

UNIVERSITY COLLEGE LONDON

University of London

EXAMINATION FOR INTERNAL STUDENTS

For The Following Qualification:–

M.Sc.

D8: Chemical Reaction Engineering

COURSE CODE : CENG00D8

DATE : 11-MAY-05

TIME : 10.00

TIME ALLOWED : 3 Hours

Answer FOUR questions. Only the first four answers will be marked.
ALL questions carry a total of 25 each, distributed as shown []

1.

Hinshelwood and Askey studied the thermal decomposition of dimethyl ether in a batch reactor. For pressures above 0.5 atm the decomposition was first order and proceeded as follows:



The expression found for the rate constant for the first-order decomposition of dimethyl ether was

$$\ln k = 30.36 - \frac{29440}{T}$$

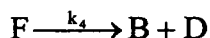
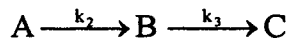
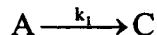
where k has the units of s^{-1} , T is in K.

It is proposed to carry this same reaction out in a perfectly mixed flow reactor operated at 550°C and 1 atm pressure. Calculate the respective space velocities (evaluated at the temperature and pressure of the reactor) which are required to achieve conversions of 20%, 50% and 80% of pure dimethyl ether in the perfectly mixed flow reactor. Assume that the mixture behaves as an ideal gas. [25]

2.

A liquid feed to a well-mixed reactor consists of 0.4 mol/dm^3 of A and the same molar concentration of F. The product C is formed from A by two different reaction mechanisms: either by direct transformation or through intermediate B. The intermediate is also formed from F. Together with B, which remains in solution, an insoluble gas D is formed, which separates in the reactor.

So, the above system is described by:



CONTINUED

All reaction steps are irreversible and first-order, except for the formation of B from F, which is second-order in F. The liquid carrier for reactants and products is an inert solvent, and no volume change results from the reaction:

$$k_1 = 0.01 \text{ min}^{-1} \quad k_2 = 0.02 \text{ min}^{-1}$$

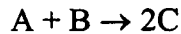
$$k_3 = 0.07 \text{ min}^{-1} \quad k_4 = 0.50 \text{ dm}^3/\text{g mol}\cdot\text{min}$$

reactor volume = 120 dm^3

- a) What is the maximum possible molar concentration of C in the product? [5]
- b) If the feed rate is $2.0 \text{ dm}^3/\text{min}$, what is the mole fraction of C in the product on a solvent-free basis? [20]

3.

The endothermic liquid-phase elementary reaction



proceeds to completion in a single steam-jacketed, continuous-stirred reactor. From the following data, calculate the steady-state reactor temperature.

Steam jacket area: 1 m^2

Jacket steam: 460K

Overall heat-transfer coefficient of jacket, U : $850 \text{ W}/(\text{m}^2\cdot\text{K})$

Heat of reaction, $\Delta H^\circ_{\text{R}} = +40,000 \text{ J/mol}$ of A

	Component		
	A	B	C
Feed (mol/h)	10.0	10.0	0
Feed temperature (K)	300	300	-
Specific heat, $\text{J}/(\text{mol}\cdot\text{K})$	204	176	190

[25]

PLEASE TURN OVER

4.

- (a) A liquid phase hydrogenation of an unsaturated hydrocarbon is catalyzed by porous pellets about 3 mm in diameter. The reaction is approximately first order with respect to the limiting reactant, hydrogen, and it is hoped to achieve useful (observable) reaction rates of the order

$$-r_{H_2} = 10^{-8} \text{ mol/s}\cdot\text{cm}^3_{\text{cat}}$$

From vapour-liquid equilibrium data the solubility of hydrogen in hydrocarbon fluid is estimated to be $C_{H_2} = 10^{-5} \text{ mol/cm}^3$ at 1 atm. Assuming ideal behaviour we also expect this solubility to be proportional to the pressure of hydrogen above the liquid phase. The effective diffusivity of reactants is estimated to be $D_e = 2 \times 10^{-5} \text{ cm}^2/\text{s}$ and approximately independent of concentration of the components, since this is a liquid system. From this information estimate the pressure at which we should operate to ensure that pore diffusion effects are absent, assuming that external mass transfer resistance can be neglected. [15]

- (b) What parameters need to be altered and how (increase or decrease them) to minimize external mass transfer resistances during a heterogeneous catalytic reaction? [10]

5.

This question concerns the kinetics of enzyme-catalysed chemical conversions.

- (a) Derive the Michaelis-Menten expression to describe the conversion of a single substrate to product in solution. [15]
- (b) What significant feature characterises such kinetics and how does this affect the performance of a continuous stirred tank reactor compared to a continuous plug flow reactor? [5]
- (c) Under what circumstances will the expression derived in (a) become invalid? [5]

END OF PAPER