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Family Name					
Given Name/s					
Student Number					
Teaching Period	Semester 1, 2019				

ENG443 – Reactor Design	DURATION	
	Reading Time:	10 minutes
	Writing Time:	180 minutes
INSTRUCTIONS TO CANDIDATES		
<ul style="list-style-type: none"> The paper has only one section. Answer All Questions. Please refer to Appendix at the end of the questions for lists of equations that you may need. 		
EXAM CONDITIONS		
<p><u>You may begin writing from the commencement of the examination session.</u> The reading time indicated above is provided as a guide only.</p>		
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 20 Page Book 1 x 8 Page Book 2 x Scrap Paper Graph paper	

**THIS EXAMINATION IS PRINTED
DOUBLE-SIDED.**

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LEFT BLANK.**

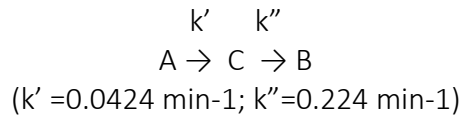
Total Number of Marks: 100

All questions should be answered in the Answer Booklet provided.
Please Note that All Questions are to be answered.

Marks for each question are indicated. Suggested time allocation: 180 mins

Question 1

A liquid phase reaction is carried out isothermally in two CSTRs connected in series. Initially 0.025 mol/L of A is fed to the first CSTR at a flow rate of 25 L/min. In this reaction, C is the intermediate and B is the desired product. Each reactor has equal volume of 500 L. The reaction follows elementary reaction law.



- i. Determine exit concentrations of A, C and B from each of the reactors.

(Marks 20)

- ii. Estimate the overall yield of the desired product.

(Marks 5)

Question 2

- (a) A batch of radioactive material is dumped into a river. At a Dam about 400km downstream, the water flows at 6000 m³/s. The flowing water was monitored for the detection of a particular radioisotope in the river. The data received by monitoring the flow are provided in the **Fig. Q2** below:

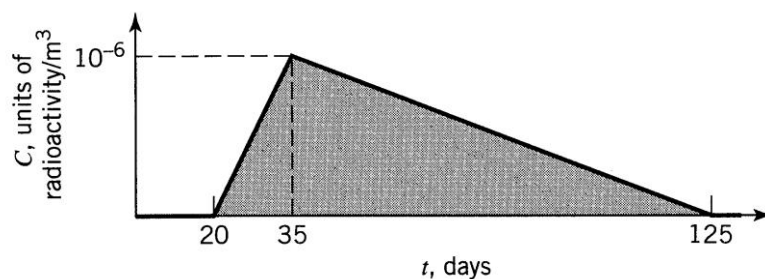


Fig. Q2: Detection of radio activity in the river

- i. Determine the amount of radioactive materials introduced into the river.

(Marks: 05)

- ii. Estimate the volume of the river waters between the Dam and the point of introduction of tracer.

(Marks: 10)

- (b) Develop possible reactor schemes suitable for the following parallel reaction with proper justification. You are required to draw schematics to describe the reactor systems.



(U: undesired product; D= desired product)

(Marks: 10)

Question 3

A first-order catalytic reaction occurs in a 1m^3 packed bed reactor. The reactor is filled with 5-mm-diameter catalyst spheres that occupy 70% of the total reactor volume. The feed concentration is $2 \times 10^{-3} \text{ mol/m}^3$ and the flow rate is $0.001 \text{ m}^3/\text{s}$.

- i. Estimate the conversion in the packed bed reactor if the pseudo-homogeneous rate constant, $k = 4 \times 10^{-3} \text{ s}^{-1}$ was obtained based on the fluid volume.

(Marks 10)

- ii. If the reaction occurs only on the external surface of the catalyst spheres with a rate, $r'' = 2 \times 10^{-6} C_A$, mol/cm².s, estimate the conversion.

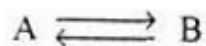
(Marks 10)

- iii. Comment on your results obtained in (i) and (ii).

(Marks: 05)

Question 4

An elementary solid-catalyzed reversible liquid-phase reaction is carried out adiabatically in a PFR.



Pure A enters the reactor at temperature 300K. Equilibrium conversion is 42%.

Additional information are: *Universal gas constant, $R = 1.987 \text{ cal/mol.K}$*

$$\begin{aligned} H_A^\circ(298 \text{ K}) &= -40,000 \text{ cal/mol} & H_B^\circ(298 \text{ K}) &= -60,000 \text{ cal/mol} \\ C_{P_A} &= 50 \text{ cal/mol} \cdot \text{K} & C_{P_B} &= 50 \text{ cal/mol} \cdot \text{K} \\ K_e &= 100,000 \text{ at } 298 \text{ K} \end{aligned}$$

- i. Determine the adiabatic equilibrium temperature of the reactor. (Marks: 07)
- ii. Estimate the equilibrium rate constant, K_e at the equilibrium temperature. (Marks: 04)
- iii. If the reactor would operate in such a way that equilibrium temperature is obtained as 500K, predict the equilibrium conversion and inlet temperature to the reactor? (Marks: 10)
- iv. Qualitatively discuss the effect of different inlet temperatures on the equilibrium conversion. (Marks: 04)

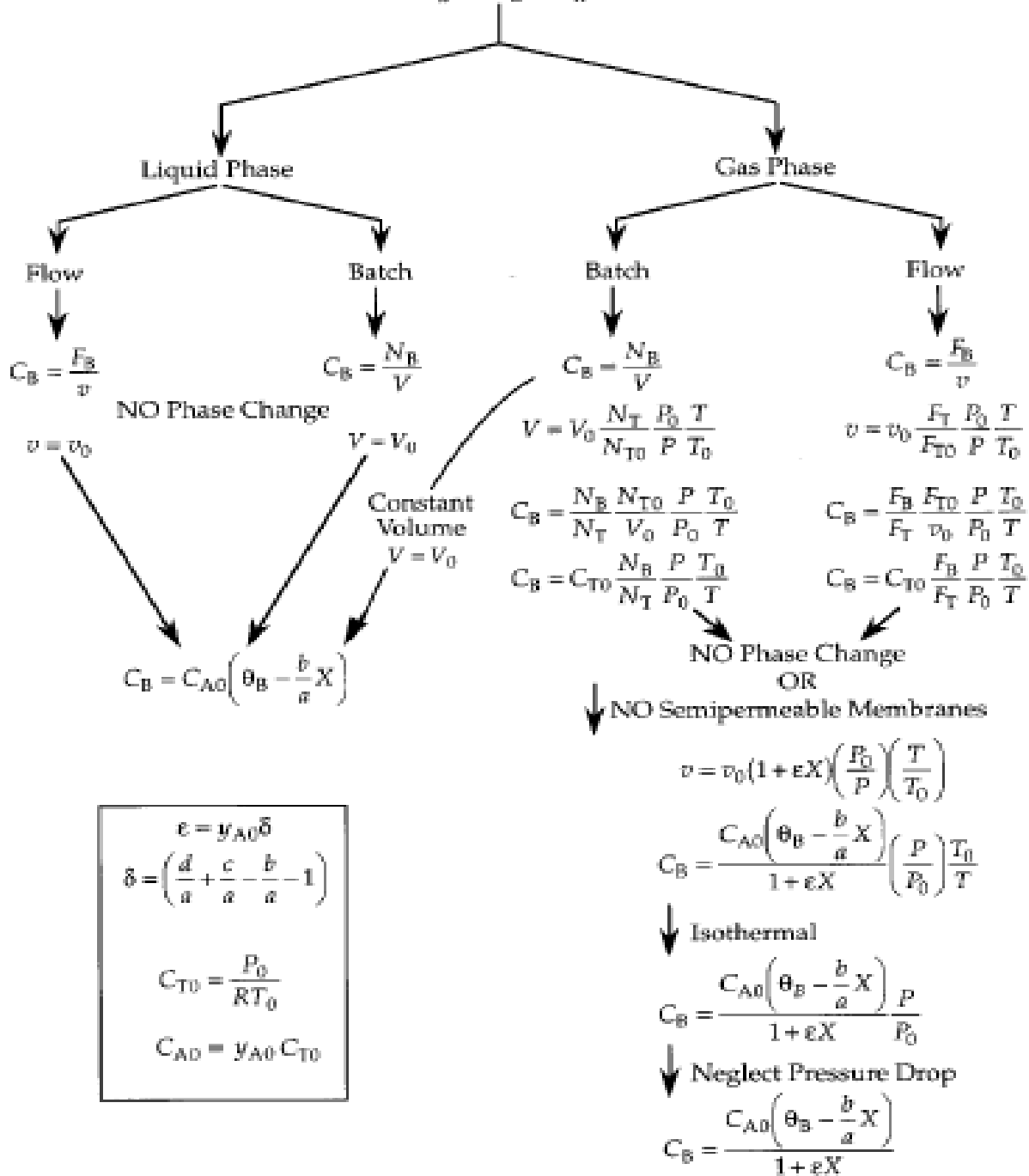
APPENDIX

- I. The general mole balance equation applied to the four major reactor types of reactors for the general reaction $A \rightarrow B$

Reactor	Differential form	Algebraic form	Integral form
Batch	$\frac{dN_A}{dt} = r_A V$ or $N_{A0} \frac{dX}{dt} = -r_A V$	-	$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$ or $t = N_{A0} \int_0^X \frac{dX}{-r_A V}$
CSTR	-	$V = \frac{F_{A0} - F_A}{-r_A}$ or $V = \frac{F_{A0} X}{-r_A}$	-
PFR	$\frac{dF_A}{dV} = r_A$ or $F_{A0} \frac{dX}{dV} = -r_A$	-	$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{dr_A}$ or $V = \int_0^X \frac{F_{A0} dX}{-r_A}$
PBR	$\frac{dF_A}{dW} = r'_A$ or $F_{A0} \frac{dX}{dW} = -r'_A$	-	$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A}$ or $W = \int_0^X \frac{F_{A0} dX}{-r'_A}$

APPENDIX

II. Expressing concentration as a function of conversion for generic reaction:



$$\epsilon = y_{A0} \delta$$

$$\delta = \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \right)$$

$$C_{T0} = \frac{P_0}{RT_0}$$

$$C_{A0} = y_{A0} C_{T0}$$

APPENDIX

III. Pseudo-homogeneous reaction rates for 1st order catalytic reaction:

Basis	r	Units of r	Units of k
volume of fluid in reactor	$-r_A = -\frac{1}{V_{fluid}} \frac{dN_A}{d\tau} = kC_A$	$\frac{mols_reacted}{m^3\ fluid - s}$	$\frac{1}{s}$
weight of catalyst pellets	$-r_A' = -\frac{1}{W} \frac{dN_A}{d\tau} = k'C_A$	$\frac{mols_reacted}{kg_cat - s}$	$\frac{m^3}{kg_cat - s}$
catalyst surface area	$-r_A'' = -\frac{1}{S} \frac{dN_A}{d\tau} = k''C_A$	$\frac{mols_reacted}{m^2\ cat_surface - s}$	$\frac{m}{s}$
volume of catalyst pellets	$-r_A''' = -\frac{1}{V_{cat}} \frac{dN_A}{d\tau} = k'''C_A$	$\frac{mols_reacted}{m^3\ solid - s}$	$\frac{1}{s}$
total reactor volume	$-r_A'''' = -\frac{1}{V_R} \frac{dN_A}{d\tau} = k''''C_A$	$\frac{mols_reacted}{m^3\ reactor - s}$	$\frac{1}{s}$

$$[C] = \frac{moles}{volume} \quad kV_{fluid} = k'W = k''S = -\frac{1}{C_A} \frac{dN_A}{dt}$$

Reactor volume , $V_R = V_{fluid} + V_{cat}$

IV. Residence time distribution for pulse input:

V = vessel volume in [m³]

v = volumetric flow of fluid through the vessel in [m³/s].

M = units of tracer (kg or moles) in to the vessel

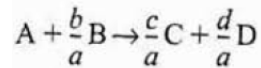
\bar{t} = mean residence time in [s]

(Area under the C_{pulse} curve): $A = \int_0^\infty C dt \cong \sum_i C_i \Delta t_i = \frac{M}{v} \quad \left[\frac{kg \cdot s}{m^3} \right]$

(Mean of the C_{pulse} curve): $\bar{t} = \frac{\int_0^\infty tC dt}{\int_0^\infty C dt} \cong \frac{\sum_i t_i C_i \Delta t_i}{\sum_i C_i \Delta t_i} = \frac{V}{v} \quad [s]$

APPENDIX

V. Equations for non-isothermal reactors for the general reaction:



The heat of reaction at temperature T , per mole of A, is

$$\Delta H_{R_x}(T) = \frac{c}{a}H_C(T) + \frac{d}{a}H_D(T) - \frac{b}{a}H_B(T) - H_A(T)$$

i.

The mean heat capacity difference, ΔC_p , per mole of A is

$$\Delta C_p = \frac{c}{a}C_{pC} + \frac{d}{a}C_{pD} - \frac{b}{a}C_{pB} - C_{pA}$$

ii.

When there are no phase changes, the heat of reaction at temperature T is related to the heat of reaction at the standard reference temperature T_R by

iii.

$$\Delta H_{R_x}(T) = H_{R_x}^\circ(T_R) + \Delta C_p(T - T_R)$$

For adiabatic operation of a PFR, PBR, CSTR, or batch reactor, the temperature conversion relationship is

iv.

$$X = \frac{\sum \Theta_i C_{p_i} (T - T_{i0})}{-[\Delta H_{R_x}^\circ(T_R) + \Delta C_p (T - T_R)]} ; \quad T = \frac{X[-\Delta H_{R_x}^\circ(T_R)] + \sum \Theta_i C_{p_i} T_{i0} + X \Delta C_p T_R}{[\sum \Theta_i C_{p_i} + X \Delta C_p]}$$

The temperature dependence of the specific reaction rate is given

v.

$$k(T) = k_1(T_1) \exp\left[\frac{E}{R} \left(\frac{T - T_1}{TT_1}\right)\right]$$

vi.

Temperature dependant equilibrium rate constant is given as

$$K_e(T) = K_e(T_1) \exp\left[\frac{\Delta H_{R_x}^\circ}{R} \left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$$