Dr. Trent L. Silbaugh, Instructor

ChE 344 Winter 2016 **Chemical Reaction Engineering** Final Exam Study Guide

to be used with *Elements of Chemical Reaction Engineering, 5th Ed., H. Scott Fogler*

Chapter 1 Mole balances:

- Know the definitions of the rate of reaction, rate of disappearance and rate of appearance
- Know what a rate law is
- Be able to write a general mole balance and know what each term means (you will be given the equation on your sheet but note an explanation of each term)
- Units, units, units → what are the units of all of the different variables in the GMBE
- What assumptions are made in developing the design equations
- CSTR, the outlet species concentration is the same as what?
- What is the difference between a PFR and a PBR? What is the difference in the design equations?

Chapter 2 Conversion and reactor sizing:

- What is conversion?
- When can conversion be used and when can it not be used?
- What is a Levenspiel plot, how is it made, and what can it be used for?
- Reactors in series: why would we want to use multiple reactors and how can we determine number, size and type of reactors that should be used for a particular reaction?
- What is space time and why is it a useful parameter?
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Chapter 3 Rate Laws:

- What is a rate law?
- If a rate law is elementary, does that mean that the reaction is elementary?
- How can one write an elementary rate law?
- What is reaction order?
- How can reaction order information be used to write a rate law? (i.e. first order in A and half order in B → what is the rate law)
- How can a rate law be converted from partial pressures to concentrations or vice-versa?
- Write a rate law for a reversible reaction.
- What is the equilibrium constant?
- The Arrhenius law: know it, love it, take it on a date this Sunday before your exam.
- What is an activation barrier, why does it exist and how does it affect your life?
- Do all molecules have the same amount of energy?

Chapter 4 Stoichiometry:

- Write relative rates
- Can you make a stoichiometric table?

- Are you sure you can make a stoichiometric table?
- Like, seriously, you are completely sure? … OK I believe you ☺
- What are δ and ε and how can they be calculated?
- When do we need to use δ and ε and when do we get to neglect them?
- PSO: Did you know that your stoich table should be based on the limiting reactant?
- Know how to write concentration in terms of conversion and also know how concentration is affected by temperature, pressure etc.
- Equilibrium conversions

Chapter 5 Design of Isothermal Reactors: Conversion

- Can you put together the pieces from the previous chapters to solve for things like conversion or reactor volume?
- Are you sure that you can put together the pieces to solve a problem?
- Even if we try to trick you with seemingly little information like you have seen in the PE exam problems?
- What is the Damkoehler number? Is it useful for anything? (See your textbook)
- Pressure drop and the Ergun Equation (worst movie title of all time: I'm guessing Keanu Reeves and Nick Cage would be in this one). Know what every variable is and what it is a function of. I heard that G is a function of cross-sectional area!
- How can we analytically account for pressure drop in a reactor?
- How does changing aspects of your reactor (e.g. particle diameter, cross-sectional area, initial pressure) affect conversion?

Chapter 6 Isothermal reactor design: DON'T USE CONVERSION

- Calculating concentrations without using conversion
- Membrane reactors: why we would use one and how we can design it?
- Semi-batch reactors: why we would use on and how we can design it?
- How does equilibrium conversion change in a membrane or semi-batch reactor?

Chapter 7 Collection and Analysis of Rate Data

- Know what the method of excess is and how and why it is used
- Integral method: why and how is it used?
- What is the differential method for constant volume systems?
- Nonlinear regression → thanks Excel
- How would one use a differential flow reactor (PFR or PBR) to determine rate information?

Chapter 8 Multiple Reactions

- Cannot use conversion for multiple reactions → use moles or molar flow rates

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- Be familiar with definitions of selectivity (instantaneous and overall) and yield
- Know the different types of multiple reactions schemes (e.g. parallel, series)
- How do we maximize selectivity, concentration, molar flow rate of a desired product, etc?
  - How would you approach solving this type of problem analytically?
- How would you select operating conditions or a reactor type to maximize yield?

Chapter 11 Nonisothermal Reactor Design

- Know how we obtained the energy balance equations used in the course so far
  - This includes knowing what assumptions were made in derivations
- Know what variables are a function of temperature (e.g. rate constant, equilibrium constant, heat capacity (?), ΔH_{rxn})
- Be able to use the energy balance equation to solve nonisothermal reactor problems
  - Which terms are required to solve a particular problem? Adiabatic → Q=0
- How does one determine the ΔHrxn from tabulated enthalpy data or from rate constant data? Is ΔHrxn a function of temperature?
- Know how to solve adiabatic reactor problems
- How can we determine the number of stages (with interstage cooling) required to reach a given conversion for a reversible reaction? Be able to do this graphically and/or analytically with a calculator

Chapter 12 Steady-State Nonisothermal Reactor Design – Flow Reactors with Heat Exchange

- How was the expression for dT/dV developed, what assumptions were made?
- Be able to develop expressions for heat transfer fluid temperature for:
  - Co-current
  - Countercurrent
- How does the type of heating or cooling configuration affect reactor operation and performance?
- Multiple reactions with heat exchange:
  - How does this type of problem change relative to the isothermal case?
  - How does the energy balance expression change for multiple reactions?

Above is the same guide provided to you for Midterm 2. Below is all new!

- Multiple Steady States: know why multiple steady states can exist and how to determine what they will be for a given system.
- Know what G(T) and R(T) represent and how to use them to answer relevant questions (Note that G(T) and R(T) are specific to the reactor that you are working with and elements present, such as W_S, in a specified problem). They are more of a concept than a set of specific equations.

Chapter 13 Unsteady-State Nonisothermal Reactor Design

- Know how we derived the unsteady state energy balance and how it can be used to describe unsteady state CSTR, Semibatch or, with a simplification, a batch reactor
- How did we use unsteady state analysis for safety problems?

Chapter 10 Catalysis and Catalytic Reactors

- Be familiar with the Quasi Equilibrium Approximation (QEA) and how it is used to develop catalytic rate laws from a given mechanism
- Understand how a catalytic mechanism is developed for a given reaction
- Know how to identify likely catalytic mechanisms for a given rate law based on the terms present (e.g. adsorbed species show up in denominator, species in numerator participate in rate determining step)
- Know what the Langmuir-Hinshelwood and Eley-Rideal mechanisms are and how they differ from one another.
- Be able to sketch rate versus partial pressure for a given rate law or be able to propose a rate law (and mechanism) from given rate vs. partial pressure data.

Chapter 14 Mass Transfer Limitations in Reacting Systems

- Be able to determine the role external mass transport plays in a given reacting system
- Be comfortable using correlations and dimensionless numbers to determine mass transfer coefficients
- Be able to describe conceptually (and numerically) how mass transport affects your system and how to eliminate such effects.
- Know what surface area is important in external mass transport limited systems (Important distinction when discussing external versus internal limitations)

Chapter 15 Diffusion and Reaction

- Understand how we derived the effectiveness factor for a single pore and what all variables mean.
- Understand how we extended the use of these concepts to catalyst pellets of varying geometries from our treatment of a single pore.
    - This includes, but is not limited to concepts of tortuosity, changes in pore cross-sectional area (think constriction factor), and an “effective diffusivity”
- Be able to use definitions of Thiele Modulus and Effectiveness factor for different geometries to solve relevant problems.
- Know the differences between all of the different rate constants we have used to describe our system and that the total surface area (generally dominated by internal surface area) is what matters when calculating the effectiveness factor.

Chapter 9 Reaction Mechanisms, Pathways, Bioreactions and Bioreactors

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- Be able to use the PSSH to develop rate laws: note that you can always develop catalytic rate laws using the PSSH. In some cases it may be the best method!
- Be familiar with enzyme kinetics rate laws (Michaelis-Menten) and how such a rate law can be affected by the presence of an inhibitor
- Confidence that you can derive enzyme rate laws for different types of inhibition using PSSH
- Be generally aware that you need only be generally aware of bioreactor topics we covered in the last lecture ☺ GOOD LUCK ON THE EXAM!