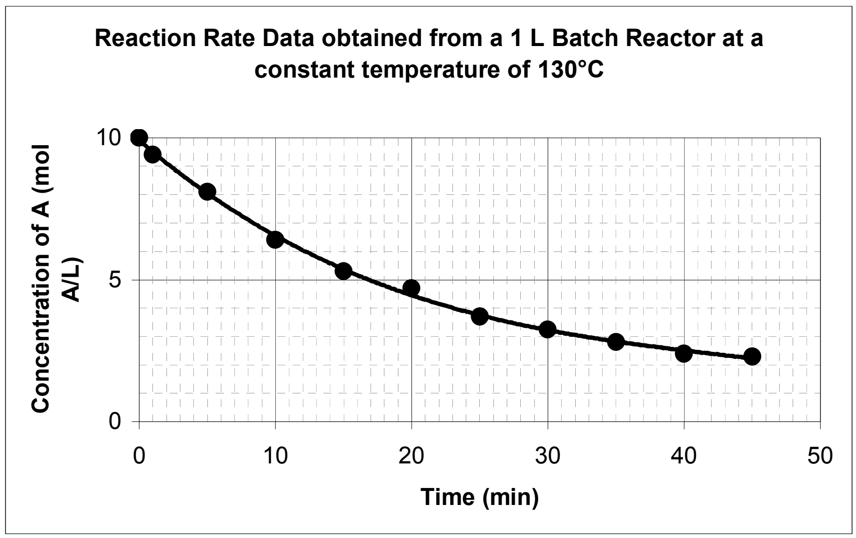
Exam 2
Chemical Reaction Engineering
2 April 2001
Closed Book and Notes

(30 pts) 1. You have been requested to troubleshoot problems with a well stirred reactor in your Texas chemical production plant. After taking the red eye flight and a long taxi ride to your hotel and then the plant your arrive exhausted, but eager to solve this problem. Apparently the problem with this 165 L reactor is that the conversion of the reactant, Anychemical, is too low at $X_A = 0.53$. This reactor is heated using steam and you measure the temperature of the liquid inside the reactor at 130°C. The initial concentration of Anychemical, A, is 10 mol A/L. The total flowrate of the liquid into the reactor is 5 L/min. You ask for reaction rate data, and are given the following table and graph from a 1 L batch reactor conducted at a temperature of 130°C.

t (min)	CA (mol A/L)
0	10
1	9.4
5	8.1
10	6.4
15	5.3
20	4.7
25	3.7
30	3.25
35	2.8
40	2.4
45	2.3



a) In your eagerness to work on your first reactor troubleshooting problem, you have left your laptop with your luggage at the hotel. The best calculator that the plant can find is a basic ACME calculator without a regression program or any plotting features. After your initial disappointment, you realize that the reactor is a CSTR and you should be able to compare the measured values with the rate data provided by the lab (given above). Determine if there is a problem with this reactor.

b) Based on the above answer give a recommendation for improving the conversion of Anychemical.

(30 pts) 2. The new products department has proposed a new chemical reaction to produce a chemical, Desiredchemical, D. This is a liquid phase reaction between Allchemical, A and Bestchemical, B. Unfortunately, undesired chemicals are also produced by this reaction, Undesiredone, U1, and Undesiredtoo, U2. The reaction scheme is given below:

$A + B \xrightarrow{k_{1A}} C + D$ where $r_{1A} = -k_{1A} C_A C_B \; [=] \; \frac{molA}{m^3 s}$

$A + 2C \xrightarrow{k_{2A}} U1 + U2$ where $r_{2A} = -k_{2A} C_A C_C^2 \; [=] \; \frac{molA}{m^3 s}$

where $k_{1A} = 2.1 \times 10^{-3} \frac{\mathrm{m}^3}{\mathrm{mol\,B\,s}} \exp\left(-\frac{3{,}300\ \mathrm{J/mol}}{RT}\right)$

and $k_{2A} = 1.1 \times 10^{-5} \frac{\mathrm{m}^6}{(\mathrm{mol\,C})^2\ \mathrm{s}} \exp\left(-\frac{5{,}200\ \mathrm{J/mol}}{RT}\right)$

a) Suggests operating conditions of concentration and temperature for these proposed reactions that would maximize the selectivity, $S = \frac{r_{\mathrm{Desired}}}{r_{\mathrm{Undesired}}}$.

b) Suggest the best reactor scheme that would maximize the selectivity for this proposed reaction network. Draw a graph of the expected concentrations as a function of reactor volume.

c) Explain the next steps that you would take to optimize this reactor configuration.

FIGURE 6-3: Different reactors and schemes for minimizing the unwanted product.

(40 pts) 3. Maleic anhydride (MA, $C_4H_2O_3$) was one of the products studied in a previous years reactor design project. One method to produce maleic anhydride is the partial oxidization of benzene (B, C_6H_6) with air. This gas phase reaction takes place in a tubular reactor with a solid vanadium pentoxide catalyst. Benzene enters the reactor at a molar flowrate of 26 mol/s and air at 1,555 mol/s. The feed temperature for this reaction is 848K and the pressure is at 5 atm. The following reactions are known to occur:

$$C_6H_6 + \frac{9}{2}O_2 \xrightarrow{k_1} C_4H_2O_3 + 2CO_2 + 2H_2O$$

$$C_4H_2O_3 + 3O_2 \xrightarrow{k_2} 4CO_2 + H_2O$$

$$C_6H_6 + \frac{15}{2}O_2 \xrightarrow{k_3} 6CO_2 + 3H_2O$$

The reaction rates are:

$$r_1 = -k_1 C_{C_6H_6} C_{O_2}$$

$$r_2 = -k_2 C_{C_4H_2O_3} C_{O_2}$$

$$r_3 = -k_3 C_{C_6H_6} C_{O_2}$$

with

$$k_1 = 0.0637\ \text{m}^6/(\text{mol O}_2\ \text{kgcat s})$$

$$k_2 = 0.0664\ \text{m}^6/(\text{mol O}_2\ \text{kgcat s})$$

$$k_3 = 0.00348\ \text{m}^6/(\text{mol O}_2\ \text{kgcat s})$$

Assuming that the tubular reactor contains 25 kg of catalyst and is isothermal and isobaric, construct a model of this reactor that will be used in a POLYMATH program. Your model should be able to predict the molar flowrate of each compound that enters or is produced in the reactor. Number each equation used in the POLYMATH program. Specify your initial conditions and final integration value.

Exam 2 Spring 2001 Solutions

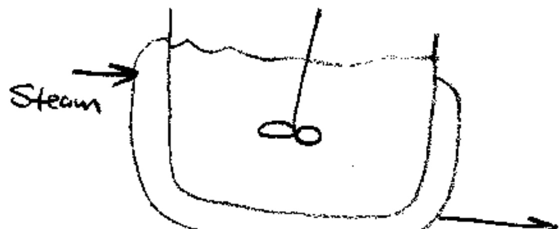
I $V = 170.3\ L$

$X_A = 0.53$

$T = 130°C$

$C_{A_0} = 10 \frac{mol\ A}{L}$

$\nu_0 = 5\ L/min$



mole balance

$$0 = F_{A0} - F_A + r_A V$$

$$X_A = \frac{F_{A0} - F_A}{F_{A0}}$$

$$0 = F_{A0} X_A + r_A V$$

$$r_A = \frac{-F_{A0} X_A}{V} = \frac{-\left(\frac{10\ mol\ A}{L}\right)(0.53)\ 5 \frac{L}{min}}{165\ L} = -0.161 \frac{mol\ A}{L\ s}$$

from graph at $X = 0.53$

$$F_A = F_{A0}(1 - X) = \frac{10\ mol}{L} \frac{5\ L}{min}(1 - 0.53) = 23.5 \frac{mol}{min}$$

$$C_A = \frac{F_A}{\nu} = \frac{23.5\ mol/min}{5\ L/min} = 4.7\ mol/L$$

4:20

USING GRAPH – the slope of the curve at $C_A = 4.7\ mol/L$ is

$$\frac{dC_A}{dt} = \frac{7.7 - 0}{0 - 47.7} = -0.161\ \frac{mol/L}{min}$$

7:22

Remember Batch Reactor $\frac{d\,C_A V}{dt} = r_A V$ const V $\boxed{\frac{dC_A}{dt} = r_A}$

Alternatively from rate data the expected conversion is:

$$X_A = \frac{-r_A V}{F_{A0}} = \frac{-(0.161\ \text{mol/L min})(165\ \text{L})}{10\ \frac{\text{mol A}}{\text{L}}\ \frac{5\ \text{L}}{\text{min}}} = 0.53$$

This reactor is working as expected

b) To increase conversion the reaction rate must be higher - see about increasing the reactor temperature.

8 min

2.

$$A + B \rightarrow C + D$$
$$A + 2C \rightarrow U1 + U2$$

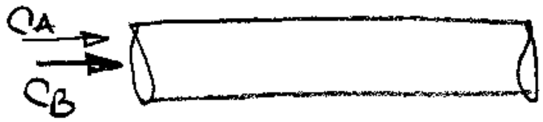
$$S = \frac{+\,2.1\times10^{-3}\, e^{\left(-\frac{3300}{RT}\right)} C_A C_B}{2.1\times10^{-4}\, \exp\left(-\frac{5200}{RT}\right) C_A C_C^2}$$

$$= 10 \exp\left[1{,}900/RT\right) \frac{C_B}{C_C^2}$$

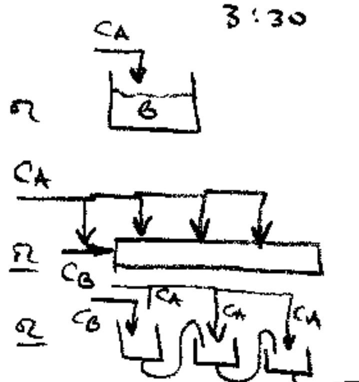
a) Conditions — T low; C_B high; C_C Low

3:30

b) Reactor operating conditions

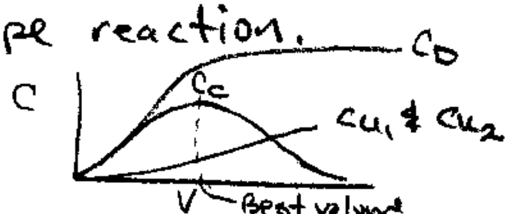


tubular



This appears to be the best reactor since this reaction appears to be primarily a series type reaction.

1:30



c) next steps

5min

- construct a model and determine the appropriate volume for this reaction.

3.5/

7min

3.

$F_{B_0} = 26$ mol/s benzene

$F_{A_0} = 1{,}555$ mol/s air

$T_0 = 848\text{K} = T$

$P_0 = 5$ atm $= P$

$W = 10$ kg

mole balances

① $\frac{dF_B}{dW} = r_B \; [=] \; \frac{\text{mol B}}{\text{s kgcat}}$ $r_1 = -0.0637 \frac{m^6}{\text{kgcat mol}\,O_2\,s}$ $\frac{\text{mol}\,O_2}{m^3}$ $\frac{\text{mol B}}{m^3}$

② $\frac{dF_O}{dW} = r_O$

③ $\frac{dF_{mA}}{dW} = r_{mA}$

④ $\frac{dF_{CO_2}}{dW} = r_{CO_2}$

⑤ $\frac{dF_W}{dW} = r_W$

⑥ $r_B = r_1 + r_3$

⑦ $r_O = r_1 \frac{9}{2} \frac{\text{mol}\,O_2}{\text{mol B}} + \frac{3\,\text{mol}\,O_2}{\text{mol MA}} r_2 + \frac{15}{2} \frac{\text{mol}\,O_2}{\text{mol B}} r_3$

⑧ $r_{MA} = -r_1 + r_2$

⑨ $r_{CO_2} = -\frac{2\,\text{mol}\,CO_2}{\text{mol B}} r_1 - \frac{4\,\text{mol}\,CO_2}{\text{mol MA}} r_2 - \frac{6\,\text{mol}\,CO_2}{\text{mol B}} r_3$

⑩ $r_W = -\frac{2\,\text{mol W}}{\text{mol B}} r_1 - \frac{1\,\text{mol W}}{1\,\text{mol MA}} r_2 - \frac{3\,\text{mol W}}{1\,\text{mol B}} r_3$ 8 min

(11) $C_B = \frac{F_B}{\upsilon}$

(12) $C_O = \frac{F_O}{\upsilon}$

(13) $C_{MA} = \frac{F_{MA}}{\upsilon}$

(14) $F_T = F_B + F_O + F_{MA} + F_{CO_2} + F_W + F_N$

$$\frac{P\upsilon}{P_O\upsilon_o} = \frac{F_T RT}{F_{T_O} RT_O}$$

(15) $\upsilon = \frac{F_T}{F_{TO}} \upsilon_o$

at $W = 0$ $F_B = 26 \text{ mol/s}$

$F_O = 0.21 (1,555 \text{ mol/s}) = 326.55$

$F_{MA} = F_{CO_2} = F_W = 0$

(21) $F_N = 0.79 (1555 \text{ mol/s})$

(16) $r_1 = -0.0637 \frac{m^6}{mol\, O_2\, kg cat\, s} C_B C_O$

(17) $r_2 = -0.0464 \frac{m^6}{mol\, O_2\, kg cat\, s} C_{MA} C_O$

(18) $r_3 = -0.00348 \frac{m^6}{mol\, O_2\, kg cat\, s} C_B C_O$

stop at $W = 10$ kg

12.5 min

(19) $\upsilon_o = \frac{\left(1,555 \frac{mol}{s}\right)\left(8.314 \frac{Pa\, m^3}{mol\, K}\right)(848 K)}{(5 atm)(1.01325 \times 10^5 \text{ Pa/atm})}$ $P\upsilon_o = F_{T_O} RT_O$

(20) $F_{TO} = 26 + 1555$

Exam 2:
Homework for a maximum of 10 points added to exam score
Chemical Reaction Engineering
Due: Tuesday 10 April 2001
OPEN Book and Notes

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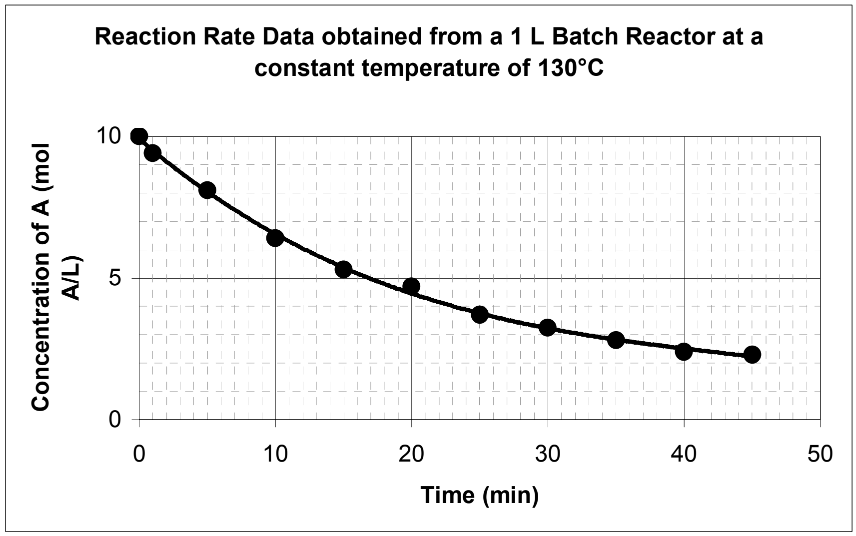


a) In your eagerness to work on your first reactor troubleshooting problem, you have left your laptop with your luggage at the hotel. The best calculator that the plant can find is a basic ACME calculator without a regression program or any plotting features. After your initial disappointment, you realize that the reactor is a CSTR and you should be able to compare the measured values with the rate data provided by the lab (given above). Determine if there is a problem with this reactor.
b) Based on the above answer give a recommendation for improving the conversion of Anychemical.
c) Using either Excel or POLYMATH, determine the reaction rate constant and order for this reaction.

(30 pts) 2. The new products department has proposed a new chemical reaction to produce a chemical, Desiredchemical, D. This is a liquid phase reaction between Allchemical, A and Bestchemical, B. The desired production rate of D is 8 mol/s. You have feed concentrations of both A and B available in the range of 1 to 40 mol/L. Unfortunately, undesired chemicals are also produced by this reaction, Undesiredone, U1, and Undesiredtoo, U2. The reaction scheme is given below:

$$A + B \xrightarrow{k_{1A}} C + D \qquad \text{where } r_{1A} = -k_{1A} C_A C_B \; [=] \; \frac{molA}{L\,s}$$

$$A + 2C \xrightarrow{k_{2A}} U1 + U2 \qquad \text{where } r_{2A} = -k_{2A} C_A C_C^2 \; [=] \; \frac{molA}{L\,s}$$

$$\text{where } k_{1A} = 2.1 \frac{\text{L}}{\text{mol B s}} \exp\left(-\frac{6{,}200 \text{ J/mol}}{RT}\right)$$

$$\text{and } k_{2A} = 1.1 \frac{\text{L}^2}{(\text{mol C})^2 \text{ s}} \exp\left(-\frac{7{,}000 \text{ J/mol}}{RT}\right)$$

a) Suggest general operating conditions of concentration and temperature for these proposed reactions that would maximize the selectivity, $S = \frac{r_{\text{Desired}}}{r_{\text{Undesired}}}$. (e.g. high or low)

b) Suggest the best reactor scheme that would maximize the selectivity for this proposed reaction network.

c) Develop a POLYMATH model for a single PFR. Make a plot selectivity as a function of of the molar feed ratio of A to B. Make a second plot of temperature as a function of selectivity for a given feed ratio of A to B.

d) Suggest a reactor volume, flowrate, and feed concentrations that you would recommend for this reaction to produce 8 mol/s of D.

(40 pts) 3. Maleic anhydride (MA, $C_4H_2O_3$) was one of the products studied in a previous years reactor design project. One method to produce maleic anhydride is the partial oxidization of benzene (B, C_6H_6) with air. This gas phase reaction takes place in a tubular reactor with a solid vanadium pentoxide catalyst. Benzene enters the reactor at a molar flowrate of 26 mol/s and air at 1,555 mol/s. The feed temperature for this reaction is 848K and the pressure is at 5 atm. The following reactions are known to occur:

$$\text{C}_6\text{H}_6 + \frac{9}{2}\text{O}_2 \xrightarrow{k_1} \text{C}_4\text{H}_2\text{O}_3 + 2\text{CO}_2 + 2\text{H}_2\text{O}$$

$$\text{C}_4\text{H}_2\text{O}_3 + 3\text{O}_2 \xrightarrow{k_2} 4\text{CO}_2 + \text{H}_2\text{O}$$

$$\text{C}_6\text{H}_6 + \frac{15}{2}\text{O}_2 \xrightarrow{k_3} 6\text{CO}_2 + 3\text{H}_2\text{O}$$

The reaction rates are:

$$r_1 = -k_1 C_{\text{C}_6\text{H}_6} C_{\text{O}_2}$$

$$r_2 = -k_2 C_{\text{C}_4\text{H}_2\text{O}_3} C_{\text{O}_2}$$

$$r_3 = -k_3 C_{\text{C}_6\text{H}_6} C_{\text{O}_2}$$

with

$$k_1 = 0.0637 \text{ m}^6/(\text{mol O}_2 \text{ kgcat s})$$

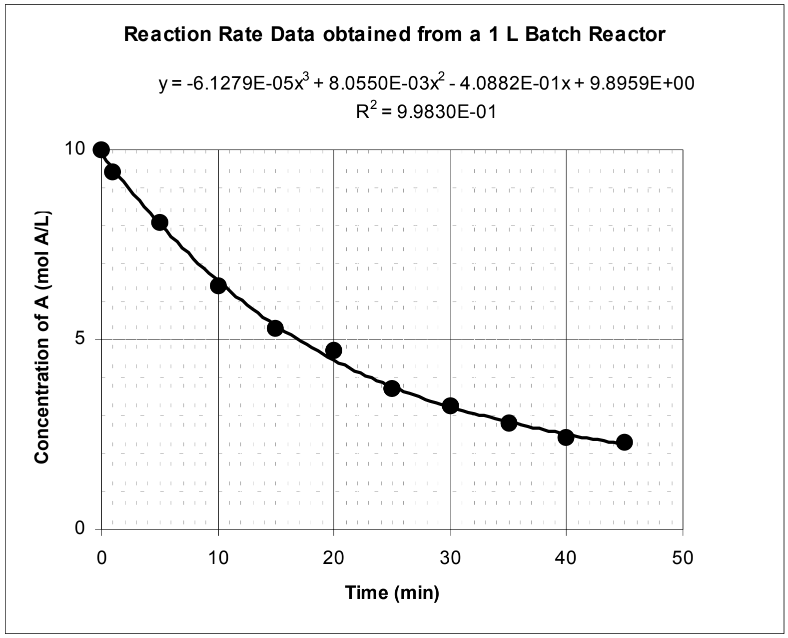
$$k_2 = 0.0664 \text{ m}^6/(\text{mol O}_2 \text{ kgcat s})$$

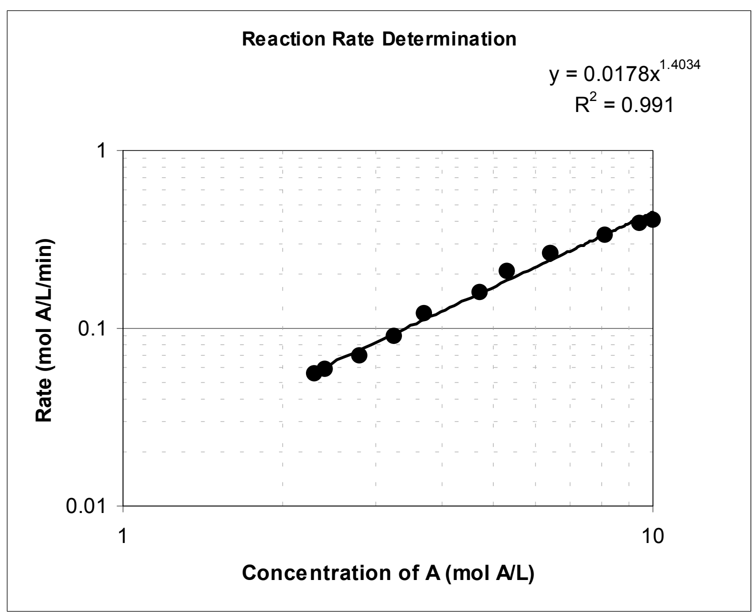
$$k_3 = 0.00348 \text{ m}^6/(\text{mol O}_2 \text{ kgcat s})$$

Assuming that the tubular reactor contains 25 kg of catalyst and is isothermal and isobaric, construct a model of this reactor that will be used in a POLYMATH program. Your model should be able to predict the molar flowrate of each compound that enters or is produced in the reactor. Number each equation used in the POLYMATH program. Specify your initial conditions and final integration value.

Exam 2: Problem 1
Rate Determination

t (min)	CA (mol A/L)	dC/dt
0	10	0.409
1	9.4	0.393
5	8.1	0.333
10	6.4	0.266
15	5.3	0.209
20	4.7	0.160
25	3.7	0.121
30	3.25	0.091
35	2.8	0.070
40	2.4	0.059
45	2.3	0.056





Reaction rate is:

$$r_A = -0.0178\left(\frac{\text{L}}{\text{mol}}\right)^{0.4}\frac{1}{\text{min}}C_A^{1.4}$$

POLYMATH Results

Exam 2 Problem 2Homework Solution- Selectivity in a PFR   04-03-2001, Rev5.1.224

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
V	0	0	10	10
FA	10	1.364E-26	10	1.364E-26
FB	40	30.634437	40	30.634437
FC	0	0	8.0966888	8.0966888
FD	0	0	9.3655629	9.3655629
FU1	0	0	0.6344371	0.6344371
FU2	0	0	0.6344371	0.6344371
flow	1	1	1	1
CB	40	30.634437	40	30.634437
T	300	300	300	300
k1	0.1748495	0.1748495	0.1748495	0.1748495
k2	0.0664569	0.0664569	0.0664569	0.0664569
CC	0	0	8.0966888	8.0966888
CA	10	1.364E-26	10	1.364E-26
r2	0	-1.6811659	0	-1.115E-26
r1	-69.939803	-69.939803	-7.306E-26	-7.306E-26
S	0	0	4.8428526	3.2759328
Soverall	0	0	10.859248	7.3810022

ODE Report (RKF45)

Differential equations as entered by the user

[1] d(FA)/d(V) = r1+r2
[2] d(FB)/d(V) = r1
[3] d(FC)/d(V) = -r1+2*r2
[4] d(FD)/d(V) = -r1
[5] d(FU1)/d(V) = -r2
[6] d(FU2)/d(V) = -r2

Explicit equations as entered by the user

[1] flow = 1
[2] CB = FB/flow
[3] T = 300
[4] k1 = 2.1*exp(-6200/8.314/T)
[5] k2 = 1.1*exp(-7000/8.314/T)
[6] CC = FC/flow
[7] CA = FA/flow
[8] r2 = -k2*CA*CC^1.2
[9] r1 = -k1*CA*CB
[10] S = if (r2<0) then (r1/r2/2) else (0)
[11] Soverall = if (FU1 >0) then (FD/(FU1+FU2)) else (0)

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: 6
number of explicit equations: 11
Data file: G:\Courses 14 june 2000\Reaction Engineering\Exams&Quizzes\exam2problem2selectivity_hmwk.pol

Problem 3
POLYMATH Results
Exam 2 Multiple Rates Maleic Anhydride 04-02-2001, Rev5.1.224

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
W	0	0	25	25
FB	26	6.2902951	26	6.2902951
FO	326.55	240.91275	326.55	240.91275
FMA	0	0	8.2091187	8.0513837
FCO2	0	0	55.627586	55.627586
FW	0	0	35.865177	35.865177
FT0	1581	1581	1581	1581
FN	1228.45	1228.45	1228.45	1228.45
FT	1581	1575.1972	1581	1575.1972
flowrate0	22.001441	22.001441	22.001441	22.001441
flowrate	22.001441	21.920688	22.001441	21.920688
CO	14.84221	10.9902	14.84221	10.9902
CMA	0	0	0.3743857	0.3672961
r2	0	-0.2880872	0	-0.2680341
CB	1.1817408	0.286957	1.1817408	0.286957
r1	-1.1172753	-1.1172753	-0.2008916	-0.2008916
r3	-0.061038	-0.061038	-0.0109749	-0.0109749
rB	-1.1172753	-1.1172753	-0.4689257	-0.4689257
rO	-5.4855238	-5.4855238	-1.7904266	-1.7904266
rMA	1.1172753	-0.0671424	1.1172753	-0.0671424
rCO2	2.6007785	1.5397692	2.6596228	1.5397692
rW	2.4176646	0.7027421	2.4176646	0.7027421
X	0	0	0.7580656	0.7580656

ODE Report (RKF45)

Differential equations as entered by the user

[1] d(FB)/d(W) = rB
[2] d(FO)/d(W) = rO
[3] d(FMA)/d(W) = rMA
[4] d(FCO2)/d(W) = rCO2
[5] d(FW)/d(W) = rW

Explicit equations as entered by the user

[1] FT0 = 26+1555
[2] FN = 0.79*1555
[3] FT = FB+FO+FMA+FCO2+FW+FN
[4] flowrate0 = FT0*8.314*848/5/1.01325e5
[5] flowrate = FT/FT0*flowrate0
[6] CO = FO/flowrate
[7] CMA = FMA/flowrate
[8] r2 = -0.0664*CMA*CO
[9] CB = FB/flowrate
[10] r1 = -0.0637*CB*CO
[11] r3 = -0.00348*CB*CO
[12] rB = r1+r2
[13] rO = 9/2*r1+3*r2+15/2*r3
[14] rMA = -r1+r2
[15] rCO2 = -2*r1-4*r2-6*r3
[16] rW = -2*r1-r2-3*r3
[17] X = (26-FB)/26

Independent variable

variable name : W
initial value : 0
final value : 25

Precision

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

General

number of differential equations: 5
number of explicit equations: 17
Data file: G:\Courses 14 june 2000\Reaction Engineering\Exams&Quizzes\maleicanhydride.pol