ChE 344
Chemical Reaction Engineering
Winter 2000

Exam II

Computer Portion

Name ______ SOLUTION ________________________________

Honor Code ____

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Signed ______________________________

1) ____ / 25 pts

2) ____ / 25 pts

3) ____ / 50 pts

Total 100 pts

NOTE: Store your problem immediately after typing in the program and before typing F7.

Saving While in POLYMATH:

Anytime after you enter your equations you may save them by hitting "shift-F8" from the equations screen. This will take you to a menu where you may type "S" to save your problem. When you type "S" you will be asked for a directory. Enter "A:". Then you will be asked for a filename. Type in the problem number (e.g. Pb3). Be careful not to save over previous work (like accidentally saving problem 3 material over problem 2 material by using the same name). Once the file is saved, you can go back to working on your problem.

The option to do this will be listed on your screen. The procedure for loading saved problems is similar, you just type "L" rather than "S" at the appropriate step.

Note: At the end of the exam, after saving all your files to a disk, delete all your problems from the library.

(25%) 1) Let's go back to Problem 8-30 once more. Ethyl-benzene is fed at a rate (in the problem statement) of 0.00344 kmol/s. The inlet steam to EB ratio is 14.5 to 1. The inlet temperature is To = 900 K. All parameter values are the same as given in the problem. However, we now want to operate the reactor **isothermally**.

a) What is the required heat exchanger duty (in Watts, i.e. J/s) to achieve isothermal operation? Explain your result.
b) Now, say the inlet temperature is 500 K. How does the required heat exchanger duty change? How is it different from the previous case **qualitatively**? Explain your result.

[Hint: only two-three lines of Polymath code change/addition maybe required to answer part (a)]

Isothermal Operation of PFR:

Isothermal $\frac{dT}{dV} = 0$

$$\frac{dT}{dV} = \frac{Q + \sum \Delta H_{ij} r_{ij}}{\sum F_i C_{Pi}} = 0 \text{ where } Q = Ua(T_a - T)$$

$$|Q| = \left|\sum \Delta H_{ij} r_{ij}\right|$$

Below are the results and Polymath code

POLYMATH 5.0 Results

PROBLEM 1:

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
v	0	0	10	10
fb	0	0	0.0023026	0.0023019
fa	0.00344	5.348E-04	0.00344	5.348E-04
fc	0	0	0.0020592	0.0020335
fd	0	0	3.348E-04	3.348E-04
fe	0	0	3.348E-04	3.348E-04
ff	0	0	2.685E-04	2.685E-04
fg	0	0	2.685E-04	2.685E-04
T	900	900	900	900
sr	14.5	14.5	14.5	14.5
H1a	1.18E+05	1.18E+05	1.18E+05	1.18E+05
H2a	1.052E+05	1.052E+05	1.052E+05	1.052E+05
H3a	-5.39E+04	-5.39E+04	-5.39E+04	-5.39E+04
p	2137	2137	2137	2137
phi	0.4	0.4	0.4	0.4
K1	0.3679746	0.3679746	0.3679746	0.3679746
fi	0.04988	0.04988	0.04988	0.04988
ft	0.05332	0.05332	0.0559568	0.0559568
Pc	0	0	0.0883967	0.0872159
Pa	0.1548387	0.0229362	0.1548387	0.0229362
Pb	0	0	0.0987702	0.0987311
r1s	9.748E-04	-2.925E-06	9.748E-04	-2.925E-06
r2b	9.634E-05	1.427E-05	9.634E-05	1.427E-05
rd	9.634E-05	1.427E-05	9.634E-05	1.427E-05
re	9.634E-05	1.427E-05	9.634E-05	1.427E-05
r3t	0	0	3.994E-05	1.697E-05
rf	0	0	3.994E-05	1.697E-05
rg	0	0	3.994E-05	1.697E-05
Qa	125.15695	0.24158	125.15695	0.24158
rb	9.748E-04	-2.925E-06	9.748E-04	-2.925E-06
rc	9.748E-04	-1.989E-05	9.748E-04	-1.989E-05
ra	-0.0010711	-0.0010711	-2.831E-05	-2.831E-05

ODE Report (RKF45)

Differential equations as entered by the user

```
[1]  d(fb)/d(v) = rb
[2]  d(fa)/d(v) = ra
[3]  d(fc)/d(v) = rc
[4]  d(fd)/d(v) = rd
[5]  d(fe)/d(v) = re
[6]  d(ff)/d(v) = rf
[7]  d(fg)/d(v) = rg
```

Explicit equations as entered by the user

```
[1]  T = 900
[2]  sr = 14.5
[3]  H1a = 118000
[4]  H2a = 105200
[5]  H3a = -53900
[6]  p = 2137
[7]  phi = .4
[8]  K1 = exp(-17.34-1.302e4/T+5.051*ln(T)+((-2.314e-10*T+1.302e-6)*T-4.931e-3)*T)
[9]  fi = sr*.00344
[10] ft = fa+fb+fc+fd+fe+ff+fg+fi
[11] Pc = fc/ft*2.4
[12] Pa = fa/ft*2.4
[13] Pb = fb/ft*2.4
[14] r1s = p*(1-phi)*exp(-.08539-10925/T)*(Pa-Pb*Pc/K1)
[15] r2b = p*(1-phi)*exp(13.2392-25000/T)*Pa
[16] rd = r2b
[17] re = r2b
[18] r3t = p*(1-phi)*exp(.2961-11000/T)*Pa*Pc
[19] rf = r3t
[20] rg = r3t
[21] Qa = (r1s*H1a+r2b*H2a+r3t*H3a)
[22] rb = r1s
[23] rc = r1s-r3t
[24] ra = -r1s-r2b-r3t
```

Independent variable
variable name : v
initial value : 0
final value : 10

Precision
Step size guess. h = 0.000001
Truncation error tolerance. eps = 0.000001

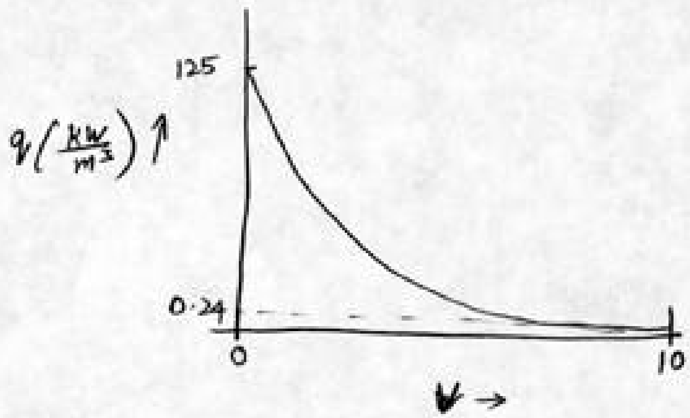
General
number of differential equations: 7
number of explicit equations: 24

Note:

we're eliminating the $\frac{dT}{dV}$ equation - so we're actually cutting down the number of variables.

Thus, there is no way POLYMATH will give errors of "too many variables", if the initial program was running okay.

As seen, we require a profile like this:



Why? The reaction rates are high at the inlet – so more heat is consumed, hence more needs to be put in. Then as the reaction rates die down, we need to put in less heat.

Is this possible? Yes, if we operate the coolant co-currently with sufficiently small flow rates, this can, theoretically, be achieved.

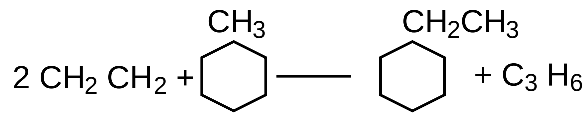
(b.) T_0=500 K

Now, the heat exchanger duty is much lower – also the percentage change along the length of the reactor is small.

Why? Because, at this temperature, reaction rates are so small, and practically no reaction occurs.

(25%) 2)The following elementary reaction was <u>also</u> found to occur in the production of styrene (P8-30).

$$\text{(4)}\quad 2\ \text{ethylene} + \text{toluene} \longrightarrow \text{ethylbenzene} + \text{propylene}$$

(4) 

Plot the exit temperature and exiting molar flow rates of ethylbenzene, styrene, toluene and benzene as a function of entering temperature from 900 K to 1100 K and compare your results with the case from the homework when the fourth reaction did not take place.

$$\Delta H_{Rx4T} = -30{,}000\ \text{kJ/kmole toluene}$$

$$\text{Heat capacity of propylene} = 120\ \text{J/mole K}$$

$$-r_{4T} = \rho(1-\varphi)\ \exp\left[10.4 - \frac{12000\text{K}}{T}\right] P_{C_2H_4} P_T \ \text{ in kmol toluene}/\text{m}^3 \cdot \text{s}$$

Just add another reaction. Modify the reaction rates of EB, Toluene, and Ethylene. Modify the dT/dV equation and F_{total}. See program and results below.

POLYMATH 5.0 Results

Problem 2

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
v	0	0	10	10
fb	0	0	0.0025208	0.0025208
fa	0.00344	3.142E-04	0.00344	3.142E-04
fc	0	0	0.002469	0.002469
fd	0	0	1.857E-06	1.124E-06
fe	0	0	0.0011051	0.0011051
ff	0	-5.002E-04	0	-5.002E-04
fg	0	0	5.186E-05	5.186E-05
fh	0	0	5.52E-04	5.52E-04
T	1015	970.89363	1015	970.89363
H1a	1.18E+05	1.18E+05	1.18E+05	1.18E+05
H2a	1.052E+05	1.052E+05	1.052E+05	1.052E+05
H3a	-5.39E+04	-5.39E+04	-5.39E+04	-5.39E+04
H4t	-3.0E+04	-3.0E+04	-3.0E+04	-3.0E+04
p	2137	2137	2137	2137
phi	0.4	0.4	0.4	0.4
K1	2.4427051	1.245584	2.4427051	1.245584
sr	58	58	58	58
fi	0.19952	0.19952	0.19952	0.19952
ft	0.20296	0.20296	0.206034	0.206034
Pa	0.040678	0.0036597	0.040678	0.0036597
Pb	0	0	0.029364	0.029364
Pc	0	0	0.0287599	0.0287599
Pd	0	0	2.194E-05	1.31E-05
r1s	0.0010132	4.554E-05	0.0010132	4.554E-05
r2b	5.89E-04	1.731E-05	5.89E-04	1.731E-05
r3t	0	0	8.427E-06	2.179E-06
r4t	0	0	2.32E-04	8.66E-06
rd	5.89E-04	-3.661E-07	5.89E-04	-1.164E-08
re	5.89E-04	1.731E-05	5.89E-04	1.731E-05
rf	0	-2.282E-04	0	-6.481E-06
rg	0	0	8.427E-06	2.179E-06
rb	0.0010132	4.554E-05	0.0010132	4.554E-05
rc	0.0010132	4.336E-05	0.0010132	4.336E-05
ra	-0.0016022	-0.0016022	-5.637E-05	-5.637E-05
rh	0	0	2.32E-04	8.66E-06

ODE Report (RKF45)

Differential equations as entered by the user

```
[1] d(fb)/d(v) = rb
[2] d(fa)/d(v) = ra
[3] d(fc)/d(v) = rc
[4] d(fd)/d(v) = rd
[5] d(fe)/d(v) = re
[6] d(ff)/d(v) = rf
[7] d(fg)/d(v) = rg
[8] d(fh)/d(v) = rh
[9] d(T)/d(v) = -
(r1s*H1a+r2b*H2a+r3t*H3a+r4t*H4t)/(fa*299+fb*273+fc*30+fd*201+fe*90+ff*249+fg*68+fh*120+fi*40)
```

Explicit equations as entered by the user

```
[1] H1a = 118000
[2] H2a = 105200
[3] H3a = -53900
[4] H4t = -30000
[5] p = 2137
[6] phi = .4
[7] K1 = exp(-17.34-1.302e4/T+5.051*ln(T)+((-2.314e-10*T+1.302e-6)*T-4.931e-3)*T)
[8] sr = 58
[9] fi = sr*.00344
[10] ft = fa+fb+fc+fd+fe+ff+fg+fh+fi
[11] Pa = fa/ft*2.4
[12] Pb = fb/ft*2.4
[13] Pc = fc/ft*2.4
[14] Pd = fd/ft*2.4
[15] r1s = p*(1-phi)*exp(-.08539-10925/T)*(Pa-Pb*Pc/K1)
[16] r2b = p*(1-phi)*exp(13.2392-25000/T)*Pa
[17] r3t = p*(1-phi)*exp(.2961-11000/T)*Pa*Pc
[18] r4t = p*(1-phi)*exp(10.4-12000/T)*Pd*Pa
[19] rd = r2b-2*r4t
[20] re = r2b
[21] rf = r3t-r4t
[22] rg = r3t
[23] rb = r1s
[24] rc = r1s-r3t
[25] ra = -r1s-r2b-r3t+r4t
[26] rh = r4t
```

Independent variable
variable name : v
initial value : 0
final value : 10

Precision
Step size guess. h = 0.000001
Truncation error tolerance. eps = 0.000001

General
number of differential equations: 9
number of explicit equations: 26

Here, Polymath CAN cause problems of "too many variables". Just have to be careful to put in numerical values of constants, instead of defining it by some variable name.

(50%) 3)Study Problem 8-9 revisited. The formation of styrene from vinylacetylene is essentially irreversible and follows an elementary rate law:

$$2A \longrightarrow B$$

a) Determine the conversion achieved in a 5 dm^3 PFR for an entering temperature of 675 K. Plot the temperature and conversion down the length (volume) of the reactor.

b) Vary the entering temperature and plot the conversion as a function of entering temperature.

All other conditions of P8-9 remain the same.

$2A \rightarrow B$

It is a gas phase reaction, but no points were deducted if assumed liquid phase

All further calculations assume gas phase

Mole Balance: $\frac{dX}{dV} = \frac{-r_A}{F_{Ao}}$

Rate Law : $-r_A = -kC_A^2$

Stoichiometry: $C_A = \frac{C_{Ao}(1-X)}{(1+\varepsilon X)}$

where $= y_{Ao}\delta = 1*(0.5-1) = -0.5$

Energy Equation : $\frac{dT}{dV} = \frac{Ua(T_a - T) + (-r_A)(-\Delta H_{rx})}{\sum F_i C_{Pi}}$

$C_{PA} = 0.12222$ kJ/mol K

$\Delta H_{rx} = -231-0.012(T-298)$

$\Delta C_P = -0.012$

$C_{PB} = C_{PA} + \Delta C_P$

Note : ΔC_P is an order of magnitude lower than C_{PA}

Therefore, $C_{PA} \quad C_{PB}$

Hence, $\sum F_i C_{Pi} = F_A C_{PA} + F_B C_{PB} \quad F_{Ao} C_{PA}$ (as used in the code below)

Or $\sum F_i C_{Pi} = F_{Ao}\left(\sum \Theta_i C_{Pi} + \Delta C_P X\right) = F_{Ao}\left(F_{Ao} C_{Pi} + \Delta C_P X\right)$

POLYMATH 5.0 Results

Prob 3: Version 2 04-12-2000

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
v	0	0	5	5
x	0	0	0.2394186	0.2394186
T	675	675	713.63314	709.32955
cao	1	1	1	1
To	675	675	675	675
Ua	5	5	5	5
k	0.0734336	0.0734336	0.3402318	0.2893287
dH	-235.524	-235.98743	-235.524	-235.93595
Ta	700	700	700	700
fao	5	5	5	5
cpa	0.1222	0.1222	0.1222	0.1222
ca	1	0.8221959	1	0.8221959
ra	-0.0734336	-0.2905362	-0.0734336	-0.1955879

ODE Report (RKF45)

Differential equations as entered by the user
[1] d(x)/d(v) = -ra/fao
[2] d(T)/d(v) = (Ua*(Ta-T)+(-ra)*(-dH))/(fao*cpa)

Explicit equations as entered by the user
[1] cao = 1
[2] To = 675
[3] Ua = 5
[4] k = 1.48e11*exp(-19124/T)
[5] dH = -231-.012*(T-298)
[6] Ta = 700
[7] fao = 5
[8] cpa = .1222
[9] ca = cao*(1-x)/(1-0.5*x)*(To/T)
[10] ra = -k*ca^2

Independent variable
variable name : v
initial value : 0
final value : 5

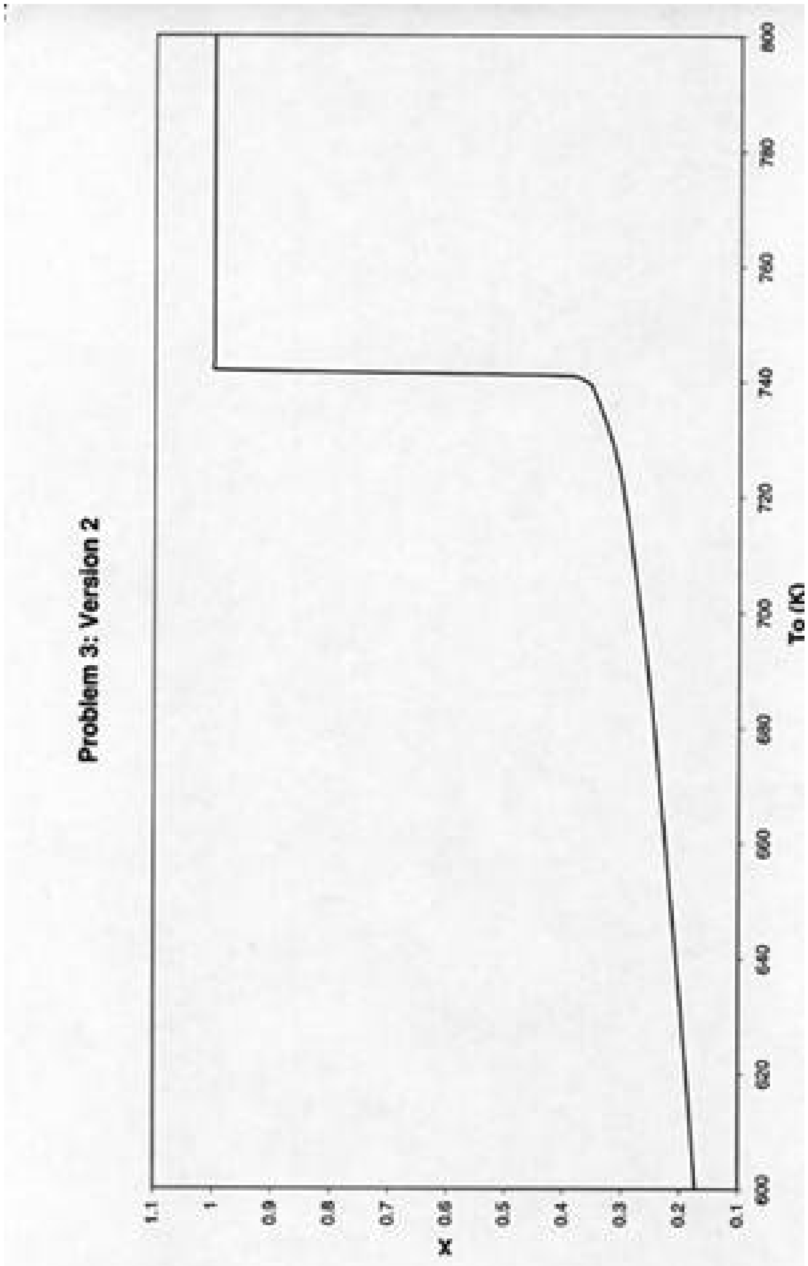
Precision
Step size guess. h = 0.000001
Truncation error tolerance. eps = 0.000001

General
number of differential equations: 2
number of explicit equations: 10
Elapsed time: 1.1574 sec
Data file: C:\WINNT\Profiles\Administrator\Desktop\ChE 344\Exam2\E2P3n.pol

VERSION 2 =>

(Ga)

To(K)	X
500	0.1103861
600	0.1729784
675	0.2394186
700	0.2683576
725	0.3062504
739	0.3521352
740	0.3630167
741	0.3895732
742	0.99999
743	0.9999919
750	0.9999945
800	0.9999968


Problem 3: Version 2
X
To (K)
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
600
620
640
660
680
700
720
740
760
780
800