B. Chemical Engineering 3rd Year 2nd Semester Examination, 2017

Chemical Reaction Engineering II

Time: Three Hours Full Marks: 100

Answer any five questions

All symbols have usual significance, if not stated otherwise

Assume any missing data

Information provided at the end of the question paper may be used

1.a)	The second order decomposition reaction $2A \longrightarrow B+C$ is carried out in a tubular reactor packed with spherical catalyst pellets 4mm in diameter. The reaction is strongly internal diffusion limited. Pure A enters the reactor at superficial velocity of 3m/s, C_{A0}=0.115mol/L. Experiments carried out on smaller pellets where surface reaction is limiting yielded a specific surface reaction rate of 50m^4/mol-s. Calculate the length of the bed necessary to achieve 80% conversion. Dispersion in axial and radial directions is negligible. (Data: D_{Ae}=2.66x$10^{-8}$$m^2$/s; Internal surface area=400m^2/g; ρ_b= 2x10^6 g/m^3).	15
1b)	What will be the value of critical temperature difference for a first order reaction to avoid thermal runaway condition if E/RT_r is 20 and T_r is 400K?	5
2a)	A hydrocarbon oil containing thiophene (C_4H_4S) is hydrodesulfurized in a trickle bed reactor undergoing the following reaction: $Thiophene + 4H_2 \rightarrow C_4H_{10} + H_2S$. Pure hydrogen and hydrocarbon liquid are fed to the top of the catalyst bed operated at 40 bar and 300°C.Assume that the liquid is saturated with hydrogen throughout the column. Although the reaction is of 2nd order, assume that the concentration of thiophene is very large relative to hydrogen and hence the reaction may be considered to be of pseudo-first order with respect to hydrogen. If η be unity, derive the expression for fractional removal of thiophene from oil. What will be the bed height to remove 80% thiophene if its feed concentration be 800ppm, ul=0.05m/s; 1st order rate constant k_H=0.11L//kg-s; $(k_c a_c)_{H_2}$ =0.5s^{-1}; ρ=0.96kg/L; $H_{H_2} = 50\ (kmol/L)_{gas}/(kmol/L)_{Liq}$.	8+5
2.b)	Compare your result if $\eta = 0.4$ and external mass transfer resistance is not negligible.	7
3.a)	For a batch reactor and a CSTR undergoing enzymatic reaction in presence of non-competitive inhibitor, correlate the substrate concentration with batch and residence times respectively.	
	With the increasing demand for xylene in the petrochemical industry, the production of xylene from toluene disproportionation has gained attention in recent years. The reaction $2Toluene \rightarrow Benzene + Xylene$ was studied over hydrogen mordenite catalyst that decays with time following second order, i.e., $r_d = k_d a^2$. The rate law for low conversion is $-r_T = k_T p_T a$ The rate constants k_T and k_d, as measured at 740K, are 20 mol/h-kg cat-atm and 1.6h^{-1} respectively. E_T and E_d are 25kcal/mol and 10kcal/mol respectively. A continuous flow reactor having constant coversion is required to be operated in order that subsequent operations are not affected by catalyst poisoning. Derive the equation for the	8

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	time-temperature trajectory for the reactor feed to maintain constancy in conversion if the T=740K at t=0.	
3.b)	Derive the concentration profile of the reactant within a cylindrical pellet for a first order reaction.	5
3.c)	The quantities ρ_d, $k_m a_v$, ε_d, and u_b for a fluidized bed reactor have been determined to be 0.01kg/L, $0.6s^{-1}$, 0.7 and 0.1m/s respectively. Showing all derivations, calculate the conversion in the effluent if the reactor length be 0.5m and the reaction rate constant be 50L/kg-s.	7
4.a)	A countercurrent moving bed reactor with downflow of solids and upflow of gas is to be designed for reducing FeS_2 pellets to FeS following the reaction $FeS_2(s) + H_2(g) \rightarrow FeS(s) + H_2S(g)$.The reactor is to be operated at 1atm pressure isothermally at 500°C. The reactor diameter is to be 0.9m with a gas flow rate of $2.6m^3/s$ of a mixture of 70% CO_2 (inert)and 30% H_2. Specially prepared 0.01m diameter FeS_2 pellets are fed from the top of the reactor at a rate of 0.5kg/s.The pellets are very reactive and very porous layer of FeS is formed during reaction and effective diffusivity through the product layer is $3.6x10^{-7}m^2/s$. Neglect external diffusion resistance and the change in size of pellets with reaction. The value of reaction rate constant, k at 500 °C is $1.02x10^{-3}m/s$. Total solid fraction in the bed is 0.5. The pellet density is $5000kg/m^3$. Since the molecular weights of FeS_2 and FeS are not very different, the mass flow rate of solid may be assumed to be constant over the reactor length. Correlate the conversion with the reactor length.	14
4. b)	For a chemostat, what is the value of D_{max} to avoid wash out condition? Which value of D corresponds to maximum production rate of biomass?The maximum specific growth rate and the saturation constants are μ_{max} and K_s	6
5. a)	The catalytic dehydrogenation of ethylbenzene (R) is conducted to produce styrene (B) and hydrogen(C) in a moving-bed reactor (MBR) at 880K . The reaction may be represented as R $\Longrightarrow$ Products The lumped dehydogenation rate can be represented by a 2nd order rate law: $-r_R' = 0.5 \dfrac{(dm)^6}{(g\,cat)(mol)(\min)} C_R^2$ The catalyst deactivation obeys a first order decay rate law, (decay constant, k_D = 0.65 min^{-1}). The volume changes during reaction may be neglected. The MBR contains 17 kg of catalyst that travels through the reactor at a rate of 8 kg/min. Ethyl benzene is fed at the rate of 27 kmol/min at a concentration of 0.068 $kmol/m^3$. Determine the conversion of ethyl benzene in the MBR.	10
5.b)	Considering shrinking core model and quasi steady state approximation , derive the expression to determine the time for complete regeneration of a spherical catalyst pellet.	10
6. a)	Explain determination of 'multiple steady states' in a CSTR and elucidate the significance of 'ignition' and 'extinction' and 'unstable steady state' temperatures.	6
6.(b)	A first-order reaction $R \rightarrow S, \Delta H_r = 0$ is being conducted at 1 atm and 609 K in a Mixed Flow (Basket-Type) Reactor with 0.01kg of 0.0012 m catalyst particles at a feed rate of 4x 10^{-6} m^3/s of pure R . Under these conditions, 80% conversion of R can be achieved. It is envisaged to design a high capacity commercial-sized reactor with 80% conversion at the above conditions. The choice is	14