CHMENG 142: Chemical Kinetics and Reaction Engineering

Fall 2023, Syllabus

Instructor:	Prof. Karthik Shekhar (KS)	**Email:**	kshekhar@berkeley.edu
Time:	Tu,Th 3:30-5:00pm	**Place:**	Valley Life Sciences 2040.
Course site:	bCourses CHMENG 142	**Office Hours:**	W 11-12pm; Tu 1-2pm (101D Gilman)

Description: Chemical reactions control our environment, our life processes, our food production and our energy utilization. Chemical reactions are all about how one chemical substance interconverts to the other, leading to the concept of the *rate* of a reaction. The topic of chemical kinetics is all about understanding the factors that govern the rates of reaction. We will then integrate concepts of chemical kinetics with thermodynamics and transport phenomena to develop models of chemical reactors ("reaction engineering"). The design and analysis of chemical reactors is one of the triumphs of the discipline of chemical engineering.

Much of this course will involve the description of chemical reactions, mole and energy balances at either via a continuum or compartmental (i.e. lumped) frameworks (recall 150A). These can be modeled as a system of ordinary differential equations that are posed as either initial value problems or boundary value problems. We will use this approach to understand the kinetics of homogeneous reactions (i.e. involving a single phase) occurring within isothermal and non-isothermal reactors. Temperature plays a fundamental role in reaction rates, and this influences the stability of reactors. We will also cover reactions in heterogenous systems (e.g. catalysts). Truly multiphase reactions involving hydrodynamic effects, however, will not be covered.

It must be understood, however, that chemical reactions are microscopic phenomena that occur at the level of individual molecules at extremely short timescales ($10^{-15} - 10^{-16}$ seconds). The continuum-level, deterministic description is appropriate when considering large numbers of molecules ($\sim 10^{23}$) that correspond to molar quantities. However, this is not satisfactory when one deals with a small number of molecules ($\sim 10-1000$), which often occurs in systems such such as biological cells. Here, the consideration of stochastic effects becomes necessary and one must model the chemical reaction as a probabilistic event. Time permitting, the last few lectures of the course will focus on introducing students to stochastic descriptions of chemical kinetics.

Main references: We will be drawing from a variety of sources that cover both fundamental and applied aspects of chemical kinetics, including new applications (e.g. biological systems). Those interested in getting a single textbook may get Fogler's book (ref. 1).

- H. S. Fogler, *Elements of Chemical Reaction Engineering*, 6^{th} Edition, Prentice Hall, 2016.
- K. J. Laidler, *Chemical Kinetics*, 3^{rd} edition, Harper & Row, 1987.
- R. Aris, *Elementary Chemical Reactor Analysis*, Butterworths, 1989.
- P. L. Houston *Chemical kinetics and reaction dynamics*, Courier Corporation, 2012.
- O. Levenspiel, *Chemical Reaction Engineering*, 3^{rd} edition, Wiley, 1999.
- J. M. Smith, *Chemical Engineering Kinetics*, 3^{rd} edition, McGraw Hill, 1981.

Course Schedule:

- Week 1
  - August 24: Course overview and logistics, introduction to chemical reactions and stoichiometry, definition of reaction rate, law of mass action, examples of 1^{st} and 2^{nd} order irreversible reactions.
  - August 29: General mole balances, and introduction to the basic types of chemical reactors.
- Week 2
  - August 31: Reactor design equations and conversion as a function of reactor size in isothermal systems. Concept of residence time. Graphical sizing of steady state flow reactor systems.
  - September 5: Multiple reactor systems, stoichiometric tables, gas and liquid phase concentrations and reactor design for an equilibrium reaction.
- Week 3
  - September 7: Isothermal reaction with phase change. Stoichiometric table analysis.
  - September 12: Concept of transient, steady state and equilibrium. Transient operations of isothermal reactors: Startup of CSTR and semi-batch operations.
- Week 4
  - September 14: Chemical Equilibrium of a multicomponent homogenous reacting system, definition of chemical potential, relation of equilibrium constant to activities, Illustration for ideal gases.
  - September 19: Temperature dependence of equilibrium constant, Le Chatelier's principle (temperature and pressure effects on conversion). Recorded Zoom lecture
- Week 5
  - September 21: Concepts in chemical kinetics, elementary reactions, temperature dependence of reaction rate constants.
  - September 26: Complex rate laws, pseudosteady state approximation intuition and application.
- Week 6
  - September 28: Enzyme kinetics.
  - October 3: **Midterm 1 (in class)**. Coverage: Lectures 1-7
- Week 7
  - October 5: Introduction to reactor energy balances.
  - October 10: Reactor energy balances.
- Week 8
  - October 12: Design of non-isothermal reactors.
  - October 17: Multiple steady-states and reactor stability.
- Week 9
  - October 19: Multiple steady-states and reactor stability.
  - October 24: Unsteady-state nonisothermal reactors.
- Week 10

  - October 26: Concepts in heterogeneous catalysis. Recorded Zoom Lecture
  - October 31: External transport effects in catalyst particles.

- Week 11
  - November 2: **Midterm 2 (in class)**. Coverage. Lectures 8-18.
  - November 7: Intraparticle diffusion and reaction. Catalyst effectiveness factor.

- Week 12
  - November 9: The Chemical Basis of Morphogenesis. Turing Instabilities.
  - November 14: Dispersion analysis of Turing instabilities.

- Week 13
  - November 16: Introduction to the stochastic theory of chemical reactions.
  - November 21: Chemical master equations and moment averaging.

- Week 14
  - November 23: NO CLASS (Thanksgiving break).
  - November 28: Special topic: Stochastic modeling of gene transcription

- Week 15
  - November 30: Special topic: Stochastic simulation of chemical reactions.

Final Exam: December 15, 7pm-10pm

Table 1: Homework schedule

Name	Post date	Due date
HW1	8/24	8/31
HW2	8/31	9/7
HW3	9/7	9/14
HW4	9/14	9/21
HW5	9/21	9/28
HW6	10/5	10/12
HW7	10/12	10/19
HW8	10/19	10/26
HW9	11/2	11/9
HW10	11/9	11/16
HW11-HW12*	11/16	12/03

$*$ This will be two homeworks clubbed together, but will be due 16 days from posted date.