Chemical & Biomolecular Engineering 142

Chemical Kinetics and Reaction Engineering

Midterm 1

Tuesday, October 4, 2011

The exam is 100 points total and 20% of the course grade. Please read through the questions very carefully before answering. Make sure to show all your work. Good luck !

Name ___________________ ________________________________

Student ID ____

Problems	Points (Max.)	Points Received
1	**32**	
2	**23**	
3	**10**	
4	**20**	
5	**15**	

You are allowed one 8.5"'x 11" sheet of paper and a calculator for this exam. A list of (possibly) useful integrals and constants is provided on the last page of this exam.

/

Started 12:35AM.

Changyi Li

Midterm 1.

ChE 142

1. (a). σ: 1, 2, 1.

$$(A \longleftrightarrow 2I^*) \times 1$$
$$(B + I^* \longrightarrow B^*) \times 2$$
$$(2B^* \longrightarrow P) \times 1$$
$$A + 2B \longrightarrow P.$$

0.5pt
0.5pt
0.5pt

-0.5 for wrong sign

-0.5 for missing a 2

-0.5 for missing a [ ] term

(b). I^*: $0 = 2r_1 - 2r_{-1} - r_2$ 4pt

B^* $0 = r_2 - 2r_3$. 4pt

$$r = \frac{dC_P}{dt} = r_3 = \frac{r_2}{2} = \frac{k_2}{2} C_B C_{I^*}$$ 1pt

-0.5 for wrong sign

-0.5 for off by a factor of 2

From I^* PSSH balance.

$$2k_1 C_A - 2k_{-1} C_{I^*}^2 - k_2 C_B C_{I^*} = 0.$$

$A = -2k_{-1}$ $B = -k_2 C_B$ $C = 2k_1 C_A$.

$$C_{I^*} = \frac{-B \pm \sqrt{B^2 - 4AC}}{2A} = \frac{k_2 C_B \pm \sqrt{k_2^2 C_B^2 + 4 \cdot 2k_{-1} \cdot 2k_1 C_A}}{-4k_{-1}}$$ 1pt

-0.5 for factor of 2

The sign has to be negative to be physical

$$C_I^* = -\frac{k_2 C_B - \sqrt{k_2^2 C_B^2 + 16 k_{-1} C_A k_1}}{4k_{-1}}$$ 0.5pt for correct sign choice

$$r_{PSSH} = \frac{k_2}{2} C_B \cdot \frac{-k_2 C_B + \sqrt{k_2^2 C_B^2 + 16 k_{-1} k_1 C_A}}{4k_{-1}}$$ 1pt.

-0.5 for error in $[I^*]$

-0.5 for having $\frac{k_2}{2} C_B C_{I^*}$

(c). From I^* balance:

$$2(r_1 - r_{-1}) = r_2 \qquad \Rightarrow 2(r_1 - r_{-1}) = r_2$$ [0.5pt.]

$r_1 > r_{-1}$ is required to be physical [0.5pt]

From B^* balance.

$$r_2 = 2r_3 \qquad \Rightarrow r_1 - r_{-1} = r_3.$$

[0.5pt] [0.5pt]

other acceptable forms involve $r_{1,net}$

(d) QE on I:

$$r_1 = r_{-1}$$

$$k_1 C_A = k_{-1} C_{I^*}^2$$ [3pt.] −0.5 for leaving out $\sqrt{\ }$

$$C_{I^*} = \left(\frac{k_1 C_A}{k_{-1}}\right)^{1/2}$$ [1pt.] −0.5 for a factor of 2

$$r_{0B} = r_3 = \frac{r_2}{2} = \frac{k_2}{2} C_B C_{I^*} = \frac{k_2}{2} C_B \cdot \left(\frac{k_1}{k_{-1}} C_A\right)^{1/2}$$ [1pt.] usually rules for "−0.5" as stated above.

(e). By imposing QE, we mandate that.

$$r_1 \approx r_{-1} \gg \frac{r_2}{2} = r_3.$$

$$\Rightarrow r_1 \cdot r_{-1} \gg \left(\frac{r_2}{2}\right)^2$$

$$k_1 k_{-1} C_A C_I^{*2} \gg \frac{1}{4} k_2^2 C_B^2 C_I^{*2}$$

$$k_1 k_{-1} C_A \gg \frac{1}{4} k_2^2 C_B^2$$ [2pt]

$\Rightarrow$ Term in the sqrt: $k_2^2 C_B^2 + 16 k_{-1} k_1 C_A \approx 16 k_{-1} k_1 C_A.$

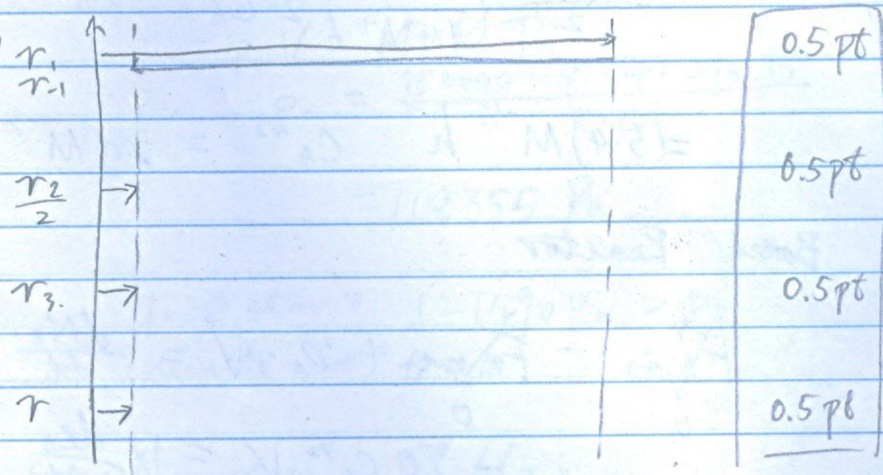
By the same inequality,

$$-k_2 C_B + \sqrt{16 k_{-1} k_1 C_A} \approx \sqrt{16 k_{-1} k_1 C_A}$$ [2pt.]

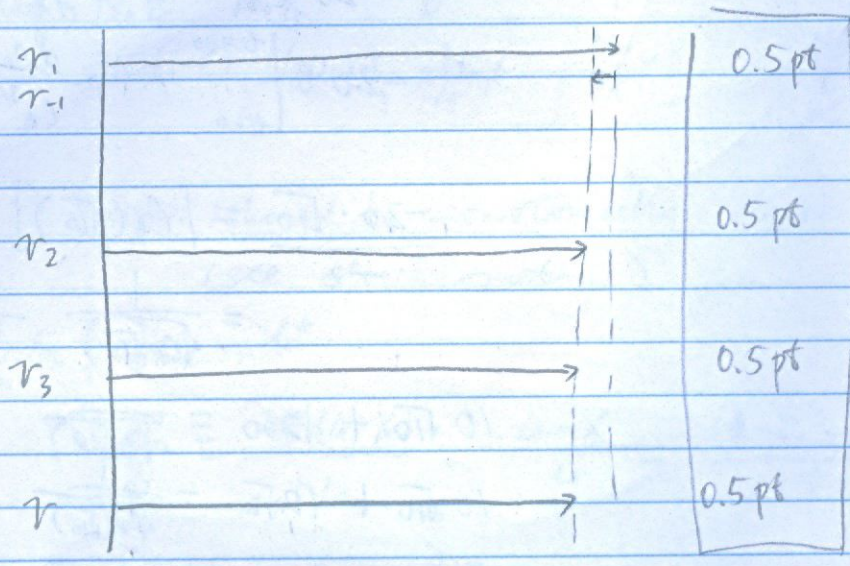
$$r_{pssH} \approx \frac{k_2}{2} C_B \cdot \frac{\sqrt{16 k_1 k_{-1} C_A}}{4 k_{-1}}$$

$$= \frac{k_2}{2} C_B \cdot \sqrt{\frac{k_1}{k_{-1}} C_A} = r_{QE}$$

(f)



(g).



−0.5 each for (f) (g) for missing σ_i

extra −0.5 for failure to demonstrate order of magnitude

(h)

$$r = \frac{k_2}{2}\left(\frac{k_1}{k_{-1}}\right)^{1/2} C_B C_A^{1/2}$$

Since we have stoichiometric amount of A and B

$$\Rightarrow C_B(t) = 2C_A(t) \quad t \in [0, \infty)$$ [1pt]

Plug in: $r = \frac{5\,M^{-1}h^{-1}}{2}\left(\frac{16h^{-1}}{1M^{-1}h^{-1}}\right)^{1/2} 2 \cdot C_A^{3/2}$

$$= (5 \cdot 4) M^{-1/2} h^{-1} \quad C_A^{3/2} = 20\,M^{-1/2} h^{-1} C_A^{3/2}$$

Batch Reactor:

$$\cancel{F_{A,in}} - \cancel{F_{A,out}} + \nu_A r V = \frac{dN_A}{dt}$$ [2pt]

(0, 0)

$$-20\,C_A^{3/2} V = V\frac{dC_A}{dt}$$

$$-20\,C_A^{3/2} = \frac{dC_A}{dt}$$

$$-20t\Big|_{t=0}^{t=\sqrt{10}} = \frac{dC_A}{C_A^{3/2}} = -2C_A^{-1/2}\Big|_{C_{A0}}^{C_A(\sqrt{10})}$$

$$\frac{-20\cdot\sqrt{10}}{-2} = \left[C_A(\sqrt{10})\right]^{-1/2} - (0.005)^{-1/2}$$

$$= \frac{1}{\sqrt{C_A(\sqrt{10})}} - \frac{1}{\sqrt{\frac{1}{200}}}$$

$$10\sqrt{10} + \sqrt{200} = \frac{1}{\sqrt{C_A(\sqrt{10})}}$$

$$10\sqrt{10} + 10\sqrt{2} = \frac{1}{\sqrt{C_A(\sqrt{10})}}$$

$$\left[10(\sqrt{10} + \sqrt{2})\right]^{-1} = \sqrt{C_A(\sqrt{10})} = 0.021851$$

$$C_A(\sqrt{10}) = 4.7746\text{E-}4\ M$$

$X(\sqrt{10}) \approx 0.904$ [1pt]

1:04pm

2. $V = \pi R^2 \cdot h$

$= \pi \left(\frac{22-2\times1}{2}\right)^2 \cdot 10$

$= \pi 10^3\ m^3$ [1pt.]

At $t=0$.

$p_0 V = N_0 R T$.

$p_0 = \frac{150000 \cdot 8.314 \cdot 298.15}{\pi \cdot 10^3}$

$= 118355\ Pa$ [3pt]

$1.20\ atm = 121590\ Pa > p_0$ [1pt]

Tolerable at $t=0$.

Stoichiometric Table:

	A	B	C	D.	Sum.
initial	$N_0 \frac{3}{4}$	$N_0 \frac{1}{4}$	0	0.	N_0
final	$\frac{3}{4}N_0(1-X)$	$\frac{N_0}{4}(1-X)$	$\frac{2N_0}{4}X$	$\frac{N_0}{4}X$	$\frac{N_0}{4}(4-X)$

[1pt/cell]

∵ Pressure should be monotonically decreasing (see stoichiometry) 2 pt

∴ let $p_{implode} = p^*$

$\frac{p^*}{p_0} = \frac{\frac{N_0}{4}(4-X)}{N_0} = \frac{4-X}{4} = \frac{(1-0.2)\ atm}{p_0}$ [4pt.]

$\frac{4-X}{4} = \frac{81060}{118355}$

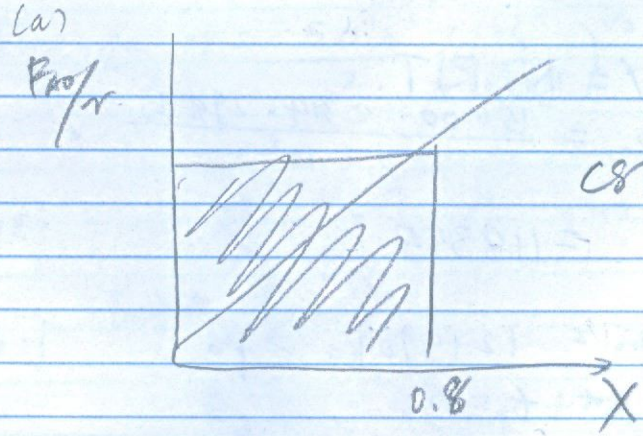
$118355(4-X) = 4 \cdot (81060)$

$X = 1.26044 \Rightarrow$ Not possible

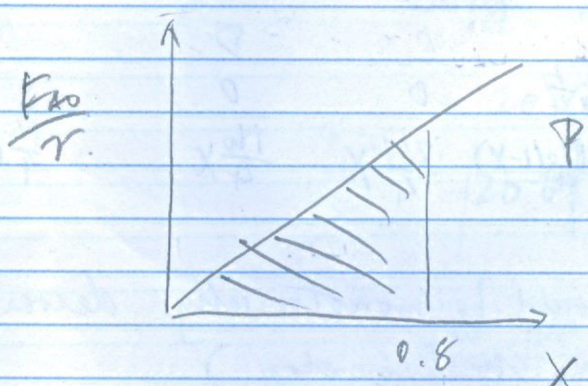
[3pt.] or if p_{final} is given.

No implosion would happen. [1pt] 1:14pm.

3. (a)



CSTR [2pt]



PFR. [2pt].

(b) PFR. [2pt]

(c). 1/2. Graphically, the triangle area = $\frac{1}{2}$ rectangle area. [2pt]

It is not 1 because it is not a ~~0th~~ order reaction.

[2pt] for the rest 1:16AM

4. (a) Short time: 3M [2pt]
Long time: 0M [2pt]

(b) CSTR:

1 pt 1 pt

$$F_{A,in} - F_{A,out} + r_A V_A = \frac{dN_A}{dt}$$ [2pt]

$F_{A,in} \to 0$ (pure solvent); $r_A V_A \to 0$ (no reaction)

$$-F_{A,out} = V\frac{dC_A}{dt}$$ [2pt]

$$-v_0 C_A = V\frac{dC_A}{dt}$$

$$-\frac{t}{\tau} = \log\frac{C_A}{C_{A0}}$$

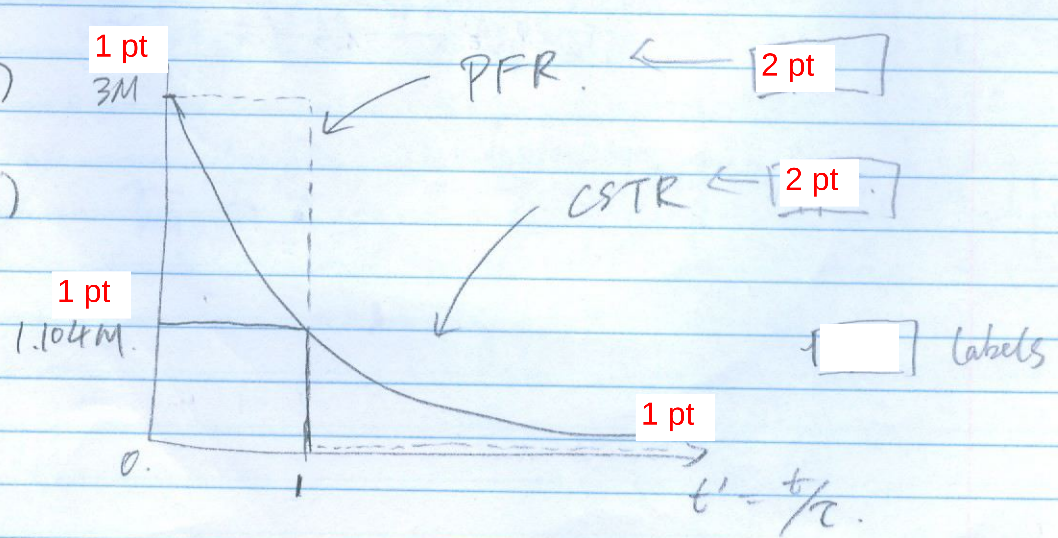
$$C_A = C_{A0}\exp\left(-\frac{t}{\tau}\right)$$ [2pt]

For $t/\tau = 1$

$$C_A = C_{A0}\cdot\exp(-1) = 1.104\,M$$ [1pt]

(c)

(d)



1:26pm

[2pt]

5. (a) PFR. Since this is a positive order reaction, PFR does not dilute reactant, therefore increasing rate. If it is gas phase, PFR will be more preferred due to the further dilution of reactant from the non-equimolar reaction. [3pt] for gas phase

-1.5 for stating PFR is more preferred.

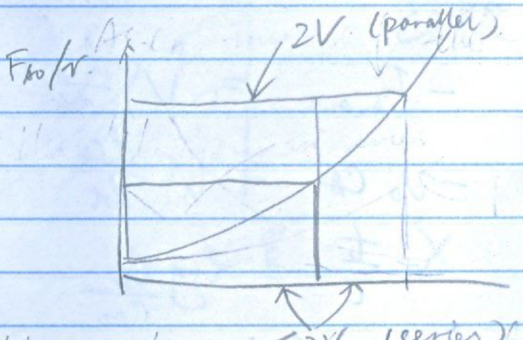
[2pt] state its positive order.

(b) $\frac{1}{r} = \frac{1+k_2C_A}{k_1C_A^2} = \frac{1}{k_1C_A^2} + \frac{k_2}{k_1C_A}$

parallel: $\frac{F_A}{2r_A(X)}X = V$

$\frac{F_A}{r_A(X)}X = 2V$ [1]

series: $\frac{F_A}{r_A(X_1)}X_1 = V$, $\frac{F_A}{r_A(X_2)}(X_2-X_1) = V$



[2pt]

~~At~~ the same conversion, $V_{parallel} > V_{series}$ ⇒ Series configuration leads to higher conversion (w/ same V). [1pt]

+1 for saying dilution and/or ΣCSTR → PFR.

(c) C_A decreases. C_B increases. C_T stays constant

[2pt] [2pt] [1pt]

A is a reactant. B is a product. Equimolar reaction.

Justification : 0.5 per quantity

1:28 AM