Problem 1 : Short Ans

Short Answers a-d, full points only for both the correct choice AND a complete explanation. No explanation = 0 pts

Solutions to MT I

CBE 142 2014

a) B - CSTR

CSTR operation dilutes the feed and therefore operates at a fixed lower concentration (+2) and since the rate is inversely proportional to concentration (ie or negative order kinetics), the rate is higher for a CSTR than that of a PFR. (+2)

b) A - constant vol CSTR

- Since $\delta > 0$ / moles are generated (+2) so volume of the reactor will expand and concentration will be diluted (+2) in a const. pressure BSTR.

OR
- $\delta > 0$ / moles are generated (+2) but the constant vol BSTR will not allow for the reactor volume change that will otherwise dilute the concentrations (+2)

c) C - equivalent (+4)

- Both reactors are at constant pressure so they accomodate changes in volume / volumetric flowrates the same way and a volume element in a PFR is its own batch reactor.

OR.
- "PFR in space is analogous to a batch reactor in time"

d) B - const. P BSTR

$$K_C = \frac{[R]^2[S]}{[P][Q]} = \frac{\frac{N_R^2}{V^2} \cdot \frac{N_S}{V}}{\frac{N_P}{V} \cdot \frac{N_Q}{V}} = \frac{N_R^2 N_S}{N_P \cdot N_Q} \cdot \frac{1}{V}$$ if $V \uparrow$, products $\uparrow$

- If volume is allowed to increase since $\delta > 0$ (+2) and in a constant pressure BSTR, the # of moles of product has to increase to maintain the value of K_C. +2

OR
- According to Le Chatelier's (+2) principle, an increase in pressure (in the case of $\delta > 0$, const. vol) will favor the side of less moles produced, which is the reverse reaction. +2

E. elementary, reversible gas phase rxn in flow reactor

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} 2C \qquad K_{eq} = \frac{k_1}{k_{-1}} = 1.25 \ \frac{mol}{L}$$

isothermal $(T = T_0)$

isobaric $(P = P_0)$

$y_{A0} = 1$ @ $T = 400K$, $P = 10\,atm$

$R = 0.082 \ \frac{L \cdot atm}{K \cdot mol}$

$X_{eq} = ?$

need to take into account Δmoles and change in volumetric flow

$$-r_A = k_1 C_A - k_{-1} C_C^2 = k_1 \left[C_A - \frac{C_C^2}{K_{eq}} \right]$$

@ equilibrium, $-r_A = 0$ thus $C_A = \frac{C_C^2}{K_{eq}}$ or $K_{eq} = \frac{C_C^2}{C_A}$

can use a stoichiometric table if needed

species	in	change	out
A	F_{A0}	$-F_{A0}X_{eq}$	$F_{A0}(1-X_{eq})$
C	0	$+2F_{A0}X_{eq}$	$2F_{A0}X_{eq}$

+1
+1

$C_A = \frac{F_A}{v}$ $\quad C_C = \frac{F_C}{v}$ and $v = v_0(1 + \varepsilon X_{eq})$ where $\varepsilon = y_{A0}\delta$, $\delta = 2-1 = 1$ +1

$v = v_0(1 + X_{eq})$

+1, MUST account for v changes in order to have the proper concentrations

$$C_A = \frac{C_{A0}(1-X_{eq})}{(1+X_{eq})}$$

$$C_C = \frac{2C_{A0}X_{eq}}{(1+X_{eq})}$$

then +1 $K_{eq} = \frac{C_C^2}{C_A}$

+1

$$K_{eq} = \frac{\frac{4C_{A0}^2(X_{eq})^2}{(1+X_{eq})^2}}{\frac{C_{A0}(1-X_{eq})}{(1+X_{eq})}} = \frac{4C_{A0}X_{eq}^2}{(1-X_{eq})(1+X_{eq})}$$

$$K_{eq} = \frac{4C_{A0}X_{eq}^2}{1-X_{eq}^2}$$

$$C_{A0} = \frac{y_{A0}P}{RT}$$

$$C_{A0} = \frac{(1)(10\,atm)}{(0.082\ \frac{L\,atm}{mol\,K})(400K)}$$

+1

$$C_{A0} = 0.305 \ \frac{mol}{L}$$

$$K_{eq} - K_{eq} X_{eq}^2 = 4 C_{A0} X_{eq}^2$$

$$K_{eq} = X_{eq}^2 (4 C_{A0} + K_{eq})$$

+1

$$X_{eq} = \sqrt{\frac{K_{eq}}{4 C_{A0} + K_{eq}}}$$

plug in values $\longrightarrow$ $$X_{eq} = \sqrt{\frac{1.25 \frac{mol}{L}}{4(0.305 \frac{mol}{L}) + 1.25 \frac{mol}{L}}}$$

+1

$$\boxed{X_{eq} = 0.71}$$

PROBLEM #2 (15 PTS)

Problem 2

Gas Phase Rxn, in a PFR

$$A_{(g)} + 2B_{(g)} \rightarrow 4D_{(g\rightarrow l)}$$

$$\begin{cases} v_0 = 5 \, L/min \\ F_{A0} = F_{B0} \\ P_{tot} = 4 \text{ atm} \\ P_{vap,D} = 1 \text{ atm} \end{cases}$$

a) $\boxed{B}$ +1

b)

	Before Condensation			After Condensation		
Species	F_{j0}	ΔF_j	F_j	F_{j0}	ΔF_j	F_j
A	$F_{A0} = F_{B0}$	$-0.5F_{B0}X_B$	$F_{B0}(1-0.5X_B)$	$F_{A0} = F_{B0}$	$-0.5F_{B0}X_B$	$F_{B0}(1-0.5X_B)$
B	F_{B0}	$-F_{B0}X_B$	$F_{B0}(1-X_B)$	F_{B0}	$-F_{B0}X_B$	$F_{B0}(1-X_B)$
D	0	$+2F_{B0}X_B$	$2F_{B0}X_B$	0		$y_D \cdot F_T'$

$$= \left(\frac{P_{vap,D}}{P_{tot}}\right) F_T' = 0.25F_T'$$

where F_T' is the total molar flow rate after condensation

In a total of 4 points in b):
1 point is deducted for each mistake made

If XA was used instead of XB, and no other mistakes were made, 2 points deducted out of 4

c)

D will condense when its partial pressure reaches its vapor pressure

+1
This may also be solved by FT = FT'

$$\boxed{y_D P_{Tot} = P_{vap,D}}$$

when $y_D = \frac{P_{vap,D}}{P_{Tot}} = \frac{1\ atm}{4\ atm} = 0.25$

when molar fraction of D in gas reaches 25%, condensation happen

$$y_D = \frac{F_D}{F_T} = \frac{2F_{B0}X_B}{F_A + F_B + F_D} = \frac{2F_{B0}X_B}{F_{B0}(1-0.5X_B) + F_{B0}(1-X_B) + 2F_{B0}X_B}$$

Correct FT +1

Correct FD (or FT') +1

$$= \frac{2F_{B0}X_B}{2F_{B0} + 0.5F_{B0}X_B}$$

$$= \frac{2X_B}{2+0.5X_B}$$

Hence when $0.25 = \frac{2X_B}{2+0.5X_B}$ condensation begins.

$0.5 + 0.125X_B = 2X_B$

$1.875X_B = 0.5$

$X_B = 0.27$

at 27% conversion of B #

Correct final solution +2

If XA was used instead of XB, and no other mistakes were made, 2 points deducted out of 5

d)

+1 For correct setup

$$\frac{(P_T v)}{(P_{T0} v_0)} = \frac{F_T' RT}{F_{T0} RT_0}$$ F_T' is the total molar flow rate after condensation

+2 For correct expression of FT'

+1 For correct expression of FT0

$$\frac{v}{v_0} = \frac{F_T'}{F_{T0}} = \frac{F_T'}{2F_{B0}}$$

$$F_T' = F_A + F_B + F_D = F_{B0}(1-0.5X_B) + F_{B0}(1-X_B) + 0.25F_T'$$

$$0.75F_T' = 2F_{B0} - 1.5F_{B0}X_B$$

$$F_T' = 2.67F_{B0} - 2F_{B0}X_B = F_{B0}(2.67 - 2X_B)$$

hence back to $\frac{v}{v_0} = \frac{F_T'}{2F_{B0}} = \frac{F_{B0}(2.67-2X_B)}{2F_{B0}} = (1.33 - X_B)$

$$\boxed{\Rightarrow v = v_0(1.33 - X_B)} \quad \#$$

+1 for correct final answer

Note that yD needs to be written out in actual numbers since yD is not given in the problem

If XA was used instead of XB, and no other mistakes were made, 2 points deducted out of 5

PROBLEM #3 (25 PTS)

$A \rightarrow 2B + 2C \quad , \quad r_{net}$

Elementary reactions :

$A \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} I_1 + 2B \qquad r_1 , r_{-1}$

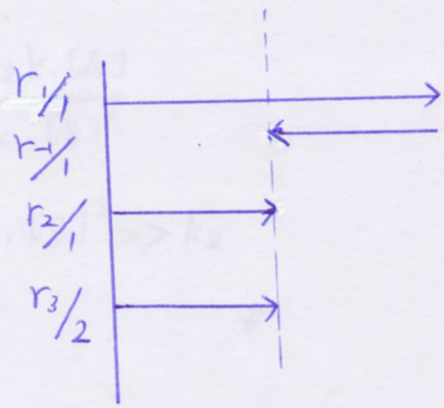
$I_1 \xrightarrow{k_2} 2I_2 \qquad r_2$

$I_2 \xrightarrow{k_3} C \qquad r_3$

a)

Total of 3 points, 1 point deducted for each mistake/ unclearity. (ex. 1 sigma value or 1 label wrong on the diagram)

	σ
$A \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} I_1 + 2B$	1
$I_1 \xrightarrow{k_2} 2I_2$	1
$I_2 \xrightarrow{k_3} C$	2



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

b) $\boxed{r_{net} = r_2 = k_2 [I_1]}$

+1 for a correct expression for setup of rnet (with correct stoichiometry)

PSSH for I_1

rnet can also be expressed as rnet = 0.5*r3

$$\frac{d[I]}{dt} = 0 = k_1 [A] - k_{-1} [I_1][B]^2 - k_2 [I_1]$$

hence

$$[I_1] = \frac{k_1 [A]}{(k_{-1}[B]^2 + k_2)}$$

$$\boxed{r_{net} = \frac{k_1 k_2 [A]}{(k_{-1}[B]^2 + k_2)}} \quad \#$$

+1 for correct expression

PSSH to find correct expression for [I1] +3

If chosen to obtain rnet from rnet=0.5*r3;
PSSH on both intermediates needed
+1 for correct expression for I2
+2 for correct expression for I1

partial credit +1 rewarded for correct rnet:
rnet = r2 or rnet = 0.5*r3

c) In case that QE applies for step 1

+3

$$\frac{k_1}{k_{-1}} = K_1 = \frac{[B]^2[I_1]}{[A]}$$

$$[I_1] = \frac{K_1 [A]}{[B]^2}$$

+1

$$r_{net} = \frac{k_2 K_1 [A]}{[B]^2} \quad \#$$

d)

From b) PSSH

The concept of comparison of the terms in the denominator +5

$$r_{net} = \frac{k_1 k_2 [A]}{k_{-1}[B]^2 + k_2}$$

Correct and clear logic +2
Note that k-1[B]^2 and k2 need to be compared (or r-1 vs r2), the sole comparison of k-1 and k2 is incomplete.

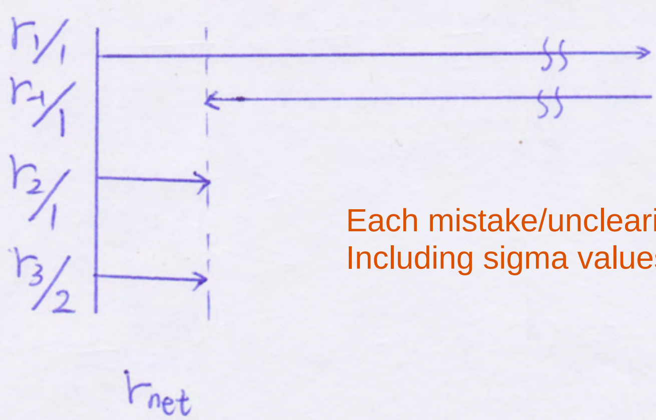
Sole comparison of k-1 and k2 leads to a deduction of 2 points

From c) QE

$$r_{net} = \frac{k_2 K_1 [A]}{[B]^2} = \frac{k_2 k_1 [A]}{k_{-1} [B]^2}$$

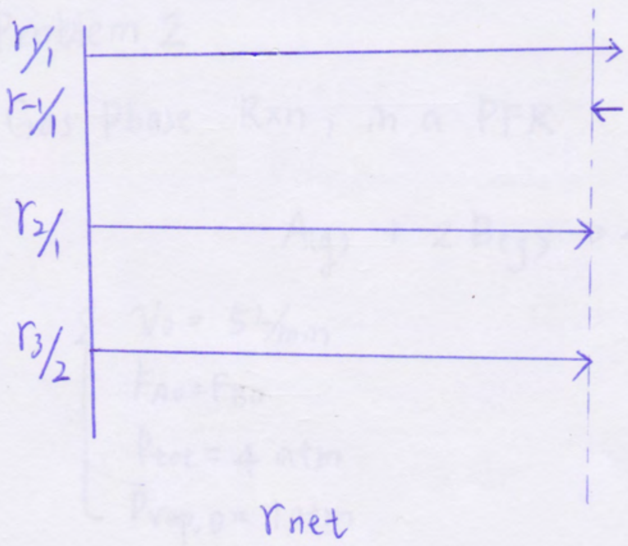
They are the same if $k_{-1}[B]^2 >> k_2$ #

e) QE for step 1



Each mistake/unclearity -1 out of 5 points.
Including sigma values, labeling of rates.

f) Step 1 is irreversible



Each mistake/unclearity -1 out of 5 points.
Including sigma values, labeling of rates.

r-1 must be included in this
diagram(or an explanation in words)
2 points deducted for not labeling r-1

Problem 4

$v = \alpha V + \beta$ } meaning the volumetric flow rate is changing as it moves down each Volume element dV. for

$\tau = \frac{V}{v}$ residence time.

a) $\alpha = 0$

, $v = \beta$ } volumetric flow rate is constant

therefore $\tau_{total} = \frac{V_f}{v} \Rightarrow \boxed{\tau_{total} = \frac{V_f}{\beta}}$ +1

b) $\alpha > 0$

see Matt's (Fall 2017) solution from recent announcement

PROBLEM #5 (25 PTS)

+1 A. from stoichiometry, know $\frac{r_A}{-2} = \frac{r_B}{+1} \rightarrow \boxed{r_A = -2r_B}$ +1/2 for negative sign
+1/2 for having two

+4 B. overall mass balance on all species
given: $\rho = \rho_0$

in − out + gen = accum

+1 $v_s \rho_0 - 0 + 0 = \frac{d(\rho V)}{dt}$ $\rho = \rho_0$, cancel out

$$\frac{dV}{dt} = v_s$$

+2 correct answer

+1 correct volume bounds $\int_{V_0}^{V} dV = \int_0^t v_s \rightarrow V - V_0 = v_s t \rightarrow \boxed{V = V_0 + v_s t}$

+5

$\boxed{\text{using } \frac{dC_A}{dt}}$ $\frac{dN_s}{dt} = C_{so} v_s$ and $\frac{dN_s}{dt} = \frac{d(C_s V)}{dt}$

$C_s \frac{dV}{dt} + V \frac{dC_s}{dt} = C_{so} v_s$

from part b, $\frac{dV}{dt} = v_s$

$V = V_0 + v_s t$

$C_s v_s + (V_0 + v_s t) \frac{dC_s}{dt} = C_{so} v_s$

$\frac{dC_s}{dt} = \frac{C_{so} v_s - C_s v_s}{V_0 + v_s t}$

+1 correct form, plugged V from your part (b) answer

$\int_0^{C_s} \frac{dC_s}{C_{so} v_s - C_s v_s} = \int_0^t \frac{dt}{V_0 + v_s t}$

@ $t=0$, $C_s = 0$ which is why C_s integrated $[0, C_s]$

+1 initial condition or correct bounds

$-\frac{1}{v_s} \left[\ln(C_{so} v_s - C_s v_s) \right]_{C_s = 0}^{C_s = C_s} = \frac{1}{v_s} \left[\ln(V_0 + v_s t) \right]_{t=0}^{t=t}$

$\left[\ln(C_{so} v_s - C_s v_s) \right]_{C_s = 0}^{C_s = C_s} = \left[\ln(V_0 + v_s t) \right]_{t=t}^{t=0}$

$\ln\left(\frac{C_{so} v_s - C_s v_s}{C_{so} v_s} \right) = \ln\left(\frac{V_0}{V_0 + v_s t} \right)$

+1 for any attempt on integration

$\frac{C_{so} v_s - C_s v_s}{C_{so} v_s} = \frac{V_0}{V_0 + v_s t}$

$(C_{so} v_s - C_s v_s)(V_0 + v_s t) = V_0 C_{so} v_s$

$C_{so} v_s V_0 + C_{so} v_s^2 t - C_s v_s V_0 - C_s v_s^2 t = V_0 C_{so} v_s$

$C_{so} v_s^2 t - C_s v_s V_0 - C_s v_s^2 t = 0$

$C_{so} v_s^2 t = C_s v_s (t v_s + V_0)$

$C_s = \frac{C_{so} v_s^2 t}{(V_0 + v_s t) v_s} \longrightarrow \boxed{C_s = \frac{C_{so} v_s t}{V_0 + v_s t}}$

+1 correct answer

+15

D. mole balance on species A

in − out + gen = accum

$$0 - 0 + r_A V = \frac{dN_A}{dt}$$

+2 mole balance

Because nothing coming out, only S enters (no A), and A is consumed based on $-r_A$

$$\frac{dN_A}{dt} = r_A V = -2r_B V$$

(from part A, know $r_A = -2r_B$)

$$\frac{dN_A}{dt} = -2kC_A C_s V$$

+1 for adding part (a) answer, +2 for correct equation or expanded via product rule correctly to dCa/dt

@ this point you can solve via $\frac{dN_A}{dt}$ or $\frac{dC_A}{dt}$. Both methods are valid, shown one by one below:

@ this point, can get +10 additional points using either dNa/dt or dCa/dt method

$\boxed{\text{Using } \frac{dN_A}{dt}}$

$$\frac{dN_A}{dt} = -2kC_A C_s V$$

(plug in C_s from part c)

+1 for Cs substitution from your part (c) answer

$$\frac{dN_A}{dt} = \frac{-2kC_A V\, C_{s0} v_s t}{V_0 + v_s t}$$

(know $N_A = C_A V$)

+1 for correct V substitution from your part (b) answer

+1 for dNa/dt term

$$\frac{dN_A}{dt} = \frac{-2k C_{s0} v_s N_A t}{V_0 + v_s t}$$

$$\int_{N_{A0}}^{N_A} \frac{dN_A}{N_A} = -2kC_{s0} v_s \int_0^t \frac{t}{V_0 + v_s t}\, dt$$

use integral table in the form

$$\int_0^x \frac{x}{ax+b}\, dx$$

$a : v_s$
$b : V_0$

$$\ln\left(\frac{N_A}{N_{A0}}\right) = (-2kC_{s0} v_s)\left[\frac{t}{v_s} + \frac{V_0}{v_s^2} \ln\left(\frac{V_0}{V_0 + v_s t}\right)\right]$$

$$\ln\left(\frac{N_A}{N_{A0}}\right) = -2kC_{s0} t - \frac{2kC_{s0} V_0}{v_s} \ln\left(\frac{V_0}{V_0 + v_s t}\right)$$

up to +2 for attempts on math with correct integration bounds

$$N_A = N_{A0} \exp\left[-2kC_{s0} t - \frac{2kC_{s0} V_0}{v_s} \ln\left(\frac{V_0}{V_0 + v_s t}\right)\right]$$

$$C_A = \frac{N_A}{V} \quad \text{and} \quad C_{A0} = \frac{N_{A0}}{V_0} \rightarrow N_{A0} = C_{A0} V_0$$

$$\boxed{C_A = \frac{C_{A0} V_0 \exp\left[-2kC_{s0} t - \frac{2kC_{s0} V_0}{v_s} \ln\left(\frac{V_0}{V_0 + v_s t}\right)\right]}{V_0 + v_s t}}$$

+5 for correct answer

using $\frac{dC_A}{dt}$

$$\frac{dN_A}{dt} = -2kC_A C_s V$$

Know $N_A = VC_A$

$$\frac{d(VC_A)}{dt} = -2kC_A C_s V$$

plug in C_s from part c)
plug in V from part b

$$V\frac{dC_A}{dt} + C_A\frac{dV}{dt} = \frac{-2kC_A C_{s0}v_s t}{V_0 + v_s t}(V_0 + v_s t)$$

$V \to V_0 + v_s t$

$\frac{dV}{dt} = v_s$

+1 for Cs substitution from your part (c) answer

+1 for correct V substitution from your part (b) answer

$$(V_0 + v_s t)\frac{dC_A}{dt} + v_s C_A = -2kC_A C_{s0} v_s t$$

+1 for dCa/dt term

$$\frac{dC_A}{dt} = \frac{-C_A(2kC_{s0}v_s t + v_s)}{V_0 + v_s t}$$

up to +2 for attempts on math with correct integration bounds

$$\int_{C_{A0}}^{C_A}\frac{dC_A}{C_A} = \int_0^t \frac{-2kC_{s0}v_s t - v_s}{V_0 + v_s t}\,dt$$

use integral table in the form

$$\int_0^x \frac{ax+b}{cx+d}\,dx$$

$a: -2kC_{s0}v_s$
$b: -v_s$
$c: v_s$
$d: V_0$

$$\ln\left(\frac{C_A}{C_{A0}}\right) = \frac{-2kC_{s0}v_s t}{v_s} + \frac{-2kC_{s0}v_s V_0 + v_s^2}{v_s^2}\ln\left(\frac{V_0}{V_0 + v_s t}\right)$$

$$\ln\left(\frac{C_A}{C_{A0}}\right) = -2kC_{s0}t + \left(1 - \frac{2kC_{s0}V_0}{v_s}\right)\ln\left(\frac{V_0}{V_0 + v_s t}\right)$$

$$\boxed{C_A = C_{A0}\exp\left[-2kC_{s0}t + \left(1 - \frac{2kC_{s0}V_0}{v_s}\right)\ln\left(\frac{V_0}{V_0 + v_s t}\right)\right]}$$

+5 correct answer