CHARLES DARWIN UNIVERSITY

Family Name	
Given Names	
Student Number	
Teaching Period	Semester 1, 2017

FINAL EXAMINATION	**DURATION**
ENG443 – Reactor Design	Reading Time: **10** minutes Writing Time: **180** minutes

INSTRUCTIONS TO CANDIDATES

EXAM CONDITIONS

<u>You may begin writing from the commencement of the examination session.</u> The reading time indicated above is provided as a guide only.

This is a CLOSED BOOK examination

Any non-programmable calculator is permitted

No handwritten notes are permitted

No dictionaries are permitted

ADDITIONAL AUTHORISED MATERIALS	**EXAMINATION MATERIALS TO BE SUPPLIED**
No additional printed material is permitted	1 x 16 Page Book 1 x Scrap Paper

THIS EXAMINATION IS PRINTED DOUBLE-SIDED.

THIS PAGE HAS BEEN INTENTIONALLY LEFT BLANK.

<u>Question 1</u> ***(30 marks)***

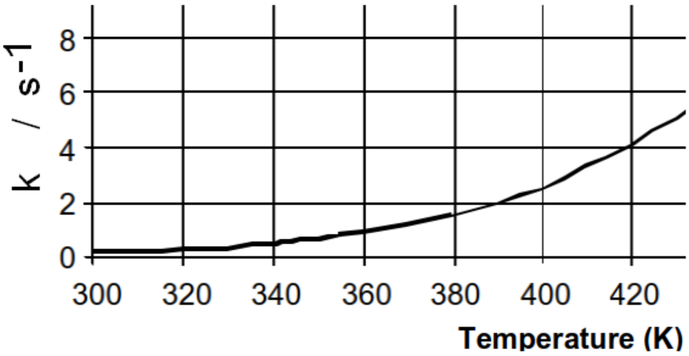
The following reversible, elementary, liquid phase reaction occurs in a CSTR:

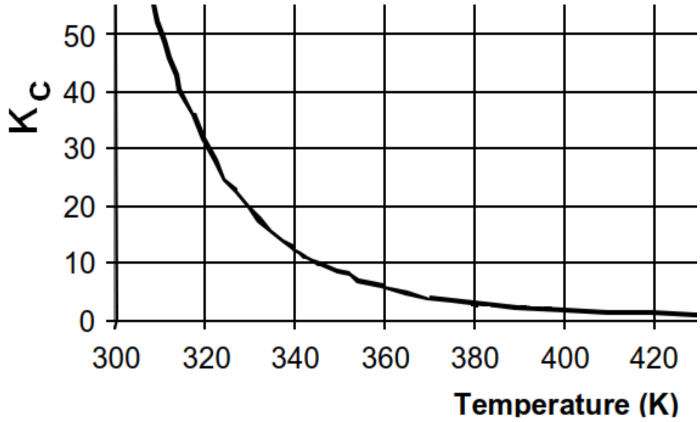
$$\mathbf{A \leftrightarrow B}$$

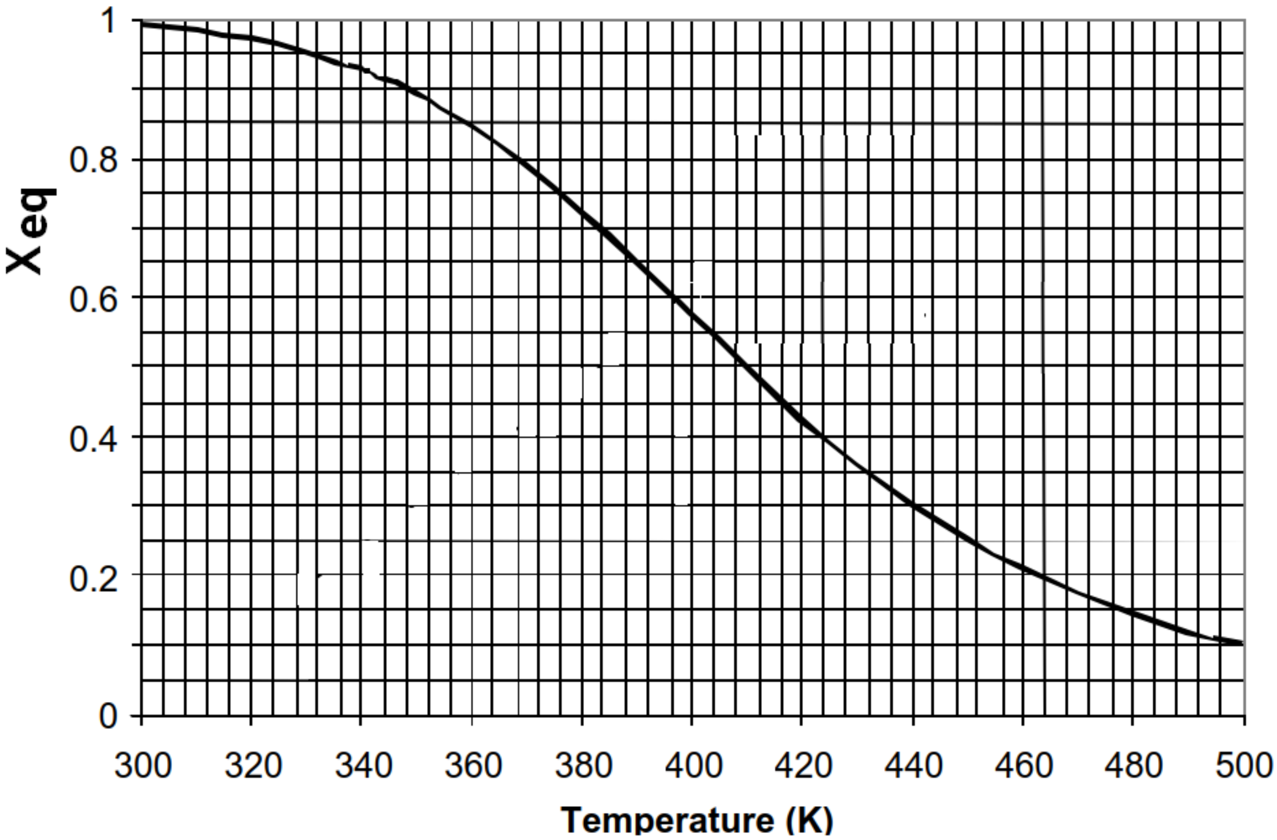
The feed enters at a temperature of 300 K, with a molar concentration of A of 2M. The input flow rate is 10 L/s.

> *What is the reactor volume necessary to achieve **90% of the equilibrium conversion** in a CSTR operated adiabatically?*

<u>Additional information:</u> $C_{pA} = C_{pB} = 60$ cal/(mol.K); $\Delta H^{\circ}_{rxn} = -10{,}000$ cal/mol A. Temperature dependencies of k, K_c and X_{eq} are given below:







Question 2 *(30 marks)*

The following irreversible elementary gas phase reaction:

$$2A \longrightarrow B + C$$

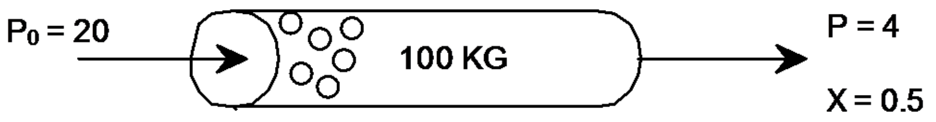
is currently carried out in a packed bed reactor containing 100 kg of catalyst. The entering pressure is 20 atm. Due to pressure drop along the catalyst bed, the exit pressure is 4 atm. A conversion of 50% is achieved with the current arrangement.

It is proposed to add a CSTR with 200 kg of catalyst downstream of the PBR. There is no pressure drop in the CSTR. The flow rate and temperature remain unchanged.

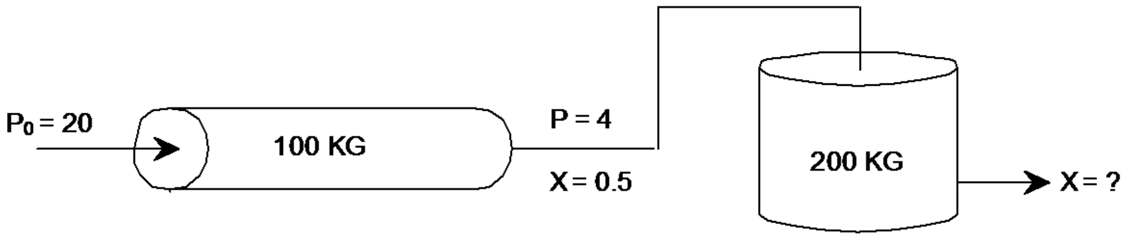
a) *What would be the overall conversion in the proposed arrangement? (Refer to the flow diagrams below).*

b) *Is there a better way to carry out the reaction, and if so what is it?*

Current



Proposed



<u>Question 3</u> ***(20 marks)***

The catalytic reaction A → B is carried out in a flow reaction system. The reaction follows the rate law given by:

$$-r_A = \frac{kC_A}{(1+K_A C_A)^2}$$

where: k = 1 min^{-1}; K_A = 1 dm^3/mol

The entering concentration of A is 2 mol/dm^3. What type of reactor or combination of reactors would have the smallest volume to achieve:

a) *50% conversion?*

b) *80% conversion?*

<u>Note:</u> You may use graph paper on page 7 to solve this problem.

<u>Question 4</u> ***(20 marks)***

The following reactions were found to occur while trying to make a desired product B

$$A \longrightarrow B \qquad -r_{A1} = k_{1A} C_A^2$$

$$A \longrightarrow X \qquad -r_{A2} = k_{2A} C_A$$

$$A + X \longrightarrow Y \qquad -r_{A3} = k_{3A} C_A C_X$$

where: $k_{1A} = 0.5\ e^{-10{,}000/T}$ *min*$^{-1}$; $k_{2A} = 50\ e^{-20{,}000/T}$ *min*$^{-1}$; $k_{3A} = 100\ e^{-5{,}000/T}$ *min*$^{-1}$
T in degrees Kelvin

Species X and Y are both pollutants.

a) *What is the instantaneous selectivity of B with respect to the pollutants X and Y?*
b) *How would you carry out this reaction to maximize the formation of B?*

Resources

Useful integrals

$$\int_0^X \frac{dX}{1-X} = \ln\frac{1}{1-X}$$

$$\int_{X_1}^{X_2} \frac{dX}{(1-X)^2} = \frac{1}{1-X_2} - \frac{1}{1-X_1}$$

$$\int_0^X \frac{dX}{(1-X)^2} = \frac{X}{1-X}$$

$$\int_0^X \frac{dX}{1+\varepsilon X} = \frac{1}{\varepsilon}\ln(1+\varepsilon X)$$

$$\int_0^X \frac{(1+\varepsilon X)dX}{1-X} = (1+\varepsilon)\ln\frac{1}{1-X} - \varepsilon X$$

$$\int_0^X \frac{(1+\varepsilon X)dX}{(1-X)^2} = \frac{(1+\varepsilon X)X}{1-X} - \varepsilon\ln\frac{1}{1-X}$$

$$\int_0^X \frac{(1+\varepsilon X)^2 dX}{(1-X)^2} = 2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon X)^2 X}{1-X}$$

$$\int_0^X \frac{dX}{(1-X)(\Theta_B - X)} = \frac{1}{\Theta_B - 1}\ln\frac{\Theta_B - X}{\Theta_B(1-X)} \quad \text{where } \Theta_B \neq 1$$

$$\int_0^X \frac{a+bX}{c+gX}dX = \frac{bX}{g} + \frac{ag-bc}{g^2}\ln\frac{c+gX}{c}$$

$$\int_0^X \frac{dX}{aX^2+bX+c} = \frac{-2}{2aX+b} + \frac{2}{b} \qquad \text{for } b^2 = 4ac$$

$$\int_0^X \frac{dX}{aX^2+bX+c} = \frac{1}{a(p-q)}\ln\left(\frac{q}{p}\cdot\frac{X-p}{X-q}\right) \qquad \text{for } b^2 > 4ac$$

where p and q are the roots of the equation:

$$aX^2 + bX + c = 0 \qquad \text{i.e., } p, q = \frac{-b \mp \sqrt{b^2 - 4ac}}{2a}$$

$$\int_0^W (1-\alpha W)^{\frac{1}{2}} dW = \frac{2}{3\alpha}\left[1 - (1-\alpha W)^{\frac{3}{2}}\right]$$

Mole balances

Batch

$$\frac{dN_A}{dt} = r_A V \qquad N_{A0}\frac{dX}{dt} = -r_A V \qquad t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V} \qquad t = N_{A0}\int_0^X \frac{dX}{-r_A V}$$

CSTR

$$V = \frac{F_{A0} - F_A}{-r_A} = \frac{F_{A0}X}{-r_A}$$

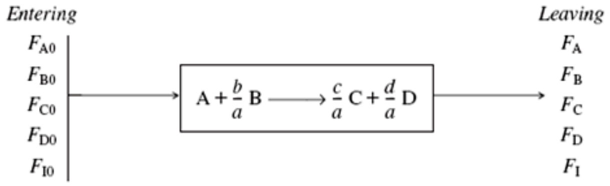
PFR

$$\frac{dF_A}{dV} = r_A \qquad F_{A0}\frac{dX}{dV} = -r_A \qquad V = \int_{F_{A0}}^{F_A} \frac{dF_A}{dr_A} = F_{A0}\int_0^X \frac{dX}{-r_A}$$

PBR

$$\frac{dF_A}{dW} = r'_A \qquad F_{A0}\frac{dX}{dW} = -r'_A \qquad W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A} = F_{A0}\int_0^X \frac{dX}{-r'_A}$$

Stoichiometry



Species	**Symbol**	**Reactor Feed**	**Change**	**Reactor Effluent**
A	A	F_{A0}	$-F_{A0}X$	$F_A=F_{A0}(1-X)$
B	B	$F_{B0}=F_{A0}\Theta_B$	$-b/aF_{A0}X$	$F_B=F_{A0}(\Theta_B-b/aX)$
C	C	$F_{C0}=F_{A0}\Theta_C$	$+c/aF_{A0}X$	$F_C=F_{A0}(\Theta_C+c/aX)$
D	D	$F_{D0}=F_{A0}\Theta_D$	$+d/aF_{A0}X$	$F_D=F_{A0}(\Theta_D+d/aX)$
Inert	I	$F_{I0}=F_{A0}\Theta_I$	----------	$F_I=F_{A0}\Theta_I$
		F_{T0}		$F_T=F_{T0}+\delta F_{A0}X$

$$\Theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}\upsilon_0}{C_{A0}\upsilon_0} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}} \qquad \delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \qquad C_A = \frac{F_A}{\upsilon}$$

$$\upsilon = \upsilon_0 \frac{F_T}{F_{T0}} \frac{P_0}{P} \frac{T}{T_0} \qquad C_i = C_{T0}\left(\frac{F_i}{F_T}\right)\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right) = C_{A0}\left(\frac{\theta_i + v_i X}{1+\varepsilon X}\right)\frac{P}{P_0}\frac{T_0}{T}$$

$$\upsilon = \upsilon_0 \left(1 + y_{A0}\delta X\right)\frac{T}{T_0}\frac{P_0}{P} = \upsilon_0\left(1+\varepsilon X\right)\frac{T}{T_0}\frac{P_0}{P} \qquad \varepsilon = y_{A0}\delta$$

Considering pressure drop

$$\frac{dX}{dW} = \frac{kC_{A0}}{v_0}\left(\frac{1-X}{1+\varepsilon X}\right)^2\left(\frac{P}{P_0}\right)^2\left(\frac{T_0}{T}\right)^2$$

$$W = (1-\varphi)A_c z \rho_c \qquad \beta_0 = -\frac{G(1-\varphi)}{\rho_0 g_c D_p \varphi^3}\left[\frac{150(1-\varphi)\mu}{D_p} + 1.75G\right]$$

$$\frac{dP}{dW} = -\frac{\beta_0}{A_c(1-\varphi)\rho_c}\frac{P_0}{P}\left(\frac{T}{T_0}\right)\frac{F_T}{F_{T0}} \qquad \frac{dy}{dW} = -\frac{\alpha}{2y}\frac{T}{T_0}\frac{F_T}{F_{T0}}$$

$$y = \frac{P}{P_0} \qquad \alpha = \frac{2\beta_0}{A_c(1-\varphi)\rho_c P_0}$$

$$\varepsilon = 0, \quad T_0 = T$$

$$y = \frac{P}{P_0} = (1-\alpha W)^{1/2} = \left(1 - \frac{2\beta_0 z}{P_0}\right)^{1/2}$$

$$g_c = 1\ \mathrm{kg{\cdot}m/N{\cdot}s^2} = 1\ \mathrm{slug{\cdot}ft/lbf{\cdot}s^2} = 32.2\ \mathrm{lbm{\cdot}ft/lbf{\cdot}s^2}$$

Adiabatic Reactors

$$K_C = K_{C1} \exp\left[\frac{\Delta H_{Rx}}{R}\left(\frac{1}{T_2} - \frac{1}{T}\right)\right]$$

$$X_{EB} = \frac{\sum \Theta_i \hat{C}_{P_i}(T - T_0)}{-\Delta H_{Rx}} \qquad X = \frac{\tilde{C}_{P_A}(T - T_0)}{-\Delta H_{Rx}}$$

$$T = T_0 + \frac{(-\Delta H_{Rx})X}{\sum \Theta_i C_{P_i}}$$