

## ChE 471- Fall 2012 – FINAL REVIEW OF KEY CONCEPTS

### Part 1

1. What is a chemical reaction? Define it.
2. What is reaction stoichiometry? What is it based on? What relationship between reactants and products does stoichiometry provide?
3. What is the difference between a single and multiple reactions?
4. What is the (molar) extent of reaction?
5. What is the concept of the limiting reactant?
6. What is (fractional) conversion of the limiting reactant,  $x_A$ ?
7. How is molar extent of reaction related to conversion?
8. How is molar concentration of any species related to conversion? Is there a difference between constant volume and constant pressure systems?
9. How is molar concentration of a species related to molar extent?
10. How is mole fraction of species  $j$  related to reaction extent? Conversion?
11. How is the thermodynamic equilibrium constant  $K$  calculated at standard conditions? Does this constant have units? Define it for a single reaction of known stoichiometry as function of appropriate species activities.
12. How do we correct the value of the thermodynamic equilibrium constant for temperature? Is this constant a function of pressure?
13. How is the thermodynamic equilibrium constant,  $K$ , related to  $K_y$ , for ideal gases?  $K_c$  for liquids?
14. What information is needed to calculate the equilibrium composition of the system in terms of mole fractions? What is the procedure?
15. How is the rate of reaction defined? What is it a function of?
16. Write down the representation of an  $n$ -th order reaction rate for an irreversible reaction and show what the Arrhenius representation of the rate constant looks like. What is the meaning of activation energy?
17. What is an elementary reaction? Can we infer its order from its molecularity?
18. What is a kinetic mechanism of reaction?
19. Using PSSA how do we develop a rate equation from the proposed mechanism?
20. Using RLSA how do we develop a rate equation from the proposed mechanism?
21. How does a catalytic mechanistic sequence differ from the non-catalytic one?
22. What is the Lindemann's mechanism for 'unimolecular' gas phase reactions? At what conditions is the expected first order rate observed? At what conditions is the rate second order?
23. What is the Michaelis-Menten reaction mechanism for enzyme promoted reactions? Show the expected rate form and discuss apparent reaction order at low and high reactant (substrate) concentrations.
24. Write the basic mass balance for reactant A for an isothermal batch reactor, list key assumptions, and relate reaction time to conversion.
25. How do you relate production rate in a batch reactor, reaction time and conversion?
26. Develop the basic design equation for an isothermal continuous flow stirred tank reactor (CSTR).
27. Develop the basic design equation for an isothermal plug flow reactor (PFR).
28. What is the meaning of space time?
29. Represent graphically the space time for a CSTR and PFR on a plot of the reciprocal of the reaction rate versus conversion.
30. What is the mean residence time (mean holding time)? How does it relate to the space time?

## Part 2

1. For a reaction with 20 kcal activation energy a 10° C temperature rise from 300 to 310K raises the rate how many times?
2. For a zeroth order reaction in a batch complete conversion is reached in 1 hour. If we doubled the initial reactant concentration what happens to the time required for complete conversion?
3. For n-th order ( $n > 0$ ) reaction at fixed feed conditions and fixed desired final conversion we need a larger space time in a PFR than in a CSTR. True or false? Explain
4. For an autocatalytic reaction the largest reactor volumetric productivity is achievable in a) PFR, b) CSTR c) reactor combination. Explain.
5. True or false. For consecutive reactions  $A \rightarrow R \rightarrow S$  the highest yield of intermediate  $R$  can be expected in a PFR not in a CSTR.
6. True or false. For competitive reactions  $A \rightarrow P, A \rightarrow S$ , the reaction of higher order is promoted in a PFR.
7. Sketch the relationship between point yield, ( $R_P/-R_A$ ) and overall yield in a) CSTR, b) PFR. Consider the relationship between point yield and concentration of reactant  $A, C_A$ , in which i) point yield is a monotonically increasing function of  $C_A$ , ii) point yield is a monotonically decreasing function of  $C_A$ , iii) point yield exhibits a maximum at a certain value of  $C_A$ . If you are free to choose the final conversion levels indicate for each case which ideal reactor (or their combination) would produce the maximum concentration of the desired product  $R$ . Also indicate how the maximum overall yield would be obtained for each case.
8. For multiple reactions  $A + 2B = R; 2A + R = S$  develop the relationship for the molar concentration of each species, their feed concentrations and the molar extents per unit volume ( $\xi_1, \xi_2$ ) for each reaction.
9. What is the design equation for a) CSTR, b) PFR, c) an isothermal recycle reactor for a homogeneous single reaction?
10. Write for a single reaction  $A \rightarrow$  products a reactant  $A$  species mass balance and the reactor energy balance for a) CSTR, b) PRF?
11. In an adiabatic CSTR how many steady states are possible for an n-th order reaction ( $n \geq 0$ ) which is a) endothermic, b) exothermic?
12. What are the necessary conditions for stability of a steady state in a CSTR?
13. Wall cooled tubular reactors are prone to hot spot formation. Can you describe why? What do we need to do to prevent a hot spot?
14. True or false. Hot spots in wall cooled tubular reactors are more likely when the reactor is operated at high conversion.
15. How should adiabatic plug flow reactors be operated to ensure safety?
16. How should an adiabatic CSTR be operated to avoid thermal runaway?
17. What is the effectiveness factor for nonporous catalysts? Can it be larger than one for n-th order ( $n \geq 0$ ) reaction that is a) exothermic, b) endothermic?
18. If a reaction on a nonporous catalyst is completely mass transfer controlled what can be assumed for the reactant concentration at the catalyst surface? Can you express catalyst surface temperature in terms of mass transfer coefficient, heat transfer

coefficient and bulk gas phase reactant concentration in the vicinity of the catalyst surface?

19. What is the Thiele modulus? What is the effectiveness factor for a porous catalyst particle that accounts for internal transport effects? How are they related?
20. What do we mean by “strong pore diffusion limitation regime”? What is the relationship between the effectiveness factor and the Thiele modulus in such regime?
21. What is the value of the catalyst effectiveness factor in absence of internal and external transport effects?
22. At very high temperatures the catalytic reaction rate is limited by external mass transfer. To enhance the reaction rate per unit mass of catalyst should we use larger or smaller particles? Explain.
23. What is the residence time distribution (RTD) in a reactor?
24. How is E-curve obtained from a tracer impulse response?
25. What is the mean of the E-curve equal to?
26. What is a segregated flow model and how does it use the E-curve?
27. What is the maximum-mixedness model for a CSTR and what is the segregated flow model for the CSTR? For n-th order reactions do they predict different reactor performance? What can you tell us about it?
28. In order to predict isothermal reactor performance for a first order reaction in a homogeneous system what do we need to know? Show the equation from which conversion can be calculated.
29. How should a fluidized bed reactor be modeled? Can its performance be bracketed by a CSTR and PFR model?
30. To maximize volumetric productivity how should packed bed adiabatic reactors be operated for exothermic reaction? Sketch on a conversion –temperature diagram!
31. In gas liquid systems where the gas reactant A absorbs in the liquid and reacts there with non-volatile reactant B what are the key dimensionless numbers that help us identify the reaction regimes in which this process may take place?
32. Considering a gas and liquid film adjacent to a gas-liquid interface and soluble reactant A dissolving in the liquid and reacting there with nonvolatile reactant B. How many possible regimes can you recall with regard to the position of reaction interface? For each, state where the reaction takes place (e.g. at gas –liquid interface, reaction interface, in reaction zone located where, and whether the behavior in the liquid film is coupled with that in the bulk gas and bulk liquid phases in the reactor. How many ‘resistances’ to reaction are present in each regime?
33. What type of gas-liquid reactors are you familiar with and how would you approximate the flow pattern of the gas and liquid phases in each?
34. Solid catalyzed gas –liquid reactions can be conducted in trickle beds or slurry systems. Enumerate advantages and disadvantages of each.
35. When a solid particle, which reacts with the surrounding fluid, exhibits a distinct reaction interface between unreacted solid reactant B and solid product layer S what model can be used to describe the progress of solid reactant conversion with time in the particle? How many resistances may be present? How does reaction time needed for complete conversion scale with particle diameter?

36. For uniform particles of unchanging size that undergo the USCM show how to relate conversion achieved to mean residence time in a reactor which behaves as a) PFR and b) CSTR.
37. Develop the basic equation for biomass production in a CSTR that follows Monod cell growth and Michaelis-Menten kinetics for substrate consumption. Explain when washout occurs and how it is related to kinetic and operational parameters.
38. What information can you obtain from the breakthrough curve (step response) of an adsorber? Explain.