Syllabus (Fall 2018)

Chemistry 662: Chemical Kinetics and Dynamics

The policies and regulations contained in this syllabus are subject to change at any point. Such changes will be announced in class and/or posted on the course website. The syllabus has been compiled to be as complete as possible but is by no means a binding document.

General Info

Instructor:	Prof. **Jörg C. Woehl**
Office:	Chemistry Building, Room 343
Office hours:	Open door and by appointment
Email:	woehl@uwm.edu
Phone:	414-229-5223

Class Meeting Times:	Tuesday and Thursday, 9:30-10:45 am
Class Location:	Chemistry Building, Room 170
First Day of Class:	Tuesday, September 4
Last Day of Class:	Thursday, December 13
Midterm (take-home):	Tuesday, November 6; due Tuesday, November 13
Final Exam:	Thursday, December 20, 7:30-9:30 am

Course Objectives

This course is both an introduction to and advanced treatment of Chemical Kinetics. In contrast to a traditional lecture course, we will make use of a computational programming environment (Matlab) in order to explore the theoretical foundations of chemical kinetics and use it as a tool for advanced simulations and problem solving.

Required Class Material

Latest version (R2018a) of either

- "MATLAB Student" + "Symbolic Math Toolbox" ($59 if ordered at the same time)

or

- "MATLAB and Simulink Student Suite" ($99; includes the "Symbolic Math Toolbox" and many other add-on products)

Recommended Textbook

Jeffrey I. Steinfeld, Joseph S. Francisco, and William L. Hase: "Chemical Kinetics and Dynamics" (518 pages), 2nd ed., Prentice Hall, Upper Saddle River, NJ (1999). ISBN 0137371233. UWM Library Call Number QD502 .S74 1999 (on Reserve).

Supplemental Textbooks

- Donald A. McQuarrie and John D. Simon: "Physical Chemistry: A Molecular Approach", University Science Books, 1997. UWM Library Call Number: QD453.2 .M394 1997.
- Keith J. Laidler: "Chemical Kinetics", McGraw Hill, 1965. UWM Library Call Number: QD501 .L17 1965.
- Paul L. Houston: "Chemical Kinetics and Reaction Dynamics", McGraw Hill, 2001. UWM Library Call Number: QD502 .H7 2001; also available online through Knovel.
- Gordon G. Hammes and Isadore Amdur: "Principles of Chemical Kinetics", Academic Press, 1978. UWM Library Call Number: QD502 .H35.
- Gordon G. Hammes: "Thermodynamics and Kinetics for the Biological Sciences", Wiley-Interscience, 2000. UWM Library Call Number: QP517.P49 H35 2000.
- Donald A. McQuarrie: "Mathematical Methods for Scientists and Engineers", University Science Books, 2003. UWM Library Call Number: QA37.3 .M36 2003.

Course Prerequisites

"Chemistry 662: Chemical Kinetics and Dynamics" (Chem-662) requires Senior Status and Grade of C or better in CHM 562 (Physical Chemistry II).

Lectures

Your attendance of all lectures is highly recommended. This is a graduate level class, and I expect you to take the necessary steps to take ownership of the material. You know best whether you have truly understood a particular topic and whether you need to read up on it using textbooks, try to solve more problem sets, or seek the help of your instructor; please use the available options accordingly.

Course Website

Canvas: https://uwm.edu/canvas/. For information on how to use Canvas, please visit https://uwm.edu/canvas/students/.
Problem sets and solutions as well as other course material will be made available on Canvas. Visit the course website regularly as important information and announcements may be posted there as well.

Problem Sets

There will be a few homework assignments at irregular intervals. You are required to turn them in by the due date, but they will not be corrected and no grade will be given. Working on these problem sets will help you in preparing for the midterm and final exam; solutions to the homework assignments will be provided on the course website. In addition, you are strongly encouraged to work on your own through more problems from kinetics textbooks.

Grading

The course will be graded as follows based on examinations and a research project:

Midterm (take-home)	35%
Final Exam (in-class)	45%
Research Project	20%
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Total	100%

The *Midterm* is a take-home exam that will be handed out and posted to Canvas after the lecture. The midterm will cover all topics discussed in class and problem sets in a format similar to the problem sets. No class will be held on Thursday during midterm week (Nov 8, 2017).
No time extensions or make-up exam will be given for the take-home midterm. If you are unable to turn it in during class, you may upload it to the Canvas dropbox.

The *Final Exam* is comprehensive. Only a calculator (programmable or non-programmable) and a single sheet of paper with handwritten notes (recto-verso) are allowed. No books or other material are admitted.

In addition, you will choose one kinetics-related *Research Project* to work on during the second part of the semester. You will present the results from this project to the other students as an oral presentation during the last week of class. The quality of this presentation will count 20% towards the final grade.

Tentative Schedule

Week		Topic
1	Sep 4 - Sep 9	Introduction to Matlab
2	Sep 10 - Sep 16	Kinetic Measurements; Basic Concepts of Chemical Kinetics
3	Sep 17 - Sep 23	First- and Second-Order Reactions
4	Sep 24 - Sep 30	Third-Order Reactions; Determination of Reaction Orders; Arrhenius Equation
	Oct 1	Last day to drop full-term courses without “W” on record
5	Oct 1 - Oct 7	Complex Reactions: Reversible and Consecutive Reactions
6	Oct 8 - Oct 14	Complex Reactions: Parallel Reactions; Single Molecule Kinetics
7	Oct 15 - Oct 21	Steady-State Approximation; The Hydrogen-Bromine Reaction
8	Oct 22 - Oct 28	Laplace Transform Method

Week		Topic
9	Oct 29 - Nov 4	Matrix Algebra; Numerical Methods
	Nov 11	Last day to drop or withdraw from full-term courses
10	Nov 5 - Nov 11	**Midterm (take-home)** - no class on Thursday, Nov 8 Stochastic Approach
11	Nov 12 - Nov 18	Catalysis
12	Nov 19 - Nov 20	Enzyme Kinetics
	Nov 21 - Nov 25	Thanksgiving Recess
13	Nov 26 - Dec 2	Autocatalysis ; Potential Energy Surfaces
14	Dec 3 - Dec 9	Transition State Theory
15	Dec 10 - Dec 13	**Research Project Presentations**
	Dec 20	**Final Exam 7:30-9:30 am (CHM 170)**

Policies

If you will need accommodations in order to meet any of the requirements of this course, please contact me and the Student Accessibility Center (SAC) as soon as possible. Special accommodations for students with disabilities can be provided, but their timely implementation can only be insured if the SAC is contacted ahead of time. For details see www4.uwm.edu/sac/SACltr.pdf.

Department of Chemistry and Biochemistry policies are posted on bulletin boards in the department.

UWM policies related to students with disabilities, religious observances, students called to active military duty, incompletes, discriminatory conduct, academic misconduct, complaint procedures, grade appeal procedures, and final examination requirements can be consulted at https://uwm.edu/secu/wp-content/uploads/sites/122/2016/12/Syllabus-Links.pdf.

Academic Misconduct

Cheating on an exam or other graded material will automatically result in a grade of zero (as a minimum consequence); failure in the course and referral to the Dean may also occur. Academic dishonesty in any form will not be tolerated.

> *"Academic misconduct is an act in which a student seeks to claim credit for the work or efforts of another without authorization or citation, uses unauthorized materials or fabricated data in any academic exercise, forges or falsifies academic documents or records, intentionally impedes or damages the academic work of others, engages in*

conduct aimed at making false representation of a student's academic performance, or assists other students in any of these acts."

"Prohibited conduct includes cheating on an examination; collaborating with others in work to be presented, contrary to the stated rules of the course; submitting a paper or assignment as one's own work when a part or all of the paper or assignment is the work of another; submitting a paper or assignment that contains ideas or research of others without appropriately identifying the sources of those ideas; stealing examinations or course materials; submitting, if contrary to the rules of a course, work previously presented in another course; tampering with the laboratory experiment or computer program of another student; knowingly and intentionally assisting another student in any of the above, including assistance in an arrangement whereby any work, classroom performance, examination or other activity is submitted or performed by a person other than the student under whose name the work is submitted or performed."

(From: Office of the Provost and Vice Chancellor)