Mark Scored:

KATHMANDU UNIVERSITY
End Semester Examination
August, 2018

Level : B.E.
Year : III
Course : CHEG 312
Semester : II
Exam Roll No. :
Time: 30 min
F. M. : 10
Registration No.:
Date AUG 15 2018

SECTION "A"

[20Q ×0.5 = 10 marks]

Attempt *ALL* questions. Tick the most appropriate answer.

1. For a reaction of $H_2 + Br_2 \rightarrow 2HBr$, the Pseudo-Steady-State-Hypothesis (PSSH) can be applied to
   a. H_2 b. Br_2 c. HBr d. Intermediates

2. The unit of the Michaelis constant in the rate equation of an enzyme reaction is
   a. mol/L b. mol/kg c. kg/m^3 d. kg/L

3. An enzyme is
   a. a reactant.
   b. is not consumed nor does it affect the chemical reaction equilibrium.
   c. more effectively involved in the reaction under strong acidic condition.
   d. combined with a product to form an intermediate.

4. In the stationary phase of a bio-reaction,
   a. cells are decreasing in concentration.
   b. the net cell growth is zero.
   c. cells are adjusting to their new environments.
   d. cells are dividing to produce more cells.

5. In the Monod equation, the unit of the maximum specific growth rate is
   a. $mol\ s^{-1}$ b. $mol\ L^{-1}\ s^{-1}$ c. s^{-1} d. dimensionless

6. In a chemostat at the steady state, a decrease in the dilution rate would result in
   a. a decrease of the nutrient at the reactor outlet.
   b. an increase of the nutrient at the reactor outlet.
   c. a decrease of the cell at the reactor outlet.
   d. the wash-out.

7. The energy balance equation for adiabatic reactor does not include
   a. reactor inlet temperature.
   b. molar heat capacities of inert species.
   c. the standard reaction enthalpy.
   d. the heat transfer coefficient

8. To increase the conversion for an exothermic reversible reaction, it is necessary to
   a. increase the reactor inlet temperature.
   b. decrease the reactor inlet temperature.
   c. decrease the space time.
   d. use an inter-stage cooling.

9. For an exothermic reversible reaction,
a. there exists an optimum feed temperature.
b. increasing the feed temperature would increase the conversion.
c. decreasing the feed temperature would increase the conversion.
d. employing small reactors in series could increase the conversion.

10. The computer program that can be used to solve a reactor in which there are radial variations in velocity, concentration, and temperature is,
a. COMSOL b. Polymath c. Pro/II d. Aspen-Plus

11. Turn over frequency (TOF) is a parameter used to quantify the activity of a catalyst.
a. TOF is defined as the number of moles reacted per active site per unit time.
b. The higher the TOF, the higher the reaction rate.
c. To convert TOF to a reaction rate, the activation energy of the reaction is required.
d. TOF is defined as the number of molecules per unit mass of catalyst per unit time.

12. For a catalytic solid-gas reaction to occur, at least one reactant must become attached to the surface of the catalyst. This attachment is known as adsorption
a. The adsorption is exothermic.
b. The adsorption is endothermic.
c. The adsorption is isothermal.
d. The adsorption is endothermic for exothermic reactions and exothermic for endothermic reactions.

13. The deactivation of a catalyst resulting from the prolonged exposure to high temperatures is called
a. fouling b. coking c. aging d. poisoning

14. If the adsorption step is known to be rate-determining in a steady-state operation of a catalytic fluid-solid reaction,
a. the adsorption step can be assumed to be in equilibrium.
b. the surface reaction rate is higher than the adsorption rate.
c. the desorption rate is higher than the adsorption rate.
d. the adsorption rate, the surface reaction rate, and the desorption rate are the same.

15. In the Langmuir molecular adsorption of CO on a catalytic surface,
a. CO is dissociated into C and O before it is adsorbed.
b. any active site is assumed to have the same attraction for an impinging CO molecule.
c. the surface coverage is independent of adsorption temperature.
d. the surface coverage increases linearly with increasing the pressure of CO.

16. The unit of residence time distribution in a reactor is,
a. min. b. min^{-1}. c. mol min^{-1}. d. mol L min^{-1}.

17. In the pulse injection of a tracer to a reactor the residence time distribution (RTD) is defined as
a. $E(t) = \frac{d}{dt}[\frac{C(t)}{C_0}]$. b. $E(t) = \frac{C(t)v}{\int_0^\infty C(t)dt}$
c. $E(t) = \frac{C(t)v}{\int_0^\infty C(t)vdt}$. d. $E(t) = \delta\,(t - \tau)$

AUG 1 5 2018

18. In a laminar flow reactor with pulse injection of tracer, the time at which the tracer appears first at the reactor outlet
    a. equals the space time.
    b. equals half the space time.
    c. equals two time the space time.
    d. is indeterminable unless further information is provided.

19. For a CSTR with dead volume, the residence time distribution (RTD) at t (time) = 0 is
    a. lower than the CSTR without dead volume.
    b. the same as in the CSTR without dead volume.
    c. higher than the CSTR without dead volume.
    d. more information is necessary compare the residence time.

20. Choose a statement that is false in describing the models for predicting conversion from residence time distribution data
    a. in the segregation model a globule does not interchange materials with the other globules in the reactor.
    b. in the maximum mixedness model, the globules are fed as side streams to a PFR and the globules are assumed to be completely mixed in both radial and axial directions.
    c. in the tanks-in-series model, a real reactor is modeled as smaller reactors in series.
    d. in the dispersion model, both radial and axial dispersions of the material are calculated.

KATHMANDU UNIVERSITY
End Semester Examination
August, 2018

AUG 15 2018

Level : B.E.
Year : III
Time : 2 hrs. 30 mins.

Course : CHEG 312
Semester: II
F. M. : 40

SECTION "B"

Attempt *ALL* questions.

1 Azomethane (AZO) is decomposed in the gas phase to produce ethane and nitrogen: $(CH_3)_2N_2 \rightarrow C_2H_6 + N_2$. The reaction is known to occur in three elementary steps:
(1) $(CH_3)_2N_2 + (CH_3)_2N_2 \rightarrow (CH_3)_2N_2 + [(CH_3)_2N_2]^*$
(2) $(CH_3)_2N_2 + [(CH_3)_2N_2]^* \rightarrow (CH_3)_2N_2 + (CH_3)_2N_2$
(3) $[(CH_3)_2N_2]^* \rightarrow C_2H_6 + N_2$

[4]

a. What is the difference between $(CH_3)_2N_2$ and $[(CH_3)_2N_2]^*$?
b. Derive the reaction rate equation for C_2H_6 ($r_{C_2H_6}$) as a function of the concentration of azomethane.
c. The rate equation you end up with may be in the form of numerator and denominator. What does a constant appearing in the denominator mean with respect to the mechanism of the decomposition?
d. Show that $r_{C_2H_6}$ is second order with respect to azomethane concentration at low azomethane concentrations and first order with respect to azomethane concentration at high azomethane concentrations.

2. Urea is decomposed into ammonia and carbon dioxide in the presence of urease as enzyme. The reaction rates of urea (r_{urea}) were measured at various urea concentrations (C_{urea}) as follows:

C_{urea} (kmol/m^3)	0.2	0.02	0.01	0.005	0.002
$-r_{urea}$, kmol/(m^3•s)	1.08	0.55	0.38	0.2	0.09

The rate equation takes the form of $-r_{urea} = \frac{V_{max}C_{urea}}{K_M + C_{urea}}$. [5]

a. Determine the constants of V_{max} and K_M.
b. If the amount of urease is doubled, estimate the reaction rate of urea at the urea concentration of 0.2 kmol/m^3.
c. Calculate the time needed to convert 90% of the urea in a 1 L batch reactor.

3. The reaction rate of the substrate of a biological reaction represented by S (substrate) + cells → more cells + P (product) was expressed by $-r_s = \frac{V_{max}C_cC_s}{K_s + C_s}$ with V_{max} =1 h^{-1}, K_s =0.25 g/L, and $Y_{c/s} =$ 0.5 g/g. [5]

a. What does $Y_{c/s}$ of 0.5 g/g mean?
b. The reaction was carried out in a batch reactor. The initial concentrations of the substrate and the cell were 5 g/L and 0.1 g/L, respectively, and the final concentration of the substrate was measured at 4 g/L. Determine the final concentration of the cell.
c. The reaction was carried out in a steady-state CSTR. Set up the mass balance equations for the substrate and the cell, respectively, assuming that the death rate of cell is negligible.
d. Determine the dilution rate at which wash-out occurs when the concentrations of the substrate and the cell that are fed to the reactor are 5 g/L and 0 g/L, respectively.
e. Calculate the cell concentration in the reactor when the dilution rate is one-third of that at the wash-out.

4. An elementary liquid-phase reversible reaction, A=B was carried out in an adiabatic CSTR. The standard reaction enthalpy is -20,000 cal/mol, and the concentration equilibrium constant at 25°C is 100,000. The reaction enthalpy is assumed to be independent of temperature. The feed to the reactor is pure A and the feed temperature is 350 K. The heat capacities of A and B are 15 cal/(mol·K), respectively. [4]

   a. Determine the equilibrium constant at 450 K.

   $$\ln\frac{K_{C2}}{K_{C1}} = -\frac{\Delta_r H^0}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

   b. Calculate the equilibrium conversion at 450 K.

   c. The energy balance equation for the adiabatic reaction can be represented by

   $$X = \frac{\sum \Theta_i C_{Pi}(T - T_{i0})}{-[\Delta_r H^0(298.15\ K) + \Delta_r C_P(T - 298.15)]}$$

   Express the equilibrium conversion as a function of equilibrium temperature.

   d. Show how to obtain the equilibrium conversion graphically.

5. For an isothermal Langmuir adsorption of hydrogen (H_2) on an adsorbent,

   a. What are the assumptions used in the derivation of Langmuir adsorption isotherm?

   b. What is the difference between molecular adsorption and dissociative adsorption?

   c. Derive the adsorption isotherm for molecular adsorption.

   d. Derive the adsorption isotherm for dissociative adsorption.

   e. Explain the method how to determine whether a hydrogen adsorption is molecular or dissociative. [5]

6. A gas-phase reaction of $CO + H_2O = CO_2 + H_2$ occurs over a supported catalyst impregnated with platinum (atomic weight: 195.09) at 0.2 wt.%. The density of the catalyst is 2000 kg/m^3, the void fraction of the catalyst bed is 0.5, and the dispersion of the platinum is 0.5. [4]

   a. Determine the bulk density of the catalyst.

   b. What does the dispersion of platinum means?

   c. Assuming that one platinum atom is one site, calculate the number of active sites that are contained in 1 gram of the catalyst

   d. The reaction rate of CO was measured at -100 mol/(g·h). Calculate the turnover frequency of the catalyst.

7. A first-order irreversible reaction represented by A → B occurs over a porous catalyst. The reaction rate constant is 0.1 m/s, bulk concentration of A (C_{Ab}) is 0.5 mol/L, the concentration of A at the external surface of the catalyst (C_{AS}) is 0.3 mol/L, and measured reaction rate is 20 mol/(m^2·s). [4]

   a. Sketch the profile of the concentration of reactant A from the bulk to the center of the catalyst particle.

   b. Calculate the mass transfer rate of reactant A (in mol m^{-2} s^{-1}) through the external boundary layer.

   c. Determine the internal effectiveness factor.

   d. Determine the overall effectiveness factor.

8. For the residence time distribution (RTD) with pulse injection of a tracer, a real reactor was modeled as two ideal reactors in series: an ideal PFR (space time = 2 min) followed by an ideal CSTR (space time = 3 min). [5]
   a. Express the RTD in the ideal PFR as a function of time.
   b. Set up the material balance for the tracer in the ideal CSTR.
   c. Express the concentration of the tracer at the outlet of the ideal CSTR as a function time.
   d. By using $E(t) = \frac{C(t)}{\int_0^\infty C(t)dt}$, express the RTD of the real reactor as a function of time.
   e. Determine the fraction of the tracer that exited the second reactor between 3 min and 4 min.

9. There are two models in predicting the conversion of a reactant in a reactor with given residence time distribution: Segregation model and Maximum mixedness model. Explain the differences in concept between the two models and the method to determine the conversion for each model. [4]