699E+08
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Operating Cost <\$/YR>	0.4367E+09
Maintenance Cost <\$/YR>	0.1831E+07
Fixed Cost <\$/YR>	0.1005E+07
Variable Cost <\$/YR>	0.4357E+09

REACTOR # 1

Capital Cost <\$>	0.6361E+08
Operating Cost <\$/YR>	0.1738E+07
Maintenance Cost <\$/YR>	0.1738E+07
Fixed Cost <\$/YR>	0.9541E+06
Variable Cost <\$/YR>	0.7842E+06

HYDRODYNAMIC PARAMETERS FOR PREHEATER

Gas Holdup	0.40607E+00
Volumetric mass transfer coefficient	0.32308E+00
Peclet Number for mass dispersion	0.35399E+03
Peclet Number for heat dispersion	0.36586E+03

HYDRODYNAMIC PARAMETERS FOR REACTOR # 1

Gas Holdup	0.42773E-01
Volumetric mass transfer coefficient	0.38696E-01
Peclet Number for mass dispersion	0.49976E+00
Peclet Number for heat dispersion	0.51651E+00

TEMPERATURE PROFILE IN PREHEATER

DISTANCE ALONG PREHEATER		TEMPERATURE	
DIMENSIONLESS	CENTIMETERS	DIMENSIONLESS	DEGREES C
0.00	0.0	0.0000	0.1270E+03
0.01	40.0	0.0899	0.1629E+03
0.02	80.0	0.1752	0.1971E+03
0.03	120.0	0.2526	0.2281E+03
0.04	160.0	0.3208	0.2553E+03
0.05	200.0	0.3751	0.2771E+03
0.06	240.0	0.4009	0.2874E+03
0.07	280.0	0.4246	0.2968E+03
0.08	320.0	0.4463	0.3055E+03
0.09	360.0	0.4663	0.3135E+03
0.10	400.0	0.4847	0.3209E+03
0.11	440.0	0.5017	0.3277E+03
0.12	480.0	0.5173	0.3339E+03
0.13	520.0	0.5317	0.3397E+03
0.14	560.0	0.5450	0.3450E+03
0.15	600.0	0.5572	0.3499E+03
0.16	640.0	0.5684	0.3544E+03
0.17	680.0	0.5788	0.3585E+03
0.18	720.0	0.5884	0.3623E+03
0.19	760.0	0.5972	0.3659E+03
0.20	800.0	0.6053	0.3691E+03
0.21	840.0	0.6127	0.3721E+03
0.22	880.0	0.6196	0.3749E+03
0.23	920.0	0.6260	0.3774E+03
0.24	960.0	0.6318	0.3797E+03
0.25	1000.0	0.6372	0.3819E+03
0.26	1040.0	0.6422	0.3839E+03
0.27	1080.0	0.6468	0.3857E+03
0.28	1120.0	0.6510	0.3874E+03
0.29	1160.0	0.6549	0.3889E+03
0.30	1200.0	0.6584	0.3904E+03
0.31	1240.0	0.6617	0.3917E+03
0.32	1280.0	0.6648	0.3929E+03
0.33	1320.0	0.6676	0.3940E+03
0.34	1360.0	0.6702	0.3951E+03

0.35	1400.0	0.6725	0.3960E+03
0.36	1440.0	0.6747	0.3969E+03
0.37	1480.0	0.6768	0.3977E+03
0.38	1520.0	0.6786	0.3984E+03
0.39	1560.0	0.6803	0.3991E+03
0.40	1600.0	0.6819	0.3998E+03
0.41	1640.0	0.6834	0.4004E+03
0.42	1680.0	0.6847	0.4009E+03
0.43	1720.0	0.6860	0.4014E+03
0.44	1760.0	0.6871	0.4018E+03
0.45	1800.0	0.6891	0.4026E+03
0.46	1840.0	0.6909	0.4034E+03
0.47	1880.0	0.6924	0.4040E+03
0.48	1920.0	0.6937	0.4045E+03
0.49	1960.0	0.6948	0.4049E+03
0.50	2000.0	0.6957	0.4053E+03
0.51	2040.0	0.6964	0.4056E+03
0.52	2080.0	0.6971	0.4058E+03
0.53	2120.0	0.6976	0.4060E+03
0.54	2160.0	0.6980	0.4062E+03
0.55	2200.0	0.6984	0.4064E+03
0.56	2240.0	0.6987	0.4065E+03
0.57	2280.0	0.6989	0.4066E+03
0.58	2320.0	0.6992	0.4067E+03
0.59	2360.0	0.6993	0.4067E+03
0.60	2400.0	0.6995	0.4068E+03
0.61	2440.0	0.6996	0.4068E+03
0.62	2480.0	0.6997	0.4069E+03
0.63	2520.0	0.6998	0.4069E+03
0.64	2560.0	0.6999	0.4069E+03
0.65	2600.0	0.6999	0.4070E+03
0.66	2640.0	0.7000	0.4070E+03
0.67	2680.0	0.7000	0.4070E+03
0.68	2720.0	0.7001	0.4070E+03
0.69	2760.0	0.7001	0.4070E+03
0.70	2800.0	0.7001	0.4070E+03
0.71	2840.0	0.7001	0.4071E+03
0.72	2880.0	0.7002	0.4071E+03
0.73	2920.0	0.7002	0.4071E+03
0.74	2960.0	0.7002	0.4071E+03
0.75	3000.0	0.7002	0.4071E+03
0.76	3040.0	0.7002	0.4071E+03
0.77	3080.0	0.7002	0.4071E+03

0.78	3120.0	0.7002	0.4071E+03
0.79	3160.0	0.7002	0.4071E+03
0.80	3200.0	0.7002	0.4071E+03
0.81	3240.0	0.7002	0.4071E+03
0.82	3280.0	0.7002	0.4071E+03
0.83	3320.0	0.7002	0.4071E+03
0.84	3360.0	0.7002	0.4071E+03
0.85	3400.0	0.7002	0.4071E+03
0.86	3440.0	0.7002	0.4071E+03
0.87	3480.0	0.7002	0.4071E+03
0.88	3520.0	0.7002	0.4071E+03
0.89	3560.0	0.7002	0.4071E+03
0.90	3600.0	0.7002	0.4071E+03
0.91	3640.0	0.7002	0.4071E+03
0.92	3680.0	0.7002	0.4071E+03
0.93	3720.0	0.7002	0.4071E+03
0.94	3760.0	0.7002	0.4071E+03
0.95	3800.0	0.7002	0.4071E+03
0.96	3840.0	0.7002	0.4071E+03
0.97	3880.0	0.7002	0.4071E+03
0.98	3920.0	0.7002	0.4071E+03
0.99	3960.0	0.7002	0.4071E+03
1.00	4000.0	0.7002	0.4071E+03

HYDROGEN PROFILE IN PREHEATER
(GAS PHASE)

DISTANCE ALONG PREHEATER		HYDROGEN CONCENTRATION	
DIMENSIONLESS	CENTIMETERS	DIMENSIONLESS	GM/CM**3
0.00	0.0	1.0000	0.4570E-02
0.01	40.0	0.9564	0.4371E-02
0.02	80.0	0.9310	0.4255E-02
0.03	120.0	0.9154	0.4183E-02
0.04	160.0	0.9054	0.4138E-02
0.05	200.0	0.8987	0.4107E-02
0.06	240.0	0.8944	0.4087E-02
0.07	280.0	0.8916	0.4075E-02
0.08	320.0	0.8897	0.4066E-02
0.09	360.0	0.8882	0.4059E-02
0.10	400.0	0.8870	0.4054E-02
0.11	440.0	0.8861	0.4049E-02
0.12	480.0	0.8852	0.4045E-02
0.13	520.0	0.8844	0.4042E-02
0.14	560.0	0.8838	0.4039E-02
0.15	600.0	0.8832	0.4036E-02
0.16	640.0	0.8826	0.4033E-02
0.17	680.0	0.8821	0.4031E-02
0.18	720.0	0.8816	0.4029E-02
0.19	760.0	0.8812	0.4027E-02
0.20	800.0	0.8808	0.4025E-02
0.21	840.0	0.8804	0.4024E-02
0.22	880.0	0.8801	0.4022E-02
0.23	920.0	0.8798	0.4021E-02
0.24	960.0	0.8795	0.4019E-02
0.25	1000.0	0.8792	0.4018E-02
0.26	1040.0	0.8790	0.4017E-02
0.27	1080.0	0.8787	0.4016E-02
0.28	1120.0	0.8785	0.4015E-02
0.29	1160.0	0.8783	0.4014E-02
0.30	1200.0	0.8781	0.4013E-02
0.31	1240.0	0.8779	0.4012E-02
0.32	1280.0	0.8778	0.4011E-02
0.33	1320.0	0.8776	0.4011E-02
0.34	1360.0	0.8774	0.4010E-02

0.35	1400.0	0.8773	0.4009E-02
0.36	1440.0	0.8771	0.4009E-02
0.37	1480.0	0.8770	0.4008E-02
0.38	1520.0	0.8769	0.4007E-02
0.39	1560.0	0.8768	0.4007E-02
0.40	1600.0	0.8766	0.4006E-02
0.41	1640.0	0.8765	0.4006E-02
0.42	1680.0	0.8764	0.4005E-02
0.43	1720.0	0.8763	0.4005E-02
0.44	1760.0	0.8762	0.4004E-02
0.45	1800.0	0.8761	0.4004E-02
0.46	1840.0	0.8760	0.4003E-02
0.47	1880.0	0.8759	0.4003E-02
0.48	1920.0	0.8757	0.4002E-02
0.49	1960.0	0.8756	0.4002E-02
0.50	2000.0	0.8755	0.4001E-02
0.51	2040.0	0.8754	0.4001E-02
0.52	2080.0	0.8753	0.4000E-02
0.53	2120.0	0.8752	0.4000E-02
0.54	2160.0	0.8752	0.3999E-02
0.55	2200.0	0.8751	0.3999E-02
0.56	2240.0	0.8750	0.3999E-02
0.57	2280.0	0.8749	0.3998E-02
0.58	2320.0	0.8749	0.3998E-02
0.59	2360.0	0.8748	0.3998E-02
0.60	2400.0	0.8747	0.3997E-02
0.61	2440.0	0.8746	0.3997E-02
0.62	2480.0	0.8746	0.3997E-02
0.63	2520.0	0.8745	0.3996E-02
0.64	2560.0	0.8744	0.3996E-02
0.65	2600.0	0.8744	0.3996E-02
0.66	2640.0	0.8743	0.3996E-02
0.67	2680.0	0.8742	0.3995E-02
0.68	2720.0	0.8742	0.3995E-02
0.69	2760.0	0.8741	0.3995E-02
0.70	2800.0	0.8740	0.3994E-02
0.71	2840.0	0.8740	0.3994E-02
0.72	2880.0	0.8739	0.3994E-02
0.73	2920.0	0.8738	0.3993E-02
0.74	2960.0	0.8738	0.3993E-02
0.75	3000.0	0.8737	0.3993E-02
0.76	3040.0	0.8736	0.3993E-02
0.77	3080.0	0.8736	0.3992E-02

0.78	3120.0	0.8735	0.3992E-02
0.79	3160.0	0.8734	0.3992E-02
0.80	3200.0	0.8734	0.3991E-02
0.81	3240.0	0.8733	0.3991E-02
0.82	3280.0	0.8732	0.3991E-02
0.83	3320.0	0.8732	0.3990E-02
0.84	3360.0	0.8731	0.3990E-02
0.85	3400.0	0.8730	0.3990E-02
0.86	3440.0	0.8730	0.3990E-02
0.87	3480.0	0.8729	0.3989E-02
0.88	3520.0	0.8729	0.3989E-02
0.89	3560.0	0.8728	0.3989E-02
0.90	3600.0	0.8727	0.3988E-02
0.91	3640.0	0.8727	0.3988E-02
0.92	3680.0	0.8726	0.3988E-02
0.93	3720.0	0.8725	0.3987E-02
0.94	3760.0	0.8725	0.3987E-02
0.95	3800.0	0.8724	0.3987E-02
0.96	3840.0	0.8723	0.3987E-02
0.97	3880.0	0.8723	0.3986E-02
0.98	3920.0	0.8722	0.3986E-02
0.99	3960.0	0.8721	0.3986E-02
1.00	4000.0	0.8721	0.3985E-02

HYDROGEN PROFILE IN PREHEATER
(LIQUID PHASE)

DISTANCE ALONG PREHEATER		HYDROGEN CONCENTRATION	
DIMENSIONLESS	CENTIMETERS	DIMENSIONLESS	GM/CM**3
0.00	0.0	0.0000	0.0000E+00
0.01	40.0	0.4628	0.9600E-03
0.02	80.0	0.7332	0.1521E-02
0.03	120.0	0.8985	0.1864E-02
0.04	160.0	1.0047	0.2084E-02
0.05	200.0	1.0763	0.2233E-02
0.06	240.0	1.1220	0.2327E-02
0.07	280.0	1.1514	0.2388E-02
0.08	320.0	1.1719	0.2431E-02
0.09	360.0	1.1874	0.2463E-02
0.10	400.0	1.1997	0.2489E-02
0.11	440.0	1.2101	0.2510E-02
0.12	480.0	1.2191	0.2529E-02
0.13	520.0	1.2270	0.2545E-02
0.14	560.0	1.2340	0.2560E-02
0.15	600.0	1.2404	0.2573E-02
0.16	640.0	1.2461	0.2585E-02
0.17	680.0	1.2513	0.2596E-02
0.18	720.0	1.2560	0.2605E-02
0.19	760.0	1.2603	0.2614E-02
0.20	800.0	1.2642	0.2622E-02
0.21	840.0	1.2677	0.2630E-02
0.22	880.0	1.2710	0.2636E-02
0.23	920.0	1.2739	0.2642E-02
0.24	960.0	1.2766	0.2648E-02
0.25	1000.0	1.2791	0.2653E-02
0.26	1040.0	1.2813	0.2658E-02
0.27	1080.0	1.2833	0.2662E-02
0.28	1120.0	1.2852	0.2666E-02
0.29	1160.0	1.2869	0.2669E-02
0.30	1200.0	1.2885	0.2673E-02
0.31	1240.0	1.2899	0.2676E-02
0.32	1280.0	1.2912	0.2678E-02
0.33	1320.0	1.2924	0.2681E-02
0.34	1360.0	1.2934	0.2683E-02

0.35	1400.0	1.2944	0.2685E-02
0.36	1440.0	1.2953	0.2687E-02
0.37	1480.0	1.2961	0.2689E-02
0.38	1520.0	1.2969	0.2690E-02
0.39	1560.0	1.2975	0.2691E-02
0.40	1600.0	1.2982	0.2693E-02
0.41	1640.0	1.2987	0.2694E-02
0.42	1680.0	1.2992	0.2695E-02
0.43	1720.0	1.2997	0.2696E-02
0.44	1760.0	1.3001	0.2697E-02
0.45	1800.0	1.3005	0.2698E-02
0.46	1840.0	1.3011	0.2699E-02
0.47	1880.0	1.3016	0.2700E-02
0.48	1920.0	1.3021	0.2701E-02
0.49	1960.0	1.3026	0.2702E-02
0.50	2000.0	1.3029	0.2703E-02
0.51	2040.0	1.3032	0.2703E-02
0.52	2080.0	1.3034	0.2704E-02
0.53	2120.0	1.3036	0.2704E-02
0.54	2160.0	1.3037	0.2704E-02
0.55	2200.0	1.3038	0.2704E-02
0.56	2240.0	1.3038	0.2705E-02
0.57	2280.0	1.3039	0.2705E-02
0.58	2320.0	1.3039	0.2705E-02
0.59	2360.0	1.3039	0.2705E-02
0.60	2400.0	1.3039	0.2705E-02
0.61	2440.0	1.3038	0.2705E-02
0.62	2480.0	1.3038	0.2704E-02
0.63	2520.0	1.3037	0.2704E-02
0.64	2560.0	1.3037	0.2704E-02
0.65	2600.0	1.3036	0.2704E-02
0.66	2640.0	1.3035	0.2704E-02
0.67	2680.0	1.3035	0.2704E-02
0.68	2720.0	1.3034	0.2704E-02
0.69	2760.0	1.3033	0.2703E-02
0.70	2800.0	1.3032	0.2703E-02
0.71	2840.0	1.3031	0.2703E-02
0.72	2880.0	1.3030	0.2703E-02
0.73	2920.0	1.3030	0.2703E-02
0.74	2960.0	1.3029	0.2702E-02
0.75	3000.0	1.3028	0.2702E-02
0.76	3040.0	1.3027	0.2702E-02
0.77	3080.0	1.3026	0.2702E-02

0.78	3120.0	1.3025	0.2702E-02
0.79	3160.0	1.3024	0.2702E-02
0.80	3200.0	1.3023	0.2701E-02
0.81	3240.0	1.3022	0.2701E-02
0.82	3280.0	1.3021	0.2701E-02
0.83	3320.0	1.3020	0.2701E-02
0.84	3360.0	1.3019	0.2701E-02
0.85	3400.0	1.3018	0.2700E-02
0.86	3440.0	1.3017	0.2700E-02
0.87	3480.0	1.3016	0.2700E-02
0.88	3520.0	1.3015	0.2700E-02
0.89	3560.0	1.3014	0.2700E-02
0.90	3600.0	1.3013	0.2699E-02
0.91	3640.0	1.3012	0.2699E-02
0.92	3680.0	1.3011	0.2699E-02
0.93	3720.0	1.3011	0.2699E-02
0.94	3760.0	1.3010	0.2699E-02
0.95	3800.0	1.3009	0.2698E-02
0.96	3840.0	1.3008	0.2698E-02
0.97	3880.0	1.3007	0.2698E-02
0.98	3920.0	1.3006	0.2698E-02
0.99	3960.0	1.3005	0.2698E-02
1.00	4000.0	1.3004	0.2697E-02

CONCENTRATION PROFILE IN PREHEATER

DISTANCE ALONG PREHEATER		CHEMICAL SPECIES		
DIMENSIONLESS	CENTIMETERS	1	2	3
0.00	0.0	.100E+01	.547E-05	.149E-10
0.01	40.0	.100E+01	.109E-04	.523E-10
0.02	80.0	.100E+01	.164E-04	.120E-09
0.03	120.0	.100E+01	.219E-04	.217E-09
0.04	160.0	.100E+01	.273E-04	.344E-09
0.05	200.0	.100E+01	.328E-04	.501E-09
0.06	240.0	.100E+01	.383E-04	.687E-09
0.07	280.0	.100E+01	.437E-04	.904E-09
0.08	320.0	.100E+01	.492E-04	.115E-08
0.09	360.0	.100E+01	.547E-04	.143E-08
0.10	400.0	.100E+01	.601E-04	.173E-08
0.11	440.0	.100E+01	.656E-04	.207E-08
0.12	480.0	.100E+01	.711E-04	.244E-08
0.13	520.0	.100E+01	.765E-04	.283E-08
0.14	560.0	.100E+01	.820E-04	.326E-08
0.15	600.0	.100E+01	.875E-04	.371E-08
0.16	640.0	.100E+01	.929E-04	.420E-08
0.17	680.0	.100E+01	.984E-04	.471E-08
0.18	720.0	.100E+01	.104E-03	.526E-08
0.19	760.0	.100E+01	.109E-03	.584E-08
0.20	800.0	.100E+01	.115E-03	.644E-08
0.21	840.0	.100E+01	.120E-03	.708E-08
0.22	880.0	.100E+01	.126E-03	.774E-08
0.23	920.0	.100E+01	.131E-03	.843E-08
0.24	960.0	.100E+01	.137E-03	.916E-08
0.25	1000.0	.100E+01	.142E-03	.991E-08
0.26	1040.0	.100E+01	.148E-03	.107E-07
0.27	1080.0	.100E+01	.153E-03	.115E-07
0.28	1120.0	.100E+01	.159E-03	.124E-07
0.29	1160.0	.100E+01	.164E-03	.132E-07
0.30	1200.0	.100E+01	.169E-03	.141E-07
0.31	1240.0	.100E+01	.175E-03	.151E-07
0.32	1280.0	.100E+01	.180E-03	.160E-07
0.33	1320.0	.100E+01	.186E-03	.170E-07
0.34	1360.0	.100E+01	.191E-03	.180E-07
0.35	1400.0	.100E+01	.197E-03	.191E-07

0.36	1440.0	.100E+01	.202E-03	.202E-07
0.37	1480.0	.100E+01	.208E-03	.213E-07
0.38	1520.0	.100E+01	.213E-03	.224E-07
0.39	1560.0	.100E+01	.219E-03	.236E-07
0.40	1600.0	.100E+01	.224E-03	.248E-07
0.41	1640.0	.100E+01	.230E-03	.261E-07
0.42	1680.0	.100E+01	.235E-03	.273E-07
0.43	1720.0	.100E+01	.240E-03	.286E-07
0.44	1760.0	.100E+01	.246E-03	.299E-07
0.45	1800.0	.100E+01	.251E-03	.313E-07
0.46	1840.0	.100E+01	.257E-03	.327E-07
0.47	1880.0	.100E+01	.262E-03	.341E-07
0.48	1920.0	.100E+01	.268E-03	.355E-07
0.49	1960.0	.100E+01	.273E-03	.370E-07
0.50	2000.0	.100E+01	.279E-03	.385E-07
0.51	2040.0	.100E+01	.284E-03	.400E-07
0.52	2080.0	.100E+01	.290E-03	.416E-07
0.53	2120.0	.100E+01	.295E-03	.432E-07
0.54	2160.0	.100E+01	.301E-03	.448E-07
0.55	2200.0	.100E+01	.306E-03	.464E-07
0.56	2240.0	.100E+01	.312E-03	.481E-07
0.57	2280.0	.100E+01	.317E-03	.498E-07
0.58	2320.0	.100E+01	.322E-03	.516E-07
0.59	2360.0	.100E+01	.328E-03	.533E-07
0.60	2400.0	.100E+01	.333E-03	.551E-07
0.61	2440.0	.100E+01	.339E-03	.570E-07
0.62	2480.0	.100E+01	.344E-03	.588E-07
0.63	2520.0	.100E+01	.350E-03	.607E-07
0.64	2560.0	.100E+01	.355E-03	.626E-07
0.65	2600.0	.100E+01	.361E-03	.646E-07
0.66	2640.0	.100E+01	.366E-03	.666E-07
0.67	2680.0	.100E+01	.372E-03	.686E-07
0.68	2720.0	.100E+01	.377E-03	.706E-07
0.69	2760.0	.100E+01	.383E-03	.727E-07
0.70	2800.0	.100E+01	.388E-03	.748E-07
0.71	2840.0	.100E+01	.393E-03	.769E-07
0.72	2880.0	.100E+01	.399E-03	.791E-07
0.73	2920.0	.100E+01	.404E-03	.813E-07
0.74	2960.0	.100E+01	.410E-03	.835E-07
0.75	3000.0	.100E+01	.415E-03	.857E-07
0.76	3040.0	.100E+01	.421E-03	.880E-07
0.77	3080.0	.100E+01	.426E-03	.903E-07
0.78	3120.0	.100E+01	.432E-03	.927E-07

0.79	3160.0	.100E+01	.437E-03	.950E-07
0.80	3200.0	.100E+01	.443E-03	.974E-07
0.81	3240.0	.100E+01	.448E-03	.998E-07
0.82	3280.0	.100E+01	.454E-03	.102E-06
0.83	3320.0	.100E+01	.459E-03	.105E-06
0.84	3360.0	.100E+01	.464E-03	.107E-06
0.85	3400.0	.100E+01	.470E-03	.110E-06
0.86	3440.0	.100E+01	.475E-03	.112E-06
0.87	3480.0	.100E+01	.481E-03	.115E-06
0.88	3520.0	.100E+01	.486E-03	.118E-06
0.89	3560.0	.100E+01	.492E-03	.120E-06
0.90	3600.0	.100E+01	.497E-03	.123E-06
0.91	3640.0	.999E+00	.503E-03	.126E-06
0.92	3680.0	.999E+00	.508E-03	.129E-06
0.93	3720.0	.999E+00	.514E-03	.131E-06
0.94	3760.0	.999E+00	.519E-03	.134E-06
0.95	3800.0	.999E+00	.525E-03	.137E-06
0.96	3840.0	.999E+00	.530E-03	.140E-06
0.97	3880.0	.999E+00	.535E-03	.143E-06
0.98	3920.0	.999E+00	.541E-03	.146E-06
0.99	3960.0	.999E+00	.546E-03	.149E-06
1.00	4000.0	.999E+00	.546E-03	.149E-06

VISCOSITY PROFILE IN PREHEATER

DISTANCE ALONG PREHEATER		VISCOSITY
DIMENSIONLESS	CENTIMETERS	POISE
0.00	0.0	0.5849E-01
0.01	40.0	0.4367E-01
0.02	80.0	0.3676E-01
0.03	120.0	0.3310E-01
0.04	160.0	0.3100E-01
0.05	200.0	0.1400E+00
0.06	240.0	0.1400E+00
0.07	280.0	0.1400E+00
0.08	320.0	0.1400E+00
0.09	360.0	0.1400E+00
0.10	400.0	0.1400E+00
0.11	440.0	0.1400E+00
0.12	480.0	0.1400E+00
0.13	520.0	0.1400E+00
0.14	560.0	0.1400E+00
0.15	600.0	0.1400E+00
0.16	640.0	0.1400E+00
0.17	680.0	0.1400E+00
0.18	720.0	0.1400E+00
0.19	760.0	0.1400E+00
0.20	800.0	0.1400E+00
0.21	840.0	0.1400E+00
0.22	880.0	0.1400E+00
0.23	920.0	0.1400E+00
0.24	960.0	0.1400E+00
0.25	1000.0	0.1400E+00
0.26	1040.0	0.1400E+00
0.27	1080.0	0.1400E+00
0.28	1120.0	0.1400E+00
0.29	1160.0	0.1400E+00
0.30	1200.0	0.1400E+00
0.31	1240.0	0.1400E+00
0.32	1280.0	0.1400E+00
0.33	1320.0	0.1400E+00
0.34	1360.0	0.1400E+00
0.35	1400.0	0.1400E+00

0.36	1440.0	0.1400E+00
0.37	1480.0	0.1400E+00
0.38	1520.0	0.1400E+00
0.39	1560.0	0.1400E+00
0.40	1600.0	0.1400E+00
0.41	1640.0	0.1400E+00
0.42	1680.0	0.1400E+00
0.43	1720.0	0.1400E+00
0.44	1760.0	0.1400E+00
0.45	1800.0	0.2647E-01
0.46	1840.0	0.2646E-01
0.47	1880.0	0.2645E-01
0.48	1920.0	0.2644E-01
0.49	1960.0	0.2644E-01
0.50	2000.0	0.2643E-01
0.51	2040.0	0.2643E-01
0.52	2080.0	0.2643E-01
0.53	2120.0	0.2642E-01
0.54	2160.0	0.2642E-01
0.55	2200.0	0.2642E-01
0.56	2240.0	0.2642E-01
0.57	2280.0	0.2642E-01
0.58	2320.0	0.2642E-01
0.59	2360.0	0.2642E-01
0.60	2400.0	0.2641E-01
0.61	2440.0	0.2641E-01
0.62	2480.0	0.2641E-01
0.63	2520.0	0.2641E-01
0.64	2560.0	0.2641E-01
0.65	2600.0	0.2641E-01
0.66	2640.0	0.2641E-01
0.67	2680.0	0.2641E-01
0.68	2720.0	0.2641E-01
0.69	2760.0	0.2641E-01
0.70	2800.0	0.2641E-01
0.71	2840.0	0.2641E-01
0.72	2880.0	0.2641E-01
0.73	2920.0	0.2641E-01
0.74	2960.0	0.2641E-01
0.75	3000.0	0.2641E-01
0.76	3040.0	0.2641E-01
0.77	3080.0	0.2641E-01
0.78	3120.0	0.2641E-01

0.79	3160.0	0.2641E-01
0.80	3200.0	0.2641E-01
0.81	3240.0	0.2641E-01
0.82	3280.0	0.2641E-01
0.83	3320.0	0.2641E-01
0.84	3360.0	0.2641E-01
0.85	3400.0	0.2641E-01
0.86	3440.0	0.2641E-01
0.87	3480.0	0.2641E-01
0.88	3520.0	0.2641E-01
0.89	3560.0	0.2641E-01
0.90	3600.0	0.2641E-01
0.91	3640.0	0.2641E-01
0.92	3680.0	0.2641E-01
0.93	3720.0	0.2641E-01
0.94	3760.0	0.2641E-01
0.95	3800.0	0.2641E-01
0.96	3840.0	0.2641E-01
0.97	3880.0	0.2641E-01
0.98	3920.0	0.2641E-01
0.99	3960.0	0.2641E-01
1.00	4000.0	0.2641E-01

TEMPERATURE PROFILE IN REACTOR # 1

DISTANCE ALONG REACTOR		TEMPERATURE	
DIMENSIONLESS	CENTIMETERS	DIMENSIONLESS	DEGREES C
0.00	0.0	1.1972	0.6059E+03
0.01	7.0	1.1998	0.6069E+03
0.02	14.0	1.2022	0.6079E+03
0.03	21.0	1.2046	0.6089E+03
0.04	28.0	1.2070	0.6098E+03
0.05	35.0	1.2092	0.6107E+03
0.06	42.0	1.2114	0.6116E+03
0.07	49.0	1.2136	0.6124E+03
0.08	56.0	1.2157	0.6133E+03
0.09	63.0	1.2177	0.6141E+03
0.10	70.0	1.2197	0.6149E+03
0.11	77.0	1.2216	0.6156E+03
0.12	84.0	1.2234	0.6164E+03
0.13	91.0	1.2252	0.6171E+03
0.14	98.0	1.2270	0.6178E+03
0.15	105.0	1.2287	0.6185E+03
0.16	112.0	1.2304	0.6191E+03
0.17	119.0	1.2320	0.6198E+03
0.18	126.0	1.2335	0.6204E+03
0.19	133.0	1.2350	0.6210E+03
0.20	140.0	1.2365	0.6216E+03
0.21	147.0	1.2379	0.6222E+03
0.22	154.0	1.2393	0.6227E+03
0.23	161.0	1.2406	0.6233E+03
0.24	168.0	1.2419	0.6238E+03
0.25	175.0	1.2432	0.6243E+03
0.26	182.0	1.2444	0.6248E+03
0.27	189.0	1.2456	0.6252E+03
0.28	196.0	1.2467	0.6257E+03
0.29	203.0	1.2478	0.6261E+03
0.30	210.0	1.2489	0.6266E+03
0.31	217.0	1.2499	0.6270E+03
0.32	224.0	1.2509	0.6274E+03
0.33	231.0	1.2519	0.6278E+03
0.34	238.0	1.2529	0.6281E+03

0.35	245.0	1.2538	0.6285E+03
0.36	252.0	1.2546	0.6289E+03
0.37	259.0	1.2555	0.6292E+03
0.38	266.0	1.2563	0.6295E+03
0.39	273.0	1.2571	0.6298E+03
0.40	280.0	1.2579	0.6301E+03
0.41	287.0	1.2586	0.6304E+03
0.42	294.0	1.2593	0.6307E+03
0.43	301.0	1.2600	0.6310E+03
0.44	308.0	1.2607	0.6313E+03
0.45	315.0	1.2613	0.6315E+03
0.46	322.0	1.2619	0.6318E+03
0.47	329.0	1.2625	0.6320E+03
0.48	336.0	1.2631	0.6322E+03
0.49	343.0	1.2637	0.6325E+03
0.50	350.0	1.2642	0.6327E+03
0.51	357.0	1.2647	0.6329E+03
0.52	364.0	1.2652	0.6331E+03
0.53	371.0	1.2657	0.6333E+03
0.54	378.0	1.2661	0.6335E+03
0.55	385.0	1.2666	0.6336E+03
0.56	392.0	1.2670	0.6338E+03
0.57	399.0	1.2674	0.6340E+03
0.58	406.0	1.2678	0.6341E+03
0.59	413.0	1.2682	0.6343E+03
0.60	420.0	1.2686	0.6344E+03
0.61	427.0	1.2689	0.6346E+03
0.62	434.0	1.2693	0.6347E+03
0.63	441.0	1.2696	0.6348E+03
0.64	448.0	1.2699	0.6350E+03
0.65	455.0	1.2702	0.6351E+03
0.66	462.0	1.2705	0.6352E+03
0.67	469.0	1.2707	0.6353E+03
0.68	476.0	1.2710	0.6354E+03
0.69	483.0	1.2713	0.6355E+03
0.70	490.0	1.2715	0.6356E+03
0.71	497.0	1.2717	0.6357E+03
0.72	504.0	1.2719	0.6358E+03
0.73	511.0	1.2721	0.6359E+03
0.74	518.0	1.2723	0.6359E+03
0.75	525.0	1.2725	0.6360E+03
0.76	532.0	1.2727	0.6361E+03
0.77	539.0	1.2729	0.6362E+03

0.78	546.0	1.2730	0.6362E+03
0.79	553.0	1.2732	0.6363E+03
0.80	560.0	1.2733	0.6363E+03
0.81	567.0	1.2735	0.6364E+03
0.82	574.0	1.2736	0.6364E+03
0.83	581.0	1.2737	0.6365E+03
0.84	588.0	1.2738	0.6365E+03
0.85	595.0	1.2739	0.6366E+03
0.86	602.0	1.2740	0.6366E+03
0.87	609.0	1.2741	0.6367E+03
0.88	616.0	1.2742	0.6367E+03
0.89	623.0	1.2743	0.6367E+03
0.90	630.0	1.2744	0.6367E+03
0.91	637.0	1.2744	0.6368E+03
0.92	644.0	1.2745	0.6368E+03
0.93	651.0	1.2746	0.6368E+03
0.94	658.0	1.2746	0.6368E+03
0.95	665.0	1.2746	0.6369E+03
0.96	672.0	1.2747	0.6369E+03
0.97	679.0	1.2747	0.6369E+03
0.98	686.0	1.2747	0.6369E+03
0.99	693.0	1.2747	0.6369E+03
1.00	700.0	1.2747	0.6369E+03

HYDROGEN PROFILE IN REACTOR # 1
(GAS PHASE)

DISTANCE ALONG REACTOR		HYDROGEN CONCENTRATION	
DIMENSIONLESS	CENTIMETERS	DIMENSIONLESS	GM/CM**3
0.00	0.0	0.8721	0.3985E-02
0.01	7.0	0.8105	0.3704E-02
0.02	14.0	0.7560	0.3455E-02
0.03	21.0	0.7076	0.3234E-02
0.04	28.0	0.6644	0.3037E-02
0.05	35.0	0.6258	0.2860E-02
0.06	42.0	0.5911	0.2701E-02
0.07	49.0	0.5598	0.2558E-02
0.08	56.0	0.5314	0.2429E-02
0.09	63.0	0.5056	0.2311E-02
0.10	70.0	0.4820	0.2203E-02
0.11	77.0	0.4603	0.2104E-02
0.12	84.0	0.4403	0.2012E-02
0.13	91.0	0.4218	0.1928E-02
0.14	98.0	0.4046	0.1849E-02
0.15	105.0	0.3886	0.1776E-02
0.16	112.0	0.3736	0.1707E-02
0.17	119.0	0.3595	0.1643E-02
0.18	126.0	0.3462	0.1582E-02
0.19	133.0	0.3336	0.1525E-02
0.20	140.0	0.3217	0.1470E-02
0.21	147.0	0.3103	0.1418E-02
0.22	154.0	0.2995	0.1369E-02
0.23	161.0	0.2892	0.1322E-02
0.24	168.0	0.2794	0.1277E-02
0.25	175.0	0.2700	0.1234E-02
0.26	182.0	0.2609	0.1192E-02
0.27	189.0	0.2522	0.1153E-02
0.28	196.0	0.2438	0.1114E-02
0.29	203.0	0.2358	0.1078E-02
0.30	210.0	0.2280	0.1042E-02
0.31	217.0	0.2205	0.1008E-02
0.32	224.0	0.2133	0.9749E-03
0.33	231.0	0.2063	0.9430E-03
0.34	238.0	0.1996	0.9122E-03

0.35	245.0	0.1931	0.8825E-03
0.36	252.0	0.1868	0.8537E-03
0.37	259.0	0.1807	0.8259E-03
0.38	266.0	0.1748	0.7990E-03
0.39	273.0	0.1691	0.7729E-03
0.40	280.0	0.1636	0.7478E-03
0.41	287.0	0.1583	0.7234E-03
0.42	294.0	0.1531	0.6998E-03
0.43	301.0	0.1481	0.6769E-03
0.44	308.0	0.1433	0.6548E-03
0.45	315.0	0.1386	0.6334E-03
0.46	322.0	0.1341	0.6127E-03
0.47	329.0	0.1297	0.5926E-03
0.48	336.0	0.1254	0.5732E-03
0.49	343.0	0.1213	0.5544E-03
0.50	350.0	0.1173	0.5363E-03
0.51	357.0	0.1135	0.5187E-03
0.52	364.0	0.1098	0.5016E-03
0.53	371.0	0.1062	0.4851E-03
0.54	378.0	0.1027	0.4692E-03
0.55	385.0	0.0993	0.4538E-03
0.56	392.0	0.0960	0.4388E-03
0.57	399.0	0.0929	0.4244E-03
0.58	406.0	0.0898	0.4104E-03
0.59	413.0	0.0869	0.3969E-03
0.60	420.0	0.0840	0.3839E-03
0.61	427.0	0.0812	0.3713E-03
0.62	434.0	0.0786	0.3591E-03
0.63	441.0	0.0760	0.3473E-03
0.64	448.0	0.0735	0.3359E-03
0.65	455.0	0.0711	0.3249E-03
0.66	462.0	0.0688	0.3142E-03
0.67	469.0	0.0665	0.3040E-03
0.68	476.0	0.0643	0.2940E-03
0.69	483.0	0.0622	0.2845E-03
0.70	490.0	0.0602	0.2752E-03
0.71	497.0	0.0583	0.2663E-03
0.72	504.0	0.0564	0.2577E-03
0.73	511.0	0.0546	0.2495E-03
0.74	518.0	0.0528	0.2415E-03
0.75	525.0	0.0512	0.2338E-03
0.76	532.0	0.0495	0.2264E-03
0.77	539.0	0.0480	0.2193E-03

0.78	546.0	0.0465	0.2124E-03
0.79	553.0	0.0450	0.2058E-03
0.80	560.0	0.0436	0.1995E-03
0.81	567.0	0.0423	0.1934E-03
0.82	574.0	0.0410	0.1876E-03
0.83	581.0	0.0398	0.1820E-03
0.84	588.0	0.0387	0.1766E-03
0.85	595.0	0.0375	0.1715E-03
0.86	602.0	0.0365	0.1667E-03
0.87	609.0	0.0355	0.1620E-03
0.88	616.0	0.0345	0.1576E-03
0.89	623.0	0.0336	0.1534E-03
0.90	630.0	0.0327	0.1494E-03
0.91	637.0	0.0319	0.1456E-03
0.92	644.0	0.0311	0.1421E-03
0.93	651.0	0.0304	0.1387E-03
0.94	658.0	0.0297	0.1356E-03
0.95	665.0	0.0290	0.1327E-03
0.96	672.0	0.0285	0.1300E-03
0.97	679.0	0.0279	0.1275E-03
0.98	686.0	0.0274	0.1253E-03
0.99	693.0	0.0270	0.1232E-03
1.00	700.0	0.0266	0.1214E-03

HYDROGEN PROFILE IN REACTOR # 1
(LIQUID PHASE)

DISTANCE ALONG REACTOR		HYDROGEN CONCENTRATION	
DIMENSIONLESS	CENTIMETERS	DIMENSIONLESS	GM/CM**3
0.00	0.0	0.6266	0.1300E-02
0.01	7.0	0.6222	0.1291E-02
0.02	14.0	0.6158	0.1277E-02
0.03	21.0	0.6078	0.1261E-02
0.04	28.0	0.5985	0.1242E-02
0.05	35.0	0.5882	0.1220E-02
0.06	42.0	0.5770	0.1197E-02
0.07	49.0	0.5652	0.1172E-02
0.08	56.0	0.5529	0.1147E-02
0.09	63.0	0.5403	0.1121E-02
0.10	70.0	0.5273	0.1094E-02
0.11	77.0	0.5143	0.1067E-02
0.12	84.0	0.5011	0.1039E-02
0.13	91.0	0.4879	0.1012E-02
0.14	98.0	0.4748	0.9849E-03
0.15	105.0	0.4618	0.9578E-03
0.16	112.0	0.4488	0.9310E-03
0.17	119.0	0.4361	0.9046E-03
0.18	126.0	0.4235	0.8785E-03
0.19	133.0	0.4112	0.8528E-03
0.20	140.0	0.3990	0.8277E-03
0.21	147.0	0.3871	0.8030E-03
0.22	154.0	0.3755	0.7788E-03
0.23	161.0	0.3641	0.7552E-03
0.24	168.0	0.3529	0.7321E-03
0.25	175.0	0.3421	0.7096E-03
0.26	182.0	0.3315	0.6876E-03
0.27	189.0	0.3212	0.6662E-03
0.28	196.0	0.3111	0.6453E-03
0.29	203.0	0.3013	0.6250E-03
0.30	210.0	0.2918	0.6053E-03
0.31	217.0	0.2826	0.5861E-03
0.32	224.0	0.2736	0.5674E-03
0.33	231.0	0.2648	0.5493E-03
0.34	238.0	0.2563	0.5317E-03

0.35	245.0	0.2481	0.5146E-03
0.36	252.0	0.2401	0.4980E-03
0.37	259.0	0.2323	0.4820E-03
0.38	266.0	0.2248	0.4663E-03
0.39	273.0	0.2175	0.4512E-03
0.40	280.0	0.2105	0.4365E-03
0.41	287.0	0.2036	0.4223E-03
0.42	294.0	0.1970	0.4085E-03
0.43	301.0	0.1905	0.3952E-03
0.44	308.0	0.1843	0.3823E-03
0.45	315.0	0.1782	0.3697E-03
0.46	322.0	0.1724	0.3576E-03
0.47	329.0	0.1667	0.3459E-03
0.48	336.0	0.1613	0.3345E-03
0.49	343.0	0.1560	0.3235E-03
0.50	350.0	0.1508	0.3129E-03
0.51	357.0	0.1459	0.3026E-03
0.52	364.0	0.1411	0.2926E-03
0.53	371.0	0.1364	0.2830E-03
0.54	378.0	0.1319	0.2737E-03
0.55	385.0	0.1276	0.2647E-03
0.56	392.0	0.1234	0.2560E-03
0.57	399.0	0.1194	0.2476E-03
0.58	406.0	0.1154	0.2395E-03
0.59	413.0	0.1117	0.2316E-03
0.60	420.0	0.1080	0.2240E-03
0.61	427.0	0.1045	0.2167E-03
0.62	434.0	0.1011	0.2097E-03
0.63	441.0	0.0978	0.2028E-03
0.64	448.0	0.0946	0.1963E-03
0.65	455.0	0.0916	0.1899E-03
0.66	462.0	0.0886	0.1838E-03
0.67	469.0	0.0858	0.1779E-03
0.68	476.0	0.0830	0.1723E-03
0.69	483.0	0.0804	0.1668E-03
0.70	490.0	0.0779	0.1615E-03
0.71	497.0	0.0754	0.1565E-03
0.72	504.0	0.0731	0.1516E-03
0.73	511.0	0.0709	0.1470E-03
0.74	518.0	0.0687	0.1425E-03
0.75	525.0	0.0666	0.1382E-03
0.76	532.0	0.0646	0.1341E-03
0.77	539.0	0.0627	0.1301E-03

0.78	546.0	0.0609	0.1264E-03
0.79	553.0	0.0592	0.1228E-03
0.80	560.0	0.0575	0.1193E-03
0.81	567.0	0.0560	0.1161E-03
0.82	574.0	0.0545	0.1130E-03
0.83	581.0	0.0531	0.1100E-03
0.84	588.0	0.0517	0.1073E-03
0.85	595.0	0.0505	0.1046E-03
0.86	602.0	0.0493	0.1022E-03
0.87	609.0	0.0482	0.9989E-04
0.88	616.0	0.0471	0.9775E-04
0.89	623.0	0.0462	0.9577E-04
0.90	630.0	0.0453	0.9395E-04
0.91	637.0	0.0445	0.9229E-04
0.92	644.0	0.0438	0.9079E-04
0.93	651.0	0.0431	0.8945E-04
0.94	658.0	0.0426	0.8828E-04
0.95	665.0	0.0421	0.8728E-04
0.96	672.0	0.0417	0.8645E-04
0.97	679.0	0.0414	0.8580E-04
0.98	686.0	0.0411	0.8533E-04
0.99	693.0	0.0410	0.8504E-04
1.00	700.0	0.0410	0.8495E-04

CONCENTRATION PROFILE IN REACTOR # 1

DISTANCE ALONG REACTOR		CHEMICAL SPECIES		
DIMENSIONLESS	CENTIMETERS	1	2	3
0.00	0.0	.961E-01	.482E-01	.856E+00
0.01	7.0	.919E-01	.483E-01	.860E+00
0.02	14.0	.879E-01	.482E-01	.864E+00
0.03	21.0	.841E-01	.481E-01	.868E+00
0.04	28.0	.804E-01	.479E-01	.872E+00
0.05	35.0	.769E-01	.477E-01	.875E+00
0.06	42.0	.735E-01	.473E-01	.879E+00
0.07	49.0	.703E-01	.469E-01	.883E+00
0.08	56.0	.672E-01	.465E-01	.886E+00
0.09	63.0	.643E-01	.460E-01	.890E+00
0.10	70.0	.615E-01	.454E-01	.893E+00
0.11	77.0	.588E-01	.448E-01	.896E+00
0.12	84.0	.562E-01	.442E-01	.900E+00
0.13	91.0	.538E-01	.435E-01	.903E+00
0.14	98.0	.514E-01	.429E-01	.906E+00
0.15	105.0	.492E-01	.422E-01	.909E+00
0.16	112.0	.470E-01	.414E-01	.912E+00
0.17	119.0	.450E-01	.407E-01	.914E+00
0.18	126.0	.430E-01	.399E-01	.917E+00
0.19	133.0	.411E-01	.392E-01	.920E+00
0.20	140.0	.393E-01	.384E-01	.922E+00
0.21	147.0	.376E-01	.376E-01	.925E+00
0.22	154.0	.360E-01	.368E-01	.927E+00
0.23	161.0	.344E-01	.361E-01	.930E+00
0.24	168.0	.329E-01	.353E-01	.932E+00
0.25	175.0	.315E-01	.345E-01	.934E+00
0.26	182.0	.301E-01	.337E-01	.936E+00
0.27	189.0	.288E-01	.329E-01	.938E+00
0.28	196.0	.275E-01	.321E-01	.940E+00
0.29	203.0	.263E-01	.314E-01	.942E+00
0.30	210.0	.252E-01	.306E-01	.944E+00
0.31	217.0	.241E-01	.299E-01	.946E+00
0.32	224.0	.230E-01	.291E-01	.948E+00
0.33	231.0	.220E-01	.284E-01	.950E+00
0.34	238.0	.211E-01	.276E-01	.951E+00
0.35	245.0	.202E-01	.269E-01	.953E+00

0.36	252.0	.193E-01	.262E-01	.954E+00
0.37	259.0	.184E-01	.255E-01	.956E+00
0.38	266.0	.176E-01	.248E-01	.958E+00
0.39	273.0	.169E-01	.242E-01	.959E+00
0.40	280.0	.161E-01	.235E-01	.960E+00
0.41	287.0	.154E-01	.229E-01	.962E+00
0.42	294.0	.148E-01	.223E-01	.963E+00
0.43	301.0	.141E-01	.216E-01	.964E+00
0.44	308.0	.135E-01	.210E-01	.965E+00
0.45	315.0	.129E-01	.204E-01	.967E+00
0.46	322.0	.124E-01	.199E-01	.968E+00
0.47	329.0	.118E-01	.193E-01	.969E+00
0.48	336.0	.113E-01	.188E-01	.970E+00
0.49	343.0	.108E-01	.182E-01	.971E+00
0.50	350.0	.104E-01	.177E-01	.972E+00
0.51	357.0	.994E-02	.172E-01	.973E+00
0.52	364.0	.951E-02	.167E-01	.974E+00
0.53	371.0	.911E-02	.162E-01	.975E+00
0.54	378.0	.872E-02	.157E-01	.976E+00
0.55	385.0	.835E-02	.153E-01	.976E+00
0.56	392.0	.799E-02	.148E-01	.977E+00
0.57	399.0	.766E-02	.144E-01	.978E+00
0.58	406.0	.733E-02	.140E-01	.979E+00
0.59	413.0	.703E-02	.136E-01	.979E+00
0.60	420.0	.673E-02	.132E-01	.980E+00
0.61	427.0	.645E-02	.128E-01	.981E+00
0.62	434.0	.619E-02	.125E-01	.981E+00
0.63	441.0	.593E-02	.121E-01	.982E+00
0.64	448.0	.569E-02	.118E-01	.983E+00
0.65	455.0	.546E-02	.114E-01	.983E+00
0.66	462.0	.524E-02	.111E-01	.984E+00
0.67	469.0	.503E-02	.108E-01	.984E+00
0.68	476.0	.483E-02	.105E-01	.985E+00
0.69	483.0	.464E-02	.102E-01	.985E+00
0.70	490.0	.446E-02	.995E-02	.986E+00
0.71	497.0	.429E-02	.969E-02	.986E+00
0.72	504.0	.413E-02	.943E-02	.986E+00
0.73	511.0	.397E-02	.919E-02	.987E+00
0.74	518.0	.383E-02	.896E-02	.987E+00
0.75	525.0	.369E-02	.873E-02	.988E+00
0.76	532.0	.356E-02	.852E-02	.988E+00
0.77	539.0	.343E-02	.832E-02	.988E+00
0.78	546.0	.332E-02	.813E-02	.989E+00

0.79	553.0	.321E-02	.794E-02	.989E+00
0.80	560.0	.310E-02	.777E-02	.989E+00
0.81	567.0	.301E-02	.761E-02	.989E+00
0.82	574.0	.292E-02	.745E-02	.990E+00
0.83	581.0	.283E-02	.731E-02	.990E+00
0.84	588.0	.275E-02	.717E-02	.990E+00
0.85	595.0	.268E-02	.704E-02	.990E+00
0.86	602.0	.261E-02	.693E-02	.990E+00
0.87	609.0	.255E-02	.682E-02	.991E+00
0.88	616.0	.249E-02	.672E-02	.991E+00
0.89	623.0	.244E-02	.663E-02	.991E+00
0.90	630.0	.239E-02	.654E-02	.991E+00
0.91	637.0	.235E-02	.647E-02	.991E+00
0.92	644.0	.232E-02	.640E-02	.991E+00
0.93	651.0	.228E-02	.635E-02	.991E+00
0.94	658.0	.226E-02	.630E-02	.991E+00
0.95	665.0	.224E-02	.626E-02	.992E+00
0.96	672.0	.222E-02	.623E-02	.992E+00
0.97	679.0	.221E-02	.621E-02	.992E+00
0.98	686.0	.220E-02	.619E-02	.992E+00
0.99	693.0	.220E-02	.619E-02	.992E+00
1.00	700.0	.220E-02	.619E-02	.992E+00

RESULTS OF PARAMETER ESTIMATION

1. ISOTHERMAL CASE:

SIM.FOR GAVE THE FOLLOWING VALUES OF OUTPUT CONCENTRATION

$$C_1 = 0.02067$$

$$C_2 = 0.0217$$

$$C_3 = 0.9567$$

PARAMETER ESTIMATION GAVE THESE RESULTS FOR KINETIC PARAMETERS

$$k_1 = 30.187 \quad E_1 = 12,500.$$

$$k_2 = 29.497 \quad E_2 = 12,501.$$

FUNCTION VALUE AND OUTPUT CONCENTRATIONS FROM FIT.FOR

$$C_1 = 0.02147$$

$$C_2 = 0.02152$$

$$C_3 = 0.957$$

$$FMIN = .77E-06$$

2. NON-ISOTHERMAL CASE:

SIM.FOR GAVE THE FOLLOWING VALUES OF OUTPUT CONCENTRATION

$$C_1 = .002475$$

$$C_2 = .006843$$

$$C_3 = .9907$$

PARAMETER ESTIMATION GAVE THESE RESULTS FOR KINETIC PARAMETERS

$$k_1 = 20.018 \quad E_1 = 12,500.$$

$$k_2 = 17.666 \quad E_2 = 12,500.$$

FUNCTION VALUE AND OUTPUT CONCENTRATIONS FROM FIT.FOR

$$C_1 = .001866$$

$$C_2 = .007214$$

$$C_3 = .99092$$

$$FMIN = 5.57E-07$$

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