CHMENG 142: Chemical Kinetics and Reaction Engineering

Fall 2024, Syllabus

Instructors: Profs. Karthik Shekhar (kshekhar@berkeley.edu) & Neil Razdan (razdan@berkeley.edu)
Time: MWF 1-2pm **Place:** Valley Life Sciences 2060 **Course website:** bCourses CHMENG 142
Office Hours: KS (Tu 11-12pm, F 3-4pm @ 101D Gilman), NR (W 4-5pm, Th 3-4pm @ 101A 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.
- M. E. Davis, R. J. Davis, *Fundamentals of Chemical Reaction Engineering*, 1^{st} Edition, McGraw Hill, 2003.
- 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 28: Course overview and logistics, introduction to chemical reactions and stoichiometry, definition of reaction rate, law of mass action.
  - August 30: Extent of reaction and conversion. Solving homogenous kinetics problems for 1st and 2nd order irreversible reactions. Introduction to general mole balances.
- Week 2
  - September 2: Holiday (no class)
  - September 4: Reactor design equations and conversion as a function of reactor size in isothermal systems. Concept of residence time.
  - September 6: Graphical sizing of steady state flow reactor systems. Multiple reactor systems, and stoichiometric tables, gas and liquid phase concentrations.
- Week 3
  - September 9: Stochiometric tables continued. Reactor design for an equilibrium reaction.
  - September 11: Isothermal reaction with phase change. Stoichiometric table analysis.
  - September 13: Concept of transient, steady state and equilibrium. Transient operations of isothermal reactors: Startup of CSTR and semi-batch operations.
- Week 4
  - September 16: Non-steady state reactors.
  - September 18: Chemical Equilibrium of a multicomponent homogenous reacting system. Review of Chemical Potential of chemical potential, relation of equilibrium constant to activities, Illustration for ideal gases.
  - September 20: Temperature dependence of equilibrium constant, Le Chatelier's principle (temperature and pressure effects on conversion).
- Week 5
  - September 23: Concepts in chemical kinetics, elementary reactions, temperature dependence of reaction rate constants.
  - September 25: Measuring rate constants from experiments
  - September 27: Complex rate laws, pseudosteady state approximation intuition and application.
- Week 6
  - September 30: Enzyme kinetics.
  - October 2: **Midterm 1 (in class)**. Coverage: Lectures 1-13
  - October 4: Enzyme Kinetics.
- Week 7
  - October 7: Introduction to heterogeneous catalysis.
  - October 9: Adsorption phenomenon. Multi-site catalytic elementary steps.
  - October 11: Reversible catalytic reactions.
- Week 8

- October 14: Electrochemical catalytic reactions.
- October 16: External mass transport effects in heterogeneous catalysis.
- October 18: External mass transport effects in heterogeneous catalysis (cont'd).

- Week 9
  - October 21: Internal mass transport effects in heterogeneous catalysis.
  - October 23: Internal mass transport effects in heterogeneous catalysis (cont'd).
  - October 25: Introduction to reactor energy balances.
- Week 10
  - October 28: Reactor energy balances.
  - October 30: Adiabatic reactor design.
  - November 1: Adiabatic reactor design (cont'd).
- Week 11
  - November 4: Non-isothermal, non-adiabatic reactor design.
  - November 6: Review.
  - November 6: **Midterm (outside class hours)** 7-9pm, 120 Latimer.
  - November 8: Multiple steady-states and reactor stability.
- Week 12
  - November 11: Holiday (no class)
  - November 13: Unsteady non-isothermal reactor design.
  - November 15: Unsteady non-isothermal reactor design (cont'd).
- Week 13
  - November 18: Introduction to residence time distributions in reactors.
  - November 20: Residence time distributions in reactors.
  - November 22: Modelling non-ideal reactor hydrodynamics.
- Week 14
  - November 25: Special topic/Case study.
  - November 27: Holiday (no class)
  - November 29: THANKSGIVING HOLIDAY (no class)
- Week 15
  - December 2: Special topic/Case study.
  - December 4: Special topic/Case study.
  - December 6: Special topic/Case study.

Final Exam: December 18, 7pm-10pm

Table 1: Homework schedule

Name	Post date	Due date
HW1	8/30	9/6
HW2	9/6	9/13
HW3	9/13	9/20
HW4	9/20	9/27
HW5	10/4	10/11
HW6	10/11	10/18
HW7	10/18	10/25
HW8	10/25	11/1
HW9	11/8	11/15
HW10	11/15	11/22
HW11-HW12*	11/22	12/06

∗ This will be two homeworks clubbed together, but will be due two weeks from the posted date.