UNIVERSITY OF
KWAZULU-NATAL

INYUVESI
YAKWAZULU-NATALI

SCHOOL OF ENGINEERING

EXAMINATIONS: NOVEMBER 2018

COURSE AND CODE: REACTOR TECHNOLOGY FUNDAMENTALS ENCH3RT

DURATION: 3 HOURS

TOTAL MARKS: 100

INTERNAL EXAMINER(S): DR M MKHIZE
MR P BIYELA

INTERNAL MODERATOR(S): DR D LOKHAT

EXTERNAL MODERATOR: PROF K MÖLLER

INSTRUCTIONS:

1. **ALL** questions should be attempted.

2. Any programmable or non-programmable calculator may be used provided it has been cleared of any information that would subvert the purpose of the examination.

3. Calculations must be shown in sufficient detail to illustrate your understanding of the procedure.

4. **Two answer books are provided. Label them Book A and Book B. Answer Section A in Book A and Section B in Book B.**

5. **A graph paper is provided for question 1. Include your student number and submit with Answer book A.**
   Detach page 7 and submit with answer Book A.

SECTION A

QUESTION 1

The following gas phase decomposition takes place in a sealed reactor vessel

$$A \rightarrow 2B + C$$

Experiments were performed at different initial concentrations of A. The data obtained is given in Table 1. Runs 1-5 were conducted at 100°C and Run 6 was conducted at 110°C.

a) Determine the reaction order and reaction rate constant, using the given data. (8)

b) Calculate the activation energy for the reaction. (5)

Run No.	1	2	3	4	5	6
Temp (°C)	100	100	100	100	100	110
C_{A0} (g.mol/L)	0.010	0.025	0.030	0.050	0.075	0.030
Half life, $t_{1/2}$ (min)	12.25	4.86	4.04	2.41	1.60	2.0

$$t_{\frac{1}{2}} = \frac{2^{n-1} - 1}{k(n-1)}\left[\frac{1}{C_{A0}^{n-1}}\right]$$

R = 8.314 J/mol.K

GRAPH PAPER IS PROVIDED. INCLUDE YOUR STUDENT NUMBER AND SUBMIT WITH ANSWER BOOK A.

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QUESTION 2

The elementary, reversible liquid-phase reaction

$$A + B \rightarrow 2C$$

is carried out in a series of adiabatic plug flow reactors with interstage cooling. The feed temperature is 325 K. The feed to the first reactor consists of stoichiometric amounts of A and B.

a) Describe in detail how you would construct the equilibrium curve on a conversion-temperature diagram for this system. Show all necessary equations and state any assumptions. Actual numerical values are not required.

(10)

b) Determine by construction, the number of reactors required to achieve an overall conversion of at least 60% in this system. Assume a 20°C approach to equilibrium in each reactor and allow for cooling back to the original feed temperature between stages. Report the final conversion from the last stage. All stages are full reactor stages up to the prescribed equilibrium approach. Equilibrium data in the form of a conversion-temperature diagram is **provided on page 7. Detach page 7 and submit with answer Book A.**

(12)

Additional Data:

Thermodynamic parameters at 25°C

H_A^o = -10 kJ.mol^{-1}	$\bar{C}_{P,A}$ = 98 J.mol^{-1}.K^{-1}
H_B^o = -20 kJ.mol^{-1}	$\bar{C}_{P,B}$ = 46 J.mol^{-1}.K^{-1}
H_C^o = -45 kJ.mol^{-1}	$\bar{C}_{P,C}$ = 72 J.mol^{-1}.K^{-1}

$K_c = 55\ 000$ at 298 K

R = 8.314 K.mol^{-1}.K^{-1}

General Energy Balance Equation

$$\dot{Q} - \dot{W}_s - \left[\Delta H_{rxn}^o(T_{ref}) + \Delta\hat{C}_p(T - T_{ref})\right]F_{A0}X = F_{A,0}\sum_{i=1}^{n}\frac{F_{i,0}}{F_{A,0}}\bar{C}_{p,i}(T_i - T_{i,0})$$

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QUESTION 3

Solid particles with a radius R = 2 mm are processed in a batch reactor up to a conversion of 70% in a time of 5 min. The gas composition in the reactor is uniform. Under the conditions of the experiment the chemical reaction step is known to be controlling.

The same solid is now processed in a rotating kiln (the flow pattern resembles that of a plug flow reactor). The feed consists of equal fractions by weight of 2 mm and 3 mm particles. If the gas composition in the kiln is uniform and the residence time of the solids is 18 min, what is the mean conversion of solids in the unit?

Rate controlling step	Complete conversion time	Plug flow/Batch $\frac{t}{\tau}$	Mixed flow $1-\bar{X}_B$
Gas film	$\frac{\rho_B R}{3bk_g C_{As}}$	X_B	$1-\frac{1-e^{-\tau/\bar{t}}}{\frac{\tau}{\bar{t}}}$
Ash layer	$\frac{\rho_B R^2}{6bD_e C_{Ag}}$	$1-3(1-X_B)^{2/3}+2(1-X_B)$	$\frac{1}{5}\frac{\tau}{\bar{t}}-\frac{19}{420}\left(\frac{\tau}{\bar{t}}\right)^2+\frac{41}{4620}\left(\frac{\tau}{\bar{t}}\right)^3 \cdots$
Reaction	$\frac{\rho_B R}{bk_s C_{Ag}}$	$1-(1-X_B)^{1/3}$	$\frac{1}{4}\frac{\tau}{\bar{t}}-\frac{1}{20}\left(\frac{\tau}{\bar{t}}\right)^2+\frac{1}{120}\left(\frac{\tau}{\bar{t}}\right)^3$

$$1-\bar{X}_B=\sum(1-X_{B_i})\Phi_i$$

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SECTION B

QUESTION 4

Consider the solid-catalysed gas-solid reaction, for which stoichiometric equation is

$$A_2 \leftrightarrows P \quad \text{(R1)}$$

In terms of elementary reaction steps the mechanism is as follows:

$$A_2 + 2S \underset{k_{dA_2}}{\overset{k_{aA_2}}{\rightleftarrows}} 2A \cdot S \quad \text{(R2)}$$

$$A \cdot S \underset{k_{rS}}{\overset{k_{fS}}{\rightleftarrows}} P \cdot S \quad \text{(R3)}$$

$$P \cdot S \underset{k_{aP}}{\overset{k_{dP}}{\rightleftarrows}} P + S \quad \text{(R4)}$$

Derive an intrinsic rate expression assuming that the surface reaction step is rate-limiting.

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QUESTION 5

Pure reactant A is fed at a feed rate of 650 mol/s and converted according to the elementary reaction,

$$2A \rightarrow B$$

Estimate the mass of the catalyst required to give 75% conversion of A. The effective diffusivity is 3×10^{-4} m²/s, the particles are spheres with a particle diameter of 4 mm, and density of the catalytic bed particles is 1 000 kg/m³ bed. The voidage is 0.5 and the volumetric flow rate through the bed is assumed constant at 5 m³/s. External mass transfer resistances can be ignored but internal diffusion resistances are significant.

$$\phi = L\sqrt{\frac{n+1}{2}\frac{\rho_p S_g k C_s^{n-1}}{D_{Ae}}}$$

$$\eta_{int} = \frac{1}{\phi}$$

$$k_m = 2 \times 10^{-2}\ \mathrm{m^6/mol/kg/s}$$

Simpson's rule: $\int_{X_0}^{X_3} f(X)dX = \frac{3}{8}h[f(X_0) + 3f(X_1) + 3f(X_2) + f(X_3)]$

Where:

$h = \frac{X_3 - X_0}{3}$; $X_1 = X_0 + h$; $X_2 = X_0 + 2h\ldots.$

Catalytic fixed bed reactor design equation: $\frac{dF_A}{dW} = -\eta_{int} k_m C_A^2$

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QUESTION 6

Given the first-order reaction:

$$A \rightarrow B$$

The external-age residence time function is shown in the Figure 1 below:

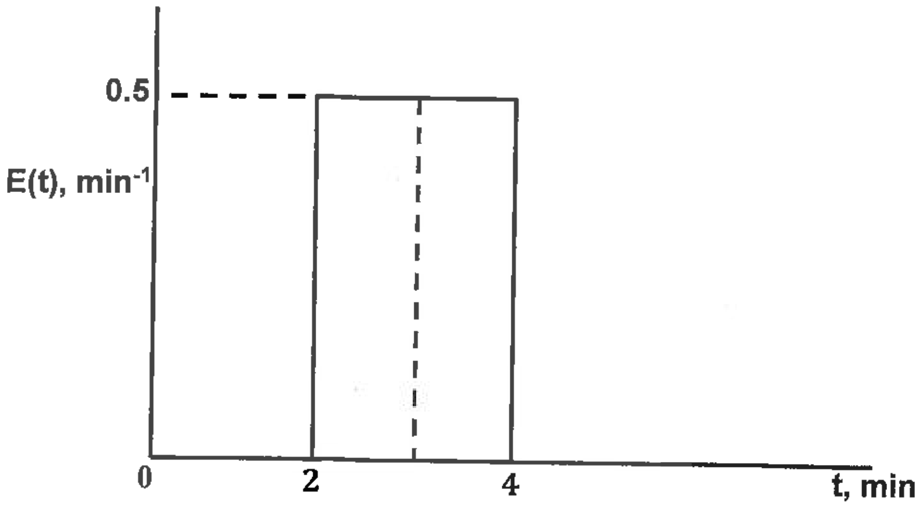

Figure 1

For $t < 2, \Rightarrow E(t) = 0;$
For $2 \leq t \leq 4, \Rightarrow E(t) = 0.5$
For $t > 4, \Rightarrow E(t) = 0$

Determine the,

a) Mean residence time, t_m, (2)

b) Variance, σ^2, (6)

c) Conversion X, predicted by the segregation model, (5)

$$\int_0^\infty E(t)dt = 1$$

$$\sigma^2 = \int_0^\infty (t-\tau)^2 E(t)dt = \int_0^\infty t^2 E(t)dt - \tau^2$$

$k = 0.8\ min^{-1}$

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CONVERSION-TEMPERATURE DIAGRAM FOR QUESTION 2

DETACH THIS PAGE AND SUBMIT WITH ANSWER BOOK A

STUDENT NUMBER