UNIVERSITY OF
KWAZULU-NATAL

INYUVESI
YAKWAZULU-NATALI

SCHOOL OF ENGINEERING

MAIN EXAMINATIONS: NOVEMBER 2019

COURSE AND CODE: REACTOR TECHNOLOGY FUNDAMENTALS ENCH3RT

DURATION: 3 HOURS

TOTAL MARKS: 100

INTERNAL EXAMINER(S): PROF R RAWATLAL
DR M MKHIZE

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. **Two graph papers are provided for question 1 and 2. Include your student number and submit with Answer book A.**

SECTION A

QUESTION 1

A small-batch constant volume reactor is filled with pure reactant A at a pressure of 1 atm. The reactor is at 25 °C, a temperature low enough that the reaction does not proceed to any appreciable extent. The temperature is then raised as rapidly as possible to 100°C by plunging the reactor into boiling water, and the readings in Table 1 below are obtained. The stoichiometry of the reaction is,

$$2A \longrightarrow B$$

After leaving the reactor in the bath over the weekend the contents are analysed for A. None can be found.

Find a rate equation in units of moles, liters, and minutes which will satisfactorily fit the data.

Table 1: Pressure versus time data

t (min)	1	2	3	4	5	6	7	8	9	10	15	20
P (atm)	1.14	1.04	0.982	0.94	0.905	0.87	0.85	0.832	0.815	0.8	0.754	0.728

Additional data:

R = 82.057 $cm^3.atm.mol^{-1}.K^{-1}$

Batch

$$\frac{dX_i}{dt} = \frac{-r_i V}{N_{i,0}}$$

$$t = N_{i,0}\int_0^{X(t)} \frac{dX_i}{-r_i V}$$

CSTR

$$V = \frac{F_{i,0}X_i}{-r_i}$$

PFR

$$\frac{dX_i}{dV} = \frac{-r_i}{F_{i,0}}$$

$$V = F_{i,0}\int_0^{X} \frac{dX_i}{-r_i}$$

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

TOTAL /15/

QUESTION 2

A three-stage CSTR is used for the reaction A $\longrightarrow$ products. The reaction occurs in an aqueous solution, and is second-order with respect to A, with k_A = 0.040 L.mol^{-1}.min^{-1}. The inlet concentration of A and the inlet volumetric flow rate are 1.5 mol.L^{-1} and 2.5 L.min^{-1}, respectively.

Determine the fractional conversion (X_A) obtained at the outlet, if V_1 = 10 L, V_2 = 20 L, and V_3 = 50 L. Use the graphical method.

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

TOTAL /20/

QUESTION 3

A kinetics study of the reaction,

$$A(g) + 2B(s) \longrightarrow products\ (s, g)$$

yielded the following values of parameters for 2 cm spherical particles at 323 °C and $p_A = 200$ kPa:

$$\tau = 4.92 \times 10^{5}\ s; \qquad k_{Ag} = 9.2 \times 10^{-5}\ m.s^{-1}$$

$$k_{As} = 48.85 \times 10^{-5}\ m.s^{-1} \qquad D_e = 8.37 \times 10^{-7}\ m^{2}.s^{-1}$$

3.1. Determine the mean fractional conversion ($\bar{X}_B$) for the mean time $\bar{t} = 75$ h assuming:

a) Reaction rate control,

b) Ash-layer diffusion control, and

c) Gas-film mass transfer control.

(10)

3.2. Comment on the significance of the error due to the assumption of the single rate-controlling step.

(5)

Additional data:

Rate controlling step	Batch reactor or Plug flow reactor		
Gas film	$\tau = \frac{\rho_B R}{3bk_g C_{Ag}}$	$X_B = \frac{t}{\tau} = 1 - \left(\frac{r_c}{R}\right)^3$	$\bar{X}_B = \frac{\bar{t}}{\tau}\left(1 - e^{-\tau/\bar{t}}\right)$
Ash layer	$\tau = \frac{\rho_B R^2}{6bD_e C_{Ag}}$	$\frac{t}{\tau} = 1 - 3(1 - X_B)^{\frac{2}{3}} + 2(1 - X_B)$	$1 - \bar{X}_B = \frac{1}{5}\frac{\tau}{\bar{t}} - \frac{19}{420}\left(\frac{\tau}{\bar{t}}\right)^2 + \frac{41}{4620}\left(\frac{\tau}{\bar{t}}\right)^3 - 0.00149\left(\frac{\tau}{\bar{t}}\right)^4$
Reaction	$\tau = \frac{\rho_B R}{bk_s C_{Ag}}$	$\frac{t}{\tau} = 1 - \frac{r_c}{R} = 1 - (1 - X_B)^{\frac{1}{3}}$	$1 - \bar{X}_B = \frac{1}{4}\frac{\tau}{\bar{t}} - \frac{1}{20}\left(\frac{\tau}{\bar{t}}\right)^2 + \frac{1}{120}\left(\frac{\tau}{\bar{t}}\right)^3$

TOTAL /15/

SECTION B

QUESTION 4

In the catalysed conversion of components A and B to form C whose overall reaction is given by

$$A_2 + B \rightarrow C$$

it is known that A reversibly dissociates and adsorbs onto two vacant sites in one step before being reversibly attacked by B (directly from the gas phase) to yield one absorbed C and one free site. The adsorbed C then reversibly desorbs. Determine the intrinsic rate expression for the case of C desorption being limiting.

TOTAL /10/

QUESTION 5

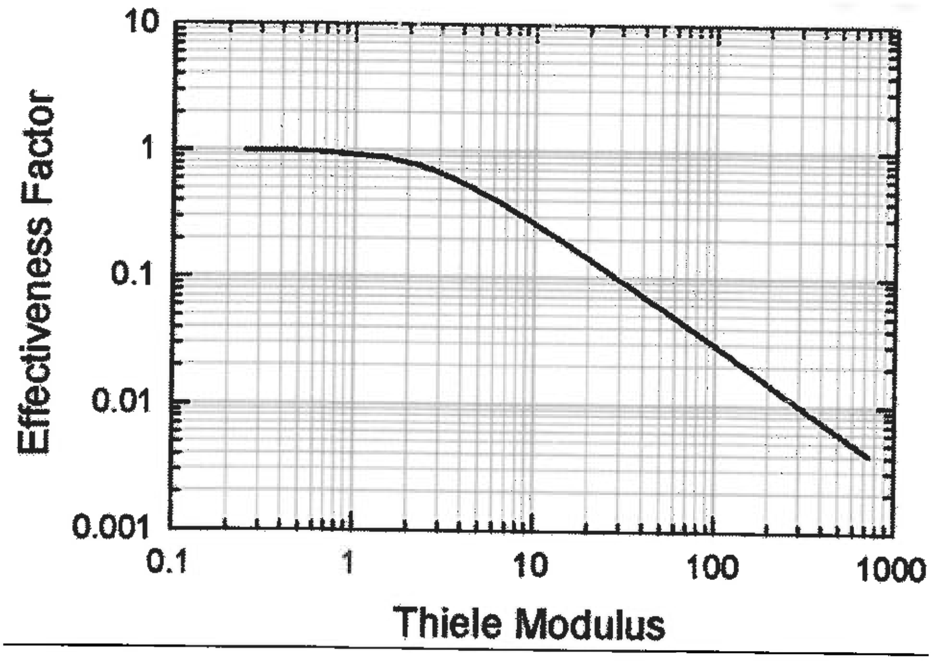
Consider a reaction carried out in a batch reactor catalysed by 5 cm (diameter) spherical particles in which the **second order reaction** occurs

$$-r_A'' = k_s.c_A^2, \quad k_s = 6.3 \times 10^{-12} m/s$$

Due to the porous highly reactive nature of the catalyst, it is suspected that the internal mass transfer resistance is significant, but that due to the high level of agitation in the reactor external transfer resistance can be ignored.

We note that for a **first order** reaction, the Thiele Modulus ϕ is given by

$$\phi = \sqrt{\frac{k_s.S_a.\rho_{crys}}{D_{AB}}}.L$$



The reactor is initially charged with a concentration of A of 35 $mol.m^{-3}$, the catalyst bed is packed at $\rho_{bed} = 700 \frac{kg}{m^3}$ and the catalyst specs are $\rho_{crys} = 8500 \frac{kg}{m^3}$, $S_a = 250 m^2/kg$. The effective diffusivity is $5.3 \times 10^{-9} m^2/s$.

QUESTION 5 continued ...

a) Propose a modified version of the material balance such that a pseudo-first-order reaction expression can be used.

(5)

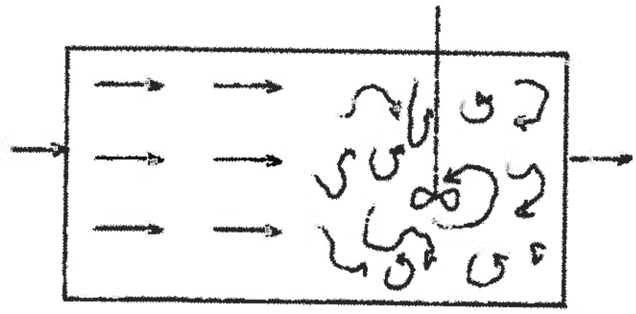
b) Estimate the overall conversion after 15 hrs of batch operation. (If you cannot convert to a first order reaction, develop your answer assuming it is first order.) (Apply a maximum of 3 iterations.)

(15)

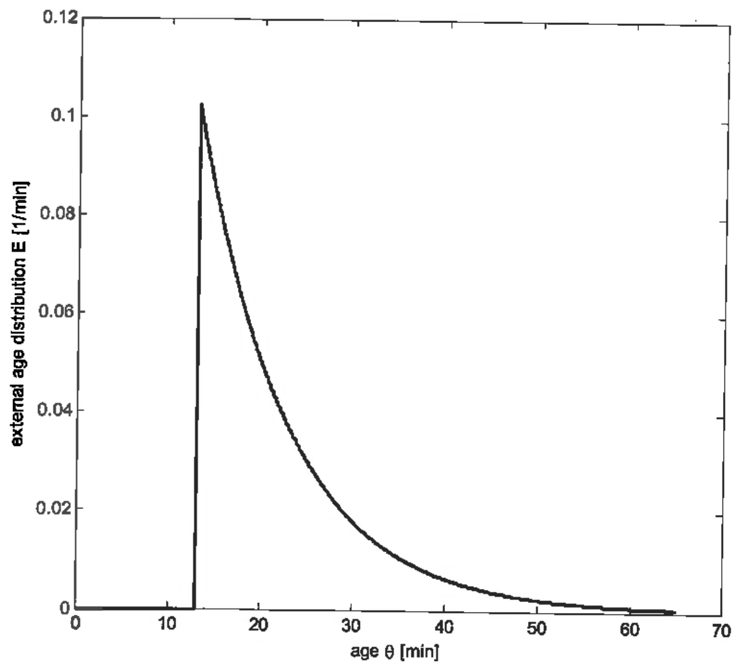
TOTAL /20/

QUESTION 6

In a certain reactor, there are indications that the flow pattern is as shown in the figure below. In addition, there is concern that there exists a significant dead zone in the reactor that effectively reduces the total reaction volume. The real volume of the reactor is 65 m^3 and the volumetric flowrate is 2 m^3/min.



A pulse tracer study yields the following exit age distribution.



a) Develop a model of the exit age distribution $E(\theta)$.

(8)

b) What is the dead zone volume in the reactor?

(7)

c) If the reactor is fed with non-coalescing oil droplets in which a first order reaction (rate constant = $2\text{x}10^{-2}$ min^{-1}) is consuming component A, what is the overall conversion in the reactor?

(5)

TOTAL /20/