Bachelor of Chemical Engineering Examination, 2017

(4th Year, 1st Semester)

Catalysis and Catalytic Reactor Design

Time: Three Hours   Full Marks: 100

Answer _Any Four (4)_ questions.

1.

   a)   Fill in the blank spaces: In _____ reactors the catalyst is present in the reactor in the form of a thin packed bed or metal net. They are used for reactions with very _____ residence times and mostly for _____ operated, heterogeneously catalyzed _____ reactions at _____ temperatures.

   b)   The exothermic gas phase reaction $A+B \rightarrow C$ is carried out over a porous catalyst, in a non-isothermal /non-adiabatic fixed bed catalytic reactor. The feed stream is equi-molar in A and B.

   I.   Using a one-dimensional, pseudo-homogeneous model framework, derive steady state mass and energy balance equations and state boundary conditions to describe the behaviour of the reactor. Define your terms carefully.
   II.   Calculate the maximum temperature that the exit gas stream would attain if the reactor were to be operated adiabatically. Judging by this result, what change would you recommended in reactor operating conditions.
   III.   Discuss briefly for the present case, advantages and disadvantages of using a one dimensional reactor model over a two-dimensional model.

   Data:

Heat of reaction, ΔH_r:	-300 000	KJ(kmol A reacted)$^{-1}$
Average heat capacities		
$C_{pA} \cong C_{pB}$:	30	KJ kmol^{-1} K^{-1}
C_{pC}:	60	KJ kmol^{-1} K^{-1}

                                                                    (5+20=25)

2.

   a)   Give two process examples where a Multi-Bed reactor is used as a two-phase reactor.

b)   Name three heat transfer mediums used in Multi-Tubular reactors, when used as two-phase reactors.

c)   The exothermic catalytic gas phase cracking reaction A→ light products is carried out with a feed of 10% "A" in an inert diluent, "B". The intrinsic rate for the reaction is given by:

$$r_{A}=125 \exp\{-5000/T\}P_A \qquad\qquad kmols^{-1}(kg\text{-}cat)^{-1}$$

Where, P_A denotes the partial pressure (bar) of "A" and T denotes the local temperature in K. The catalyst pellets (dia. 0.004m) may be considered isothermal and the value of effectiveness factor is estimated as 0.08 throughout the reactor. We select a point within the reactor where , G, the superficial mass velocity of the gas stream is 0.8 Kgm^{-2}s^{-1}, the bulk temperature, T_b, is 500K , and the partial pressure of "A" in the bulk,$P_{A,B}$, is 0.05 bar. Calculate:

I.   the global rate of reaction
II.   the external concentration gradient (expressed in terms of the partial pressures), and,
III. the temperature gradient between the bulk gas stream and external catalyst pellet surfaces, at the selected point in the reactor.

Bulk gas properties may be taken as those of the diluent. The pressure drop along the reactor axis may be neglected.

Data:

Effectiveness factor, η:	0.08 (see statement of problem)
Total reactor pressure, p_T:	1bar
Void fraction of the packed bed, ε_B:	0.5
Surface area of catalyst pellets, a_m:	0.4 m^2 kg^{-1}
Heat of reaction, ΔH_r:	-20 000 KJ (kmol A reacted)$^{-1}$
Molecular diffusivity of A in B,D_{AB}:	2×10^{-4} m^{2}s^{-1}
Density of "B ", p_B:	0.1 Kg m^{-3}
Viscosity of "B", μ_B:	1.0×10^{-5} Kg m^{-1}s^{-1}
Heat capacity of "B", $C_P B$	1.0 KJ Kg^{-1} K^{-1}
Thermal conductivity of "B", λB:	1.5×10^{-5} KJ m^{-1} s^{-1} K^{-1}

$$j_{D}=\frac{k_m p_B}{G}\left\{\frac{\mu_B}{p_B D_{AB}}\right\}^{2/3}$$

$$j_{H}=\frac{h}{C_P G}\left\{\frac{C_P \mu_B}{\lambda_B}\right\}^{2/3}$$

In these equations, K_m, the bulk to surface mass transfer coefficient is defined in terms of the equation:

$$r_{A,p}=\left(k_m a_m/_{RT_b}\right)(P_b-P_s),$$

and, h, is the surface to bulk heat transfer coefficient, defined by

$$ha_m = (T_s - T_b) = (-\Delta H_r)r_{A,p}.$$

Finally, R (Gas constant) $=8.314$ KJ Kmol^{-1} K^{-1}$=0.08314$ bar m^3 K^{-1} Kmol^{-1}

(2+3+20=25)

3.
   a) What are the disadvantages of carrying out liquid phase processes in Three-Phase reactors.
   b) Give two process examples, mentioning the ranges of operating temperature, pressure and the name of the catalyst, for carrying out homogeneously catalysed reactions in a Bubble Column Reactor.
   c) The exothermic reaction $A+B \rightarrow C$ was carried out in two different particle sizes: 8mm diameter catalyst pellets and 50μ (average) diameter catalyst particles. Both sets of experiments were carried out under conditions where external temperature and concentration gradients were negligible. Global rates of reaction, measured as a function of temperature, using approximately similar external surface concentrations of A and B **for all experiments, are given in the table below.** Assuming the 50μ particles to be isothermal under all operating conditions,

       I.   Calculate from this data, the energy of activation most likely to approximate the true value for the chemical reaction step at the catalytic sites.

       II.   For the 8mm catalyst pellets, calculate the effectiveness factor at each temperature. State your assumptions clearly.

       III.   Briefly explain observed changes in the value of effectiveness factors as a function of the experimental temperature. What do values above unity imply?

Table A: Experimental global reaction rates as a function of catalyst particle size and temperature.

	Catalyst particles (50 μ)	8mm pellets
Temp (K)	Rate, $r_{A,P}$ Kmol s^{-1}	(Kg cat)$^{-1}$
425.5	9.2×10^{-8}	5.12×10^{-7}
458.7	2.5×10^{-7}	5.95×10^{-7}
495.1	6.95×10^{-7}	7.18×10^{-7}
549.5	1.85×10^{-6}	8.58×10^{-7}
637.0	4.12×10^{-6}	9.39×10^{-7}

(2+3+20=25)

4.

   a) Compare trickle-bed and suspension reactors according to the following criteria:

       I.   Temperature distribution
       II.   Selectivity
       III.   Residence-time behaviour of the liquid
       IV.   Catalyst particle diameter
       V.   Catalyst effectiveness factor
       VI.   Catalyst performance

b) What are the continuous and dispersed phases in suspension reactors.

c) The driving force of a reaction is much smaller in a reactor with back-mixing than in a reactor without back-mixing. Why?

d) Write a short note on the use of a relatively *uncommon photocatalyst*.

e) Draw a potential energy diagram of a heterogeneous catalytic-reaction, with gaseous reactants and products and a solid catalyst. Explain each of the steps.

f) In the oxidation of methane to formaldehyde, CO_2 is the main side product. At the reaction temperatures required to oxidize methane, formaldehyde is unstable and is easily oxidized to CO_2. Since both reactions are exothermic, the catalyst temperature rises, and this favors further oxidation and catalyst sintering.

Which recommendations can be made for the choice of catalyst and reactor?

- **High porosity**
- Low porosity
- High thermal conductivity
- Low thermal conductivity
- Tubular reactor
- Shallow-bed reactor
- Single-bed reactor

(6+2+2+4+4+7=25)

5.

The intrinsic rate for the *endothermic* catalytic gas phase cracking reaction "A →products", is given by the first order reaction rate expression

$$r_A = 4,000 \ \{\exp\left(\frac{-10,000}{T}\right)\}p_A \quad \text{kmol/ (Kg-cat×s)}^{-1},$$

where p_A is the partial pressure (bar) of A, and T denotes the local temperature in K. The reaction is carried out in a differential reactor, where reactant "A" is supplied, mixed 1:1 with an inert diluent. The superficial mass velocity of the gas stream flowing over the catalyst particles, G, is 1 kg m^{-2} s^{-1}, and the temperature of the bulk stream is 750 K. The overall conversion in the reactor has been determined experimentally as 3.6 %. The catalyst pellets have a diameter of 0.004 m and may be considered isothermal.

Calculate,
  I.   The global rate of reaction,
  II. The magnitude of the effectiveness factor, and
  III. The external concentration and external temperature gradients.

The bulk gas properties can be taken as those of the diluent, B. The pressure drop through the reactor may be neglected.

Data:

Molecular diffusivity of A in B, D_{AB}:	3×10^{-4}	$m^2\,s^{-1}$
Density of diluent B, p_B:	0.1	$kg\,m^{-3}$
Viscosity of B, μ_B:	1.5×10^{-5}	$kg\,m^{-1}\,s^{-1}$
Heat capacity of B, $C_{p,B}$:	1.0	$kJ\,kg^{-1}\,K^{-1}$
Thermal conductivity of B, λ_B:	2.5×10^{-5}	$kJ\,m^{-1}\,s^{-1}\,K^{-1}$
Reactor pressure, pT:	1	Bar
Void fraction of the packed bed, ε:	0.48	
Surface area of the catalyst pellets, a_m:	0.4	$m^2\,kg^{-1}$
Heat of reaction, ΔH_R:	25,000	$kJ\,(kmol\,A)^{-1}$
Pellet effective diffusivity, D_{eff}:	1×10^{-6}	$m^2\,s^{-1}$
Pellet density, p_C:	2,000	$kg\,m^{-3}$

$$j_D = (0.7)j_H = \frac{0.46}{\varepsilon_B} R_e^{-0.4}, R_e = \frac{d_p G}{\mu_B}$$

$$j_D = \frac{k_m p_B}{G}\left\{\frac{\mu_B}{p_B D_{AB}}\right\}^{2/3}$$

$$j_H = \frac{h}{C_P G}\left\{\frac{C_P \mu_B}{\lambda_B}\right\}^{2/3}$$

In these equations, k_m, the bulk to surface mass transfer coefficient is defined in terms of the equation: $r_{A,p} = \left(\frac{k_m a_m}{RT_b}\right)(P_{A,b} - P_{A,s})$.

and, h is the surface to bulk heat transfer coefficient, defined by

$$h a_m = (T_s - T_b) = (-\Delta H_r) r_{A,p}.$$

Finally, R (Gas constant) = 8.314 KJ Kmol^{-1} K^{-1} = 0.08314 bar m^3 K^{-1} Kmol^{-1}.

(25)