Chem763 – study guide

Half semester, 2 credit class: 15/2*2 = approximately 15 classes

1st midterm will cover class 1 to 8.

Class 1 – rate definition

-) How many midterms and home works will we have?
-) Read the syllabus
-) What is the difference between physical kinetics and chemical kinetics?
-) Name one major difference between thermodynamics and chemical kinetics.
-) Stoichiometric coefficients of reactants are positive. Correct/wrong?
-) Define the “advance” of a reaction.
-) Define reaction rate.
-) What is the difference between a rate law and a rate equation?
-) The rate of a reaction and the rate of conversion are always identical. Correct/wrong?
-) What is a reaction order?
-) The reaction orders simply equals the stoichiometric coefficients. Correct/wrong?
-) What is the dimension of a reaction rate?
-) What is the dimension of a rate coefficient for a 2nd order reaction?
-) The reaction rate and rate coefficients always have the same dimension. Correct/wrong?

Class 2 – how to measure rates & 0th order kinetics

-) Name and explain an experimental method to determine the reaction order.
-) Explain two methods to measure the rate of a chemical reaction.
-) How are chemical reactions classified in kinetics?
-) What is an integrated rate law?
-) Outline the calculus for 0th order kinetics.
-) Give and discuss an example for 0th order kinetics.

Class 3 – 1st order kinetics

-) Name an example of 1st order kinetics from your own field of study.
-) Write down the rate low for 1st order kinetics.
-) Integrate the rate law.
-) If you plot $\ln([A]/[A]_0)$ vs. t for a 1st order reaction what does the slope of the line equal?
-) Calculate t1/2 for a first order reaction.
-) Compare 0th order and 1st order kinetics.

Class 4 – 2nd order reactions

-) Name an example each for a 2nd order gas phase, gas-solid, biochemistry, and electro-chemistry (liquid) reaction, respectively.
-) Writ examples for reaction rates/laws for a 2nd order reaction? (What types of 2nd order kinetics do you know?)
-) Write the rate equations (differential equations) for one of those reactions.
-) Calculate the t1/2 time for a 2nd order reaction.
-) What is a pseudo 1st order reaction?
-) what is a typical titration reaction in surface science?
-) Compare 1st and 2nd order reactions: t1/2, [A](t), r?

Class 5 – Numerical/computational techniques in kinetics & tricks to solve kinetics problems (steady state approximation), sequential reactions

-) Outline the problem of a numerical integration schematics?
-) Name a technique used to integrate rate equations using a computer program.
-) Explain the idea of such a technique.
-) what are stiff differential equations?
-) Runge and Kutta are well-known for passing over the Gimpel pass in the Himalaya as the first. Yes/No?
-) What is a steady state approximation?
-) What is the basic idea of a steady state approximation, i.e., why is it used? What is the idea or the concept behind it?
-) Write down an example where the steady state approximation is used to solve a kinetics problem.
-) What is the mass balance approach?

Class 6 – tricks to solve kinetics problems II: rate determining step approximation, pre-equilibrium & nth order reactions

-) Illustrate the idea of the rate determining step approximation using an example.

-) Discuss what dynamics effects may or may not affect the kinetics of a system.

-) What is the difference between a pre-equilibrium and a rate determining step?

-) Calculate t1/2 for a n-th order reaction.

-) Discuss the half-life method.

-) List the "tricks" you know to solve a kinetics problem.

Class 7 – parallel reactions, reversible reactions, Arrhenius Eq.

-) Solve a simple example problem of a parallel reaction.

-) What are the differences in the kinetics of a parallel and sonsequtive reaction?

-) Name an example of a reversible reaction.

-) How can the temperature dependence of the reaction rate coefficient be described?

-) Is there a connection of the van't Hoff Eq. and Arrhenius equation?

-) What may be the origin of the activation energy of a gas phase reaction?

-) What is an activated complex?

Class 8 – 1st group/homework project: computational techniques in kinetics (power point class)

A brief power point introduction (10-15 min) will be provided to help you with the 1st group/homework/hands-on project. Advanced computer skills or programming skills are not required. You will use a software tool. Use the rest of the class to start working on this exercise together with your group partner. This will be graded.

-) What is a Langmuir-Hinshelwood mechanism?

-) What is an adsorbate?

Class 9: 1st midterm will cover class 1 to 8.

2^{nd} midterm context starts here:

Class 10 – Perturbation-relaxation methods, T-jump technique, and diffusion controlled reactions

-) What is a temperature jump experiment and how can one extract kinetics information? What is the idea of the data analysis?
-) Can a gas phase reaction be diffusion controlled?
-) What is the reason for diffusion controlled reaction kinetics in the liquid phase?

Class 11 – Temperature ramping techniques & 2^{nd} group/homework project (power point class)

Kinetics often implies to understand the temperature dependence of a chemical reaction. Therefore, temperature ramping techniques and T-jump experiments are quite common. This class is a power point class which will discuss those techniques. I focus here on surface science. You will need this information to work successfully on the 2^{nd} group/homework/hands-on project which is more demanding than the 1^{st} one. (It is also the last one.) However, surface science will not be part of the exams.
The power point will not require the entire time of the class. Use the rest of the class to start working on this exercise together with your group partner. This will be graded.

Class 12 – Lindemann mechanism, Catalysis

-) The Lindemann mechanism is perhaps the simplest example of a photo-catalytic reaction. What is it? Provide the mechanism in generic form: A+B etc?
-) Brows the internet or go to the library? Find an example reaction which follows this mechanism. Try to remember it.

-) How is a catalyst defined?
-) What is a catalyst doing?
-) Why does a catalyst not change the equilibrium constant?
-) Provide a generic equation for a simple catalytic reaction.
-) Provide an electrical circuit diagram in analogy to a catalytic reaction.

Class 13 – Catalysis of a surface chemist (power point class)

-) This is a supplemental section to this class discussing the surface chemistry perspective of catalysis. However, most kinetics/PChem. books do include a chapter about surface science. Surface science is not part of the exams.

The power point may not require the entire time of the class. Use the rest of the class to work on the 2nd homework project together with your group partner.

Class 14 – radical chain reactions, polymerization, explosions

-) What is a radical?
-) Provide an example for a radical chain reaction in generic form (i.e. A + B → ?? etc.)
-) The rate equations for radical chain reactions are typically very complex. What approximations can be used to solve this kind of kinetics analytically (i.e. with pencil and paper).
-) Are typically fractional or integral reaction orders observed for radical chain reactions?
-) By the way, what is a reaction order, again?
-) Write down the generic form of a radical polymerization reaction.
-) Write down the rate of the formation of the activated monomer.
-) What is a kinetic chain length?
-) Why are typically small concentrations of the initiator used in radical polymerization reactions?
-) Thermal and chain branching explosion mechanisms are distinguished. Explain these terms. Provide a simple example.

Class 15 & 16 – brief introduction to dynamics and transition state theory

-) Draw the potential energy diagram for a molecule such as H2.
-) How does the potential energy surface of a simple reaction look like?
-) Draw a 1D PES for an exothermic and endothermic process.
-) What are the conceptual differences between the “collision theory” and “transition state theory”

-) What is the relationship between the Gibs free energy change and the equilibrium constant?
-) Derive the Eyring-Polanyi Eq.
-) What is a kinetic isotope effect?
-) What dissociation rate would be larger the one for D2 or H2? Why?
-) Why would it be bad to drink deuterated water?

Class 17 - Summary

Supplemental

Depending on time and interests of the participating students I can offer a few more classes which are related to chemical kinetics or current problems of interest in science.

Class 17 – Oscillating reactions, chemical chaos, etc..

Class 18&19 – voluntarily and supplemental – concepts for an alternative energy production (power point presentation)

Class 20 – Final (does not include surface science of supplemental topics)

List of reaction types discussed