Exam 1
Chemical Reaction Engineering
26 February 2001
Closed Book and Notes

(20%) 1. Derive the **unsteady-state** mole balance for a chemical species A for a packed bed reactor using the following steps:

a) Sketch a packed bed reactor showing the control volume and all variables that you will use in the derivation.
b) State the assumption(s) that you will use in this derivation.
c) Draw a sketch of concentration of A *vs.* catalyst weight where A is a reactant.
d) Derive the mole balance using a rate of reaction with units mol A/(s kgcat).

(30) 2. A new drug, Slatearium, has tremendous market potential to increase brain function. Before full scale manufacture is possible a pilot scale run of this liquid phase reaction must be made. We currently have available two stirred tank reactors with volumes of 500 and 1000 gal. The reaction rate has been measured from previous laboratory studies and has been found to be elementary. Slaterarium is formed by mixing Newellium and Dahmium together in a batch reactor using the following stoichiometry:

$$N + D \leftrightarrow S$$

The reaction rate constants at the recommended reaction temperature of 162 K are $k_f = 2\times10^{-3}\frac{\mathrm{m^3_{liquid}}}{\mathrm{mol\,s}}$ and $\mathrm{k}_{reverse} = 5\times10^{-4}\frac{1}{\mathrm{s}}\cdot$ As in most pharmaceutical operations, the reaction is conducted in batches to guarantee a sterile product. The initial concentrations of Newellium and Dahmium are each 0.5 mol/m^3.

a) Determine the maximum conversion of Newellium that can be obtained in this batch reactor.
b) Determine the time required to obtain the conversion found in part b.
c) Which reactor would you use for this pilot plant run. Give an explanation.

(50 pts.) 3. The gas phase reaction, $A + 3B \longrightarrow C$, has a rate that is 1/2 order in A and 1/2 order in B. This reaction is to be carried out isothermally at 55°C in a packed bed reactor. The gas stream entering the reactor has three components: A, B and I (an inert compound). The flowrates of A and B into the reactor are 0.01 mol A/s and 0.03 mol B/s. The pressure drop in the reactor is given by the expression:

$$\frac{dP}{dW} = -\frac{\rho_0}{\rho}\beta_0$$

Additional information for this reactor is given below:

Pressure term	$\beta_0 = 100{,}000$ Pa/(kgcat).
Total molar flowrate	$F_{T0} = 0.3716$ mol/s
Total flowrate into the reactor, v_0,	$v_0 = 0.002$ m^3/s
Initial pressure, P_0, is	$P_0 = 506{,}625$ Pa
Catalyst particle diameter,	$d_p = 3 \times 10^{-4}$ m
Rate constant, k_A ,	$k_A = 0.001 \frac{m^3_{gas}}{\text{kgcat s}} \left(\frac{\text{mol A}}{\text{mol B}}\right)^{0.5}$
Universal Gas Law Constant	$R = 8.314$ Pa m^3/(gmol K)
Mass Balance	$\rho_0 v_0 = \rho v$

Show All Work - Including derivation of equations that have not been given!

a) Construct a stoichiometric table for the above process.

b) Develop a reactor model for this process. Your answer should be in the form of the input required for an ODE solver such as POLYMATH. Remember to given initial conditions. Number your equations that will be used in POLYMATH. Assume a weight of catalyst as your ending point that will give a conversion of $\chi_A = 0.75$. Do not solve for this weight in this part of the problem.

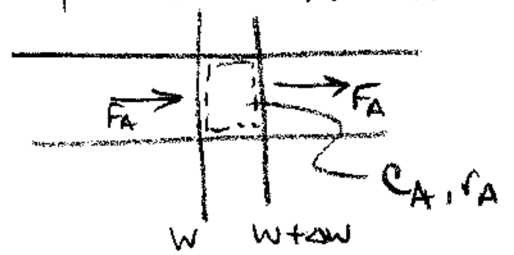
c) Estimate the pressure drop using 1 kg of catalyst in this reactor assuming that the reactants are dilute.

Extra Credit 10 points: Calculate the weight of catalyst required for a conversion of A of $\chi_A = 0.75$.

Exam 1 26 Feb 2001 Solutions

6:18

A → packed bed reactor



assumptions
uniform c, T & P in
the control volume ΔV ρ = ΔW

$$\lim_{\Delta W \to 0} \left[\frac{\partial C_A}{\partial t} \Delta w \phi/\rho_b = F_A\big|_W - F_A\big|_{W+\Delta W} + r_A \Delta W \right]$$

$$\lim_{\Delta W \to 0} \left[\frac{\phi}{\rho_b} \frac{\partial C_A}{\partial t} = \frac{-\left(F_A\big|_{W+\Delta W} - F_A\big|_W\right)}{\Delta w} + r_A \frac{\Delta W}{\Delta w} \right]$$

$$\phi/\rho_b \ \frac{\partial C_A}{\partial t} = - \frac{\partial F_A}{\partial W} + r_A$$

$$\phi/\rho_b \ \frac{\partial C_A}{\partial t} = - \frac{\partial F_A}{\partial W} + r_A$$

3.5 min

2) 6:59

elementary $N + D \rightleftarrows S$ $T = 162k$

$C_N = C_D = 0.5 \, mol/m^3$

Maximum conversion is equilibrium

species	N_i	change	final
N	N_{N_0}	$-XN_{N_0}$	$N_0(1-x)$
D	N_{N_0}	$-XN_{N_0}$	$N_0(1-x)$
S	0	$+XN_s$	$+XN_s$

$r = -k_f C_N C_D + k_r C_s$ $\frac{k_f}{k_r} = \frac{C_s}{C_N C_D}$

$$\frac{2\times10^{-3} \ m^3/mol\,s}{0.5\times10^{-3} \cdot 1/s} = \frac{\cancel{1/V}}{(1/V)^2}\frac{N_S}{N_N N_D} = V\frac{N_{N_0}X}{N_{N_0}^2(1-x)^2}$$

$$4 \frac{m^3}{mol} = \left(\frac{V}{N_{N_0}}\right)\frac{X}{(1-x)^2} = \frac{1\,m^3}{0.5\,mol}$$

$$2 = \frac{x}{(1-x)^2} \qquad 2(1-x)(1-x) = x$$

$$2(1-x-x+x^2) = x$$

$$1 - 2x + x^2 - \tfrac{1}{2}x = 0$$

$$\underset{c}{1} - \underset{b}{2.5x} + \underset{a}{x^2} = 0 \qquad \frac{-b \pm \sqrt{b^2-4ac}}{2a} = \frac{2.5 \pm \sqrt{(2.5)^2 - 4(1)(1)}}{2}$$

a) $$x = \frac{2.5 \pm \sqrt{6.25-4}}{2} = \frac{2.5 \pm 1.5}{2} = \frac{1}{2} = \boxed{0.5 = X_{max}}$$

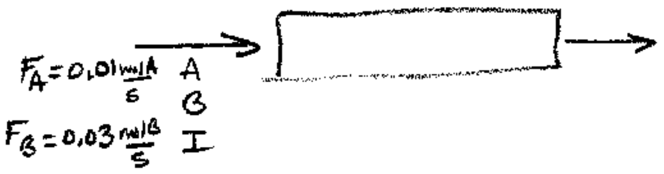
7.5 min

b) ∞

c) Either volume could be used to test the reaction

3. $A + 3B \rightarrow C$ 7:39

$-r_A = k C_A^{1/2} C_B^{1/2}$ $T = T_0 = 55°C$ PBR



$F_A = 0.01 \frac{mol A}{s}$

$F_B = 0.03 \frac{mol B}{s}$

$$\frac{dP}{dW} = -\frac{P_0}{e}\beta_0$$

Stoic table

	ini	change	
A	F_{A0}	$-F_{A0}X$	$F_A = F_{A0}(1-X)$
B	F_{B0}	$-3 F_{A0}X$	$F_B = F_{B0} - F_{A0}X(3)$
I	F_{I0}	0	F_{I0}
C	$F_{C0}=0$	$+F_{A0}X$	$F_C = F_{A0}X$
			$F_T = F_{T0} - 3F_{A0}X$

Mole Bal on A

equations for Polymath are numbered

① $\frac{dF_A}{dW} = r_A = -k C_A^{1/2} C_B^{1/2}$

② $\frac{dF_B}{dW} = r_B = \frac{3 \text{ mol} B}{1 \text{ mol} A} r_A = -3k C_A^{1/2} C_B^{1/2}$

③ $\frac{dF_C}{dW} = r_C = -r_A = +k C_A^{1/2} C_B^{1/2}$

④ $C_A = \frac{F_A}{\nu} = \frac{F_{A0}(1-X)}{\nu}$

$$\frac{P\nu}{P_0 \nu_0} = \frac{FRT}{F_0 R T_0}$$

⑤ $C_B = \frac{F_B}{\nu} = \frac{F_{B0} - 3F_{A0}X}{\nu}$

⑩ $\nu_0 = 0.002 m^3/s$

⑥ $\nu = \nu_0 \frac{F_T}{F_{T0}} \cancel{\frac{T}{T_0}} \frac{P_0}{P}$

⑨ $F_{T0} = 0.3716 mol/s$

⑧ $k = 0.001 \frac{m^3}{kgcat\ s}\left(\frac{mol A}{mol B}\right)^{1/2}$ 6:21

⑦ $F_T = F_I + F_A + F_B + F_C$

$$\frac{dP}{dW} = -\frac{\rho_0}{\rho}\beta_0 \qquad \frac{\rho_0}{\rho} = \frac{\nu}{\nu_0} = \frac{P_0}{P}\frac{F_T}{F_{T0}}\cancel{\frac{T}{T_0}}$$

$$\frac{dP}{dW} = -\frac{P_0}{P}\frac{F_T}{F_{T0}}\beta_0 = -\frac{P_0}{P}\frac{\cancel{F_{T0}} - 3y_{A0}X\cancel{F_{T0}}}{\cancel{F_{T0}}}\beta_0$$

⑪ $$\frac{dP}{dW} = -\frac{P_0}{P}\left[1-3y_{A0}X\right]\beta_0$$

⑬ $$X = \frac{F_{A0}-F_A}{F_{A0}}$$

⑫ $$y_{A0} = \frac{F_{A0}}{F_{T0}} = \frac{0.01\,\text{mol A/s}}{0.3716\,\text{mol/s}}$$

⑭ $$\beta_0 = 100{,}000\ \text{Pa/kg}_{cat}$$

at $W=0$ $\quad F_{A0}=0.01\ \text{mol/s} \quad F_{B0}=0.03\ \text{mol/s} \quad F_{I0}=(0.3716-0.04\ \frac{\text{mol}}{\text{s}})$

$P = 506{,}625\ \text{Pa}$

11 min

Since y_{A0} is small

$$\frac{dP}{dW} = -\frac{P_0}{P}\beta_0$$

$$\int P\,dP = -P_0\beta_0\int dW$$

$$\left.\frac{P^2}{2}\right|_{P_0}^{P} = -P_0\beta_0 W$$

$$P^2 - P_0^2 = -2P_0\beta_0 W$$

$$\frac{P}{P_0} = \left[1 - \frac{2\beta_0 W}{P_0}\right]^{1/2}$$

$$\frac{P}{P_0} = \left[1 - \frac{2(100{,}000\ \text{Pa/kg})(1\ \text{kg})}{506{,}625\ \text{Pa}}\right]^{1/2}$$

$$\frac{P}{P_0} = 0.778\ \text{Pa/Pa}$$

$$P = 0.778\,P_0 = 0.778(506{,}625\ \text{Pa})$$

$$\boxed{P = 394{,}154\ \text{Pa}}$$

$$\Delta P = 506{,}625 - 394{,}154 = 112471\ \text{Pa}$$

Extra Credit

$$-F_{A0}\frac{dX_A}{dW} = -kC_A^{1/2}C_B^{1/2} = -k\frac{[F_{A0}(1-X)]^{1/2}(3F_{A0}(1-X))^{1/2}\,P\,F_{T0}}{\nu_0\,F_T\,P_0}$$

$$= -k(3)^{1/2}\frac{F_{A0}}{\nu_0}(1-X)\left(\frac{P}{P_0}\right)\left[\frac{F_{T0}}{(F_{T0}-3F_{A0}X)}\right]$$

15:42

$$= -k\, 3^{1/2}\left(\frac{F_{A0}}{\nu_0}\right)(1-x)\left(\frac{P}{P_0}\right)\frac{\cancel{F_{T0}}}{\cancel{F_{T0}}}\left[\frac{1}{(1-\underbrace{3y_{A0}x}_{\text{small}})}\right]$$

$$= -3^{1/2}k\left(\frac{F_{A0}}{\nu_0}\right)(1-x)\left(\frac{P}{P_0}\right)$$

$$= -3^{1/2}k\left(\frac{F_{A0}}{\nu_0}\right)(1-x)\left[1-2\frac{\beta_0 W}{P_0}\right]^{1/2}$$

$$\frac{dx_A}{dW} = \left(\frac{3^{1/2}k}{\cancel{F_{A0}}}\right)\left(\frac{\cancel{F_{A0}}}{\nu_0}\right)(1-x)\left[1-2\frac{\beta_0}{P_0}W\right]^{1/2}$$

$$\int\frac{dx_A}{1-x_A} = \frac{3^{1/2}k}{\nu_0}\int\left[1-2\frac{\beta_0}{P_0}W\right]^{1/2}dW$$

$$-\ln(1-x_A)\Big|_0^x = \left[\frac{3^{1/2}k}{\nu_0}\right]\frac{2}{3}\frac{1}{-\alpha}\left[1-2\frac{\beta_0}{P_0}W\right]^{3/2}\Bigg|_0^W$$

$$-\ln(1-x) = -\frac{3^{1/2}k}{\nu_0}\,\frac{\cancel{2}}{3}\,\frac{P_0}{\cancel{2}\beta_0}\left[\left[1-2\frac{\beta_0}{P_0}W\right]^{3/2}-1\right]$$

$$\left[1+\frac{[\ln(1-0.75)](0.002\,\text{m}^3/\text{s})(3)(100{,}000\,\frac{\text{Pa}}{\text{kg}})}{3^{1/2}(0.001\,\frac{\text{m}^3}{\text{kg}\,\text{s}}\left(\frac{\text{mol A}}{\text{mol B}}\right)^{1/2}(506625\,\text{Pa})}\right]^{2/3} = \left(1-2\frac{\beta_0}{P_0}W\right)$$

$$(0.1395) = 1-2\frac{\beta_0}{P_0}W$$

$$W = [1-0.1395]\frac{(506{,}625\,\text{Pa})}{2(100{,}000\,\frac{\text{Pa}}{\text{kg}})}$$

$$W = 2.18\ \text{kg cat}$$

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Catalyst particle diameter,	$d_p = 3 \times 10^{-4}$ m
Rate constant, k_A,	$k_A = 0.001 \dfrac{m^3_{gas}}{\text{kgcat s}} \left(\dfrac{\text{mol A}}{\text{mol B}}\right)^{0.5}$
Universal Gas Law Constant	$R = 8.314$ Pa m^3/(gmol K)
Mass Balance	$\rho_0 v_0 = \rho v$

Show All Work - Including derivation of equations that have not been given.

a) Construct a stoichiometric table for the above process.

b) Develop a reactor model for this process. Using POLYMATH determine the weight of catalyst needed to achieve a conversion of $\chi_A = 0.75$.

c) Determine the pressure drop and weight of catalyst required to achieve a $\chi_A = 0.75$ assuming that the density is constant and equal to the inlet density.

d) Estimate the pressure drop and weight of catalyst required to achieve a $\chi_A = 0.75$ assuming that the reactants are dilute.

Exam 1 2001 Problem 3

Numerical Solution of Full Model

POLYMATH Results

Exam 1 Problem 3 Solution 03-04-2001, Rev5.1.224

Calculated values of the DEQ variables

```
Variable    initial value   minimal value   maximal value   final value
W             0               0               2.035           2.035
FA            0.01            0.0024999       0.01            0.0024999
FB            0.03            0.0074997       0.03            0.0074997
FC            0               0               0.0075001       0.0075001
P             5.066E+05       2.247E+05       5.066E+05       2.247E+05
FI            0.3316          0.3316          0.3316          0.3316
P0            5.066E+05       5.066E+05       5.066E+05       5.066E+05
FT            0.3716          0.3490997       0.3716          0.3490997
k             0.001           0.001           0.001           0.001
flow          0.002           0.002           0.004237        0.004237
CA            5               0.5900068       5               0.5900068
Beta0         1.0E+05         1.0E+05         1.0E+05         1.0E+05
CB            15              1.7700205       15              1.7700205
rA           -0.0086603      -0.0086603      -0.0010219      -0.0010219
FA0           0.01            0.01            0.01            0.01
X             0               0               0.7500116       0.7500116
```

ODE Report (RKF45)

Differential equations as entered by the user

```
[1]  d(FA)/d(W) = rA
[2]  d(FB)/d(W) = 3*rA
[3]  d(FC)/d(W) = -rA
[4]  d(P)/d(W) = -P0/P*Beta0
```

Explicit equations as entered by the user

```
[1]  FI = 0.3716-.04
[2]  P0 = 506625
[3]  FT = FI+FA+FB+FC
[4]  k = 0.001
[5]  flow = 0.002*FT/0.3716*P0/P
[6]  CA = FA/flow
[7]  Beta0 = 100000
[8]  CB = FB/flow
[9]  rA = -k*CA^0.5*CB^0.5
[10]  FA0 = 0.01
[11]  X = (FA0-FA)/FA0
```

Comments

```
[14]  X = (FA0-FA)/FA0
```

not needed for solution

Independent variable

variable name : W
initial value : 0
final value : 2.035

Precision

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

General

number of differential equations: 4
number of explicit equations: 11
Data file: C:\ACDRIVE\Courses 14 june 2000\Reaction Engineering\Exams&Quizzes\exam1problem3.pol

Numerical Solution for 1 Kg

POLYMATH Results

Exam 1 Problem 3 Solution 03-04-2001, Rev5.1.224

Calculated values of the DEQ variables

```
Variable     initial value    minimal value    maximal value    final value
W              0                0                1                1
FA             0.01             0.0045215        0.01             0.0045215
FB             0.03             0.0135646        0.03             0.0135646
FC             0                0                0.0054785        0.0054785
P              5.066E+05        3.941E+05        5.066E+05        3.941E+05
FI             0.3316           0.3316           0.3316           0.3316
P0             5.066E+05        5.066E+05        5.066E+05        5.066E+05
FT             0.3716           0.3551646        0.3716           0.3551646
k              0.001            0.001            0.001            0.001
flow           0.002            0.002            0.0024571        0.0024571
CA             5                1.8401864        5                1.8401864
Beta0          1.0E+05          1.0E+05          1.0E+05          1.0E+05
CB             15               5.5205593        15               5.5205593
rA            -0.0086603       -0.0086603       -0.0031873       -0.0031873
FA0            0.01             0.01             0.01             0.01
X              0                0                0.5478471        0.5478471
```

ODE Report (RKF45)

Differential equations as entered by the user

[1] d(FA)/d(W) = rA
[2] d(FB)/d(W) = 3*rA
[3] d(FC)/d(W) = -rA
[4] d(P)/d(W) = -P0/P*Beta0

Explicit equations as entered by the user

[1] FI = 0.3716-.04
[2] P0 = 506625
[3] FT = FI+FA+FB+FC
[4] k = 0.001
[5] flow = 0.002*FT/0.3716*P0/P
[6] CA = FA/flow
[7] Beta0 = 100000
[8] CB = FB/flow
[9] rA = -k*CA^0.5*CB^0.5
[10] FA0 = 0.01
[11] X = (FA0-FA)/FA0

Comments

[14] X = (FA0-FA)/FA0
not needed for solution

Independent variable

variable name : W
initial value : 0
final value : 1

Precision

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

General

number of differential equations: 4
number of explicit equations: 11
Data file: C:\ACDRIVE\Courses 14 june 2000\Reaction Engineering\Exams&Quizzes\exam1problem3.pol

Extra Credit Solution

Exam 1 Problem 3 Solution For Extra Credit 03-04-2001, Rev5.1.224

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
W	0	0	2.18	2.18
FA	0.01	0.0024998	0.01	0.0024998
FB	0.03	0.0074994	0.03	0.0074994
FC	0	0	0.0075002	0.0075002
P1	5.066E+05	1.892E+05	5.066E+05	1.892E+05
Beta0	1.0E+05	1.0E+05	1.0E+05	1.0E+05
P0	5.066E+05	5.066E+05	5.066E+05	5.066E+05
P	**5.066E+05**	**1.892E+05**	**5.066E+05**	**1.892E+05**
k	0.001	0.001	0.001	0.001
FI	0.3316	0.3316	0.3316	0.3316
flow	0.002	0.002	0.0053567	0.0053567
CA	5	0.466669	5	0.466669
CB	15	1.400007	15	1.400007
FT	0.3716	0.3490994	0.3716	0.3490994
FA0	0.01	0.01	0.01	0.01
X	**0**	**0**	**0.7500213**	**0.7500213**
rA	-0.0086603	-0.0086603	-8.083E-04	-8.083E-04

ODE Report (RKF45)

Differential equations as entered by the user

[1] d(FA)/d(W) = rA
[2] d(FB)/d(W) = 3*rA
[3] d(FC)/d(W) = -rA
[4] d(P1)/d(W) = -P0/P*Beta0

Explicit equations as entered by the user

[1] Beta0 = 100000
[2] P0 = 506625
[3] P = P0*(1-2*Beta0*W/P0)^0.5
[4] k = 0.001
[5] FI = 0.3716-.04
[6] flow = 0.002*P0/P
[7] CA = FA/flow
[8] CB = FB/flow
[9] FT = FI+FA+FB+FC
[10] FA0 = 0.01
[11] X = (FA0-FA)/FA0
[12] rA = -k*CA^0.5*CB^0.5

Comments

[14] X = (FA0-FA)/FA0
not needed for solution

Independent variable

variable name : W
initial value : 0
final value : 2.18

Precision

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

General

number of differential equations: 4
number of explicit equations: 12
Data file: C:\ACDRIVE\Courses 14 june 2000\Reaction Engineering\Exams&Quizzes\exam1problem3.pol