BITS, PILANI – DUBAI CAMPUS

FIRST SEMESTER 2011 – 2012

THIRD YEAR

COMPREHENSIVE EXAMINATION

Course Code: CHE C312 Date: 12.01.12

Course Title: Kinetics and Reactor Design Max Marks: 80

Duration: 3 hr (Closed Book) Weightage: 40%

Note: Attempt ALL questions. Mention appropriate units in your answers. Without units, the answer will not be deemed as correct, even if the numerical value is correct. Cleary show all calculation steps. Use graph sheets if needed.

1.(a) The exothermic reaction A → B + C was carried out adiabatically and the following data recorded. The entering molar flow rate of A was 5 mol/sec. (6 m)

X_A	0	0.2	0.4	0.5	0.6	0.8	0.9
$-r_A$ mol/lit min	10	16.67	50	50	50	12.5	9.09

i What are the PFR and CSTR volumes necessary to achieve 40% conversion? (4 m)

ii Over what range of conversions would be the CSTR and PFR reactor volumes are identical? (2 m)

1.(b) A reaction takes place in constant volume batch reactor under constant temperature. Using the following data obtain the suitable rate equation. The data are C_{A0} = 0.37 mol/lit. (13 m)

t, min	5	10	15	20	25	30	40	50	60
C_A mol/lit	0.285	0.208	0.164	0.136	0.115	0.1	0.08	0.066	0.056

2.(a) The data in table have been obtained on the decomposition of gaseous reactants A in a constant volume batch reactor at 100°C,1 atm with 100 mol of A/hr in a feed consisting of 20% inerts. The stoichiometry of the reaction is 2A → R + S. Obtain the suitable rate equation by differential method of analysis. (12 m)

t, sec	0	40	60	80	100	120	140	160
C_A, mol/L	1	0.80	0.56	0.32	0.18	0.08	0.04	0.02

2.(b) Given the two reactions

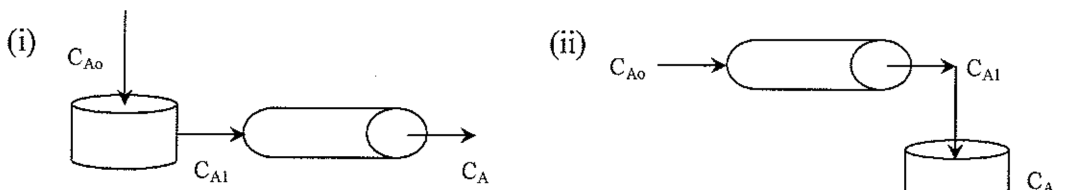
a_1 A → R (with k_1 rate constant); a_2 A → S (with k_2 rate constant)

Where R is the desired product and is to be maximized. Discuss type of the reactors and favorable conditions for the maximization of product R for the following cases (6 m)

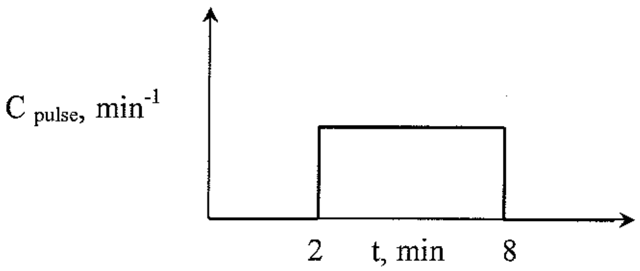
i) $a_1 > a_2$ ii) $a_1 < a_2$ iii) $a_1 = a_2$

3.(a) The kinetics of the aqueous-phase decomposition of A is investigated in two mixed flow reactors in series, the second having twice the volume of the first reactor. At steady state with a feed concentration of 1 mol A/liter and mean residence time of 96 sec in the first reactor, the concentration in the first reactor is 0.5 mol A/liter and in the second is 0.25 mol A/liter. Find the order and rate constant for the decomposition. (8 m)

3.(b) In the first system an ideal CSTR is followed by an ideal PFR; in the second system the PFR precedes the CSTR. Let τ_s and τ_p each equal 1 min, let the reaction rate constant equal $1 m^3/kmol$ min and let the initial concentration of liquid reactant, C_{Ao} equal 1 $kmol/m^3$. Find the overall conversion in each system. Comment on your results (10 m)



4.(a) Dispersed noncoalescing droplets (C_{Ao} = 2 mol/liter) react (A→R, k = 0.5 liter/mol.min) as they pass through a contactor. With E = 0.06 for 2<t<8. Find the average concentration of A remaining in the droplets leaving the contactor if their RTD is given by the curve in figure below. (6 m)



4.(b) The first-order reaction A→R is carried out in a 10-cm-diameter tubular reactor 6.36 m in length. The specific reaction rate is 0.25 min^{-1}. The results of a tracer test carried out on this reactor are shown in table

t(min)	0	1	2	3	4	5	6	7	8	9	10	12	14
C (mg/L)	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

Calculate conversion using (1) the closed vessel dispersion model, (2) PFR, (3) the tanks-in-series model, and (4) a single CSTR. (13 m)

5.(a) Discuss the steps in a heterogeneous catalytic reaction (3 m)

5.(b) Express different ways of representing the relationship of temperature, composition, and rate for a single homogeneous reaction. (3 m)

BITS, PILANI – DUBAI CAMPUS

FIRST SEMESTER 2011 – 2012

THIRD YEAR

Course Code: CHE C312 **TEST 2** Date: 22.12.11

Course Title: Kinetics and Reactor Design Max Marks: 20

Duration: 50 minutes (Open Book) Weightage: 20%

Answering Scheme

Note : Permitted to use "only prescribed Text book and original hand written notes" for the open book evaluation component. No photocopies of any sought shall be permitted.

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1. The gaseous reaction A → B has a unimolecular reaction rate constant of 0.0015 min^{-1} at 300K. This reaction is to be carried out in parallel tubes 300cm long and 2.5cm inside diameter under a pressure of 10 atm at 400K. A production rate of 453 kg/h of B is required. Assuming activation energy of 104,600 J/gmol, how many tubes are needed if the conversion of A is to be 90%? Assume perfect gas laws. A and B each have molecular weights of 58. (R = 0.0821 atm L/ mol K) (10 m)

Given data F_{Bo} = 453/58 = 7.8 kg mol/hr; F_{Ao} = 7.8/ 0.9 = 8.66 kg mol/hr

K1 = 0.0015 min^{-1} at 300K

$K_2 = K_1 \exp [E/R (1/T_1 - 1/T_2)]$

$= 0.0015 \times 60 \times \exp [(104600 / 0.0821)(1/300 - 1/400)] = 3217\ hr^{-1}$ at 400K

$$V = -\frac{F_{AO}}{KC_{AO}}\ln(1-X_A) = \frac{F_{AO}RT}{KP_A}\ln(1-X_A) = -\frac{8.66\times10^3\times0.0821\times400}{3217\times10}\ln(1-0.9) = 20\,L$$

Wkt $V = (n_t \pi D^2 L)/4$; $n_t = 4 \times 20 \times 10^3 / \pi\, 2.5^2 \times 300 = 13.7 \approx 14$ pipes

2. A RTD study was carried out in a tank for different stirring speeds. The inlet and exit flow rates were 1.15 L/min and the initial concentration of 0.8 mol/L. The tracer results for the relative concentration, C/C_o shown the below table.

	Impeller Speed (rpm)	
Time (min)	C/C_o for 170 rpm	C/C_o for 100 rpm
0	1	1
10	0.761	0.653
15	0.695	0.566
20	0.639	0.513
25	0.592	0.454
30	0.543	0.409
35	0.502	0.369
40	0.472	0.333
45	0.436	0.307
50	0.407	0.276
55	0.376	0.248
60	0.35	0.226
65	0.329	0.205

a) Calculate or plot the F curve. Give comments on dead zones and bypassing at the different stirrer speeds. (5 m)

b) What conversion can be expected (for any impeller speed) for a second order reaction with K C_o = 0.05/min at 320 K for the segregation model? (5 m)

For 170 rpm									
t	c/co	F(t)	delta t	c (t)	c(t) * delta t	E (t)	E (t) * delta t	X	mean X
0	1	0	-	0.8	-	0.029144	-	0	-
10	0.761	0.239	10	0.6088	6.088	0.022179	0.221785064	0.333333	0.073928
15	0.695	0.305	5	0.556	2.78	0.020255	0.101275046	0.428571	0.043404
20	0.639	0.361	5	0.5112	2.556	0.018623	0.093114754	0.5	0.046557
25	0.592	0.408	5	0.4736	2.368	0.017253	0.086265938	0.555556	0.047926
30	0.543	0.457	5	0.4344	2.172	0.015825	0.079125683	0.6	0.047475
35	0.502	0.498	5	0.4016	2.008	0.01463	0.073151184	0.636364	0.046551
40	0.472	0.528	5	0.3776	1.888	0.013756	0.068779599	0.666667	0.045853
45	0.436	0.564	5	0.3488	1.744	0.012707	0.063533698	0.692308	0.043985
50	0.407	0.593	5	0.3256	1.628	0.011862	0.059307832	0.714286	0.042363
55	0.376	0.624	5	0.3008	1.504	0.010958	0.054790528	0.733333	0.04018
60	0.35	0.65	5	0.28	1.4	0.0102	0.051001821	0.75	0.038251
65	0.329	0.671	5	0.2632	1.316	0.009588	0.047941712	0.764706	0.036661
					27.452		1.00007286		**0.553134**
For 100 rpm									
t	c/co	F(t)	delta t	c (t)	c(t) * delta t	E (t)	E (t) * delta t	X	mean X
0	1	0	-	0.8	-	0.038373	-	0	-
10	0.653	0.347	10	0.5224	5.224	0.025058	0.250575595	0.333333	0.083525
15	0.566	0.434	5	0.4528	2.264	0.021719	0.108595549	0.428571	0.046541
20	0.513	0.487	5	0.4104	2.052	0.019685	0.098426708	0.5	0.049213
25	0.454	0.546	5	0.3632	1.816	0.017421	0.087106677	0.555556	0.048393
30	0.409	0.591	5	0.3272	1.636	0.015695	0.078472755	0.6	0.047084
35	0.369	0.631	5	0.2952	1.476	0.01416	0.070798158	0.636364	0.045053
40	0.333	0.667	5	0.2664	1.332	0.012778	0.063891021	0.666667	0.042594
45	0.307	0.693	5	0.2456	1.228	0.011781	0.058902533	0.692308	0.040779
50	0.276	0.724	5	0.2208	1.104	0.010591	0.05295472	0.714286	0.037825
55	0.248	0.752	5	0.1984	0.992	0.009517	0.047582502	0.733333	0.034894
60	0.226	0.774	5	0.1808	0.904	0.008672	0.043361474	0.75	0.032521
65	0.205	0.795	5	0.164	0.82	0.007866	0.03933231	0.764706	0.030078
					20.848		1		**0.538499**

BITS, PILANI – DUBAI CAMPUS
FIRST SEMESTER 2011 – 2012
THIRD YEAR
TEST 1

Course Code: CHE C312 | Date: 03.11.11
Course Title: Kinetics and Reactor Design | Max Marks: 25
Duration: 50 minutes | Weightage: 25%

(Closed Book)

Answering Scheme

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1. The liquid-phase reaction

$$A + B \rightarrow C$$

follows an elementary rate law and is carried out isothermally in a flow system. The concentrations of the A and B feed streams are 2 M before mixing. The volumetric flow rate of each stream is 5 dm^3/min, and the entering temperature is 300 K. The streams are mixed immediately before entering. Two reactors are available. One is a gray 200 dm^3 CSTR operated at 77°C and the other is a white 800 dm^3 PFR operated at 300 K.

Note : k = 0.07 dm^3/mol-min at 300 K and E = 20 kcal/mol, R =1.987cal/mol K.

a) Determine conversion of the CSTR and PFR. (7 + 7 m)

(b) How long would it take to achieve 90% conversion in a 200-dm^3 batch reactor with C_{Ao}= C_{Bo}= I M after mixing at a temperature of 77°C? (3 m)

(c) What would your answer to part (b) be if the reactor were cooled to O°C? (3 m)

a) $K_2 = K_1 \exp [E/R (1/T_1 - 1/T_2)] = 8.45$ dm^3/mol.min at 350K

CSTR: at 350K; $X_A = 96\%$

PFR : $1/C_A = 1/C_{Ao} + K\tau$ at 300K; K = 0.07 dm^3/mol-min; $X_A = 85\%$

b) $1/C_A = 1/C_{Ao} + Kt$ at 300K; K = 0.07 dm^3/mol-min; $X_A = 90\%$; t = 1.06 min

c) new K = 2.54×10^{-3} dm^3/mol-min at 0°C; t = 3543 min = 2.46 days

2. The liquid-phase irreversible reaction

$$A \rightarrow B + C$$

is carried out in a CSTR. To learn the rate law the volumetric flow rate is varied and the effluent concentrations of species recorded as a function of the space time. Pure A enters the reactor at a concentration of 2 mol/dm^3. Steady-state conditions exist when the measurements are recorded.

Run	1	2	3	4	5
Space time (min)	15	38	100	300	1200
C_A (mol/dm^3)	1.5	1.25	1	0.75	0.5

Determine the reaction order and specific reaction rate (without using graph) (5 m)

CSTR: n = 1 $\tau / C_{Ao} = X_A / KC_A$; $K = (C_{Ao} - C_A)/C_A \tau$

$K_1 = 0.022$, $K_2 = 0.0157$, $K_3 = 0.01$, $K_4 = 0.005$ hence $K_1 \neq K_2 \neq K_3 \neq K_4$

n = 3 ; $\tau / C_{Ao} = X_A / KC^3{}_A$;$K = (C_{Ao} - C_A)/C^3{}_A \tau$

$K_1 = 0.009$, $K_2 = 0.01$, $K_3 = 0.01$, $K_4 = 0.0098$, $K_5 = 0.01$ hence $K_1 = K_2 = K_3 = K_4 = K_5$

Hence the rate equation is $\tau = (C_{Ao} - C_A)/C^3{}_A \; 0.01$

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FIRST SEMESTER 2011 – 2012

THIRD YEAR

QUIZ 2

Course Code: CHE C312 | Date: 14.12.11

Course Title: Kinetics and Reactor Design | Max Marks: 07

Duration : 20 minutes | (Closed Book) | Weightage: 7%

Name: .... **ID No:** .... **Sec / Prog:** ....

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1. Consider the reaction scheme: A →R and 2A →S ; R is the desired product. (2 m)

(i) The instantaneous fractional yield φ ((R+S)/R) for the reaction scheme is

(a) $\frac{k_1}{k_1 + k_2 C_A}$ (b) $\frac{k_1}{k_2 C_A}$ (c) $\frac{k_1 + k_2 C_A}{k_1}$ (d) $\frac{k_1}{k_1 + 2k_2 C_A}$

(ii) The instantaneous fractional yield φ (R /A) for the reaction scheme is

(a) $\frac{k_1}{k_1 + k_2 C_A}$ (b) $\frac{k_1}{k_2 C_A}$ (c) $\frac{k_1 + k_2 C_A}{k_1}$ (d) $\frac{k_1}{k_1 + 2k_2 C_A}$

2. Consider the reaction $A \xrightarrow{r_B = 1} B$, $A \xrightarrow{r_C = 2C_A} C$, $A \xrightarrow{r_D = C_A^2} D$. For this case φ (C/A) is given by __________ (1 m)

3. An exothermic homogeneous reaction is being conducted in an isothermal batch reactor and for a specified conversion the batch time required is t_B. If the reaction is now conducted in an adiabatic batch reactor, the batch time will be (1 m)

(a) more than t_B
(b) less than t_B
(c) equal to t_B
(d) data insufficient, so nothing can be said about the batch time in the adiabatic reactor

4. For an autocatalytic reaction A + R → R + R, the rate vs. concentration of A profile is (1 m)

(a) linear (b) parabolic

(c) exponential (d) none of these

5. An isothermal gas phase reaction, A → 5B, is being conducted by taking 65% A and 35% inert at start. ε_A= __________ (show the calculation) (1 m)

6. A homogeneous liquid phase reaction is conducted in a batch stirred reactor at a speed of agitation of 500 rpm. If the speed of agitation is doubled, (1 m)

(A) the reaction rate will remain unaffected

(B) the reaction rate will be halved

(C) the reaction rate will double

(D) the reaction rate will decrease by a factor less than two

BITS, PILANI – DUBAI CAMPUS

FIRST SEMESTER 2011 – 2012

THIRD YEAR

QUIZ 1

Course Code: CHE C312 | Date: 05.10.11

Course Title: Kinetics and Reactor Design | Max Marks: 08

Duration : 20 minutes | (Closed Book) | Weightage: 8%

Name: .... **ID No:** .... **Sec / Prog:** ....

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1. For a first order reaction the plot of ln (C_A/C_{AO}) vs. time (1 m)

(a) is linear and passes through the origin

(b) is exponential and passes through the origin

(c) is linear but does not pass through the origin

(d) is exponential but does not pass through the origin

2. A space velocity of $5hr^{-1}$ means that (1 m)

(a) five reactor volumes of feed (at specified conditions) are being fed into the reactor per hour

(b) after every 5 hours, reactor is being filled with the feed

(c) percentage conversion can be achieved in at least 5 hours

(d) a fixed conversion of a given batch of feed takes 5 hours

3. The concentration of A in first order reaction A gives B decreases (1 m)

(a) linearly with time

(b) exponentially with time

(c) very abruptly towards the end of the reaction

(d) logarithmically with time

4. In an ideal tubular flow reactor (1 m)

(a) there is no mixing in longitudinal direction

(b) mixing takes place in radial direction

(c) there is uniform velocity across the radius

(d) all of the above

5. A 200-dm^3 constant-volume batch reactor is pressurized to 20 atm with a mixture of 75% A and 25% inert. The gas-phase reaction is carried out isothermally at 227°C. Assuming that the ideal gas law is valid, how many moles of A are in the reactor initially? What is the initial concentration of A? (4 m)