Chemical Systems Modeling - A Workshop CHEM:5114

Syllabus for CHEM:5114 - Spring 2018 - 1, 2, 3 Hours

Wednesdays 6:30 pm to 9:10 pm, C139 PC

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Office Hours 21:10 to 21:40 Wednesday, after class; Thursday 10:00 to 12:00; and by appt.

General Comments on the Course: This course has a lecture portion and a workshop portion where the students will model/solve problems encountered in their research. Lectures will be on basic procedures used to solve modeling problems commonly encountered in chemical research. In the workshop, students will attempt to model/solve problems encountered in their research. Students will make presentations on their projects as they work through the steps outlined in the lectures. The first third of the course covers equilibrium. In the remainder of the course, lectures introduce kinetic and transport models as well as modeling methods and workshop begins.

Text: Information will be provided in lecture and hand outs. A text that is a good general reference is *The Chemistry Maths Book*, Erich Steiner, but is not required. For the equilibrium portion of the class, a good general reference is *Quantitative Analytical Chemistry*, Harris any edition, chapters on equilibrium calculations, usually near chapter 6. Data tables at the back are useful. Also, is the out of print text, *Chemical Equilibria* by A.J.Bard, available on the website.

Web: There is a simple class web page at https://uiowa.instructure.com/courses/74309

Prerequisites: A sense of adventure, a question and an envelope with no writing on the back.
No mathematics beyond algebra and geometry are required, although some calculus will be presented. Computer skills need not exceed use of a spreadsheet. The student's research problems may require more sophisticated methods.

Course Topics:

Visualizing the Problem - Make the Movie. See the Beaker.
Common Chemical Methods of Parameterizing Chemical Systems
- Equilibrium Methods - Conservation of mass and charge; fractional concentrations; titrations; redox
  EQ 1: Mass Balance (MB), Charge Balance (CB), constants; classes of problems (Cosmic General Rules)
  EQ 2: Fractional concentrations; titration curves; autoprotolysis; fun with buffers, CO2 equilibria
  EQ 3: Redox, Redox speciation (E vs pH), Redox Titrations (balancing redox equations), Redox potential axis
  EQ 4: In class mega problem (suggestions?)
- Kinetic Methods - the Steady State Approximation
- Governing Equations and Boundary and Initial Conditions

Parameterizing the Problem and Keeping Track of the Assumptions
- Does it Make Sense Physically ? (Back of Envelop Calculations)
- Will it Yield Values Consistent with the Experimental Observables ?
- Will the Values be in the Range of the Data ?

What Constitutes an Answer ? (Optimally/Minimally)
Methods of Solving the Equations
- Analytical Solutions
- Successive Approximations
- Computers (Spread Sheets, Symbolic Manipulators, Programming, Finite Difference, Minimization)

Is It Likely to be Solved in the Time Available ?
Simplifying Assumption - Length and Time Scales
How to Know if the Answer is Reasonable
- Dimensional Analysis
- Are all the Results Physically Reasonable ?
- Magnitude Analysis
- Can the Answer be Pushed into a Physically Unrealistic Range ?

What is the Applicable Range ? Does it Include the Experimental Range ?
Presentation and Generalization of the Result - Dimensionless Parameters
How to Make Due with a Partial Answer
Is the Model Consistent with Your Experimental Results ? (If not, repeat loop.)

Always Remember Two Things:

- Most mathematical characterizations of physical systems have been the acts of desperate people.
- Modeler's Credo: Sounds good; doesn't mean its right. Steve Feldberg

Class Requirements: The course has two components. First, various modeling protocols will be presented and the students will do some simple example of each of these protocols. This will be done on line on Canvas/ICON and will sometimes be discussed by the students in class. Second, the student will select a modeling problem of interest to them perhaps from their own research, and then attempt to the resolve the question by an appropriate modeling method. The students will discuss their process in class in a workshop style environment. A final report of the efforts is to be submitted at the end of the semester.

Online Canvas/ICON submissions serve as a rudimentary demonstration of methods presented in lecture. These will not be graded in great detail.

Selection and attempt at resolution of a modeling problem: Presentations will be made on the problem, parameterization, simplifications, and final resolution. There are no exams. Grade is determined by homework, class participation, presentations, modeling efforts, and final written statement of modeling efforts. A formal statement of the modeling effort must be submitted in written form at the end of the semester; the length will be roughly 5 to 10 pages. Modeling may be by computer or analytically. A good grade does not rely on solving the problem - modeling is not always successful.

Students with Disabilities and Learning Disabilities: Students requiring special arrangements to attend class or take exams, should notify the instructor as quickly as possible so that appropriate arrangements can be made.

Academic Misconduct: Academic misconduct will not be tolerated. Any students having questions as to what constitutes misconduct should get a copy of the University's policy on academic misconduct in the Departmental Office in1 CB.

Computer Access: Please bring your laptop to class. Install Visual Basic if necessary in Excel. One Note may also be useful and perhaps a link to Mathematica.

Exam Dates: There will be no exams. If we need the time, the final exam slot may be used to make final presentations.

Grading: Grade will be determined by homework and class participation (30%), presentations and modeling efforts (40%), and final report (30%). A good grade does not rely on necessarily solving the research problem - modeling is not always successful. (Note the total grade reported in ICON is not meaningful.)

Selection of the Individual Modeling Problem: The main objective of the course is for the student to develop a sense of the modeling "experience." This will include the student developing their own model of a problem of interest to them. Students will need to select a model question of interest to them by about the third week of class.

★Please clear your choice of modeling problem with Leddy before you begin.

From the College of Liberal Arts and Sciences: Teaching Policies & Procedures: Syllabus Content (https://clas.uiowa.edu/faculty/teaching-policies-resources-syllabus-insert)

Administrative Home: The College of Liberal Arts and Sciences is the administrative home of this course and governs matters such as the add/drop deadlines, the second-grade-only option, and other related issues. Different colleges may have different policies. Questions may be addressed to 120 Schaeffer Hall, or see the CLAS Academic Policies Handbook at https://clas.uiowa.edu/students/handbook.

Electronic Communication: University policy specifies that students are responsible for all official correspondences sent to their University of Iowa e-mail address (@uiowa.edu). Faculty and students should use this account for correspondences (Operations Manual, III.15.2).

Accommodations for Disabilities: The University of Iowa is committed to providing an educational experience that is accessible to all students. A student may request academic accommodations for a disability (which includes but is not limited to mental health, attention, learning, vision, and physical or health-related conditions). A student seeking academic accommodations should first register with Student Disability Services and then meet with the course instructor privately in the instructor's office to make particular arrangements. Reasonable accommodations are established through an interactive process between the student, instructor, and SDS. See https://sds.studentlife.uiowa.edu/ for information.

Nondiscrimination in the Classroom: The University of Iowa is committed to making the classroom a respectful and inclusive space for all people irrespective of their gender, sexual, racial, religious or other identities. Toward this goal, students are invited to optionally share their preferred names and pronouns with their instructors and classmates. The University of Iowa prohibits discrimination and harassment against individuals on the basis of race, class, gender, sexual orientation, national origin, and other identity categories set forth in the University's Human Rights policy. For more information, contact the Office of Equal Opportunity and Diversity, diversity@uiowa.edu, or visit diversity.uiowa.edu.

Academic Honesty: All CLAS students or students taking classes offered by CLAS have, in essence, agreed to the College's Code of Academic Honesty: "I pledge to do my own academic work and to excel to the best of my abilities, upholding the IOWA Challenge. I promise not to lie about my academic work, to cheat, or to steal the words or ideas of others; nor will I help fellow students to violate the Code of Academic Honesty." Any student committing academic misconduct is reported to the College and placed on disciplinary probation or may be suspended or expelled (CLAS Academic Policies Handbook).

CLAS Final Examination Policies: The final examination schedule for each class is announced by the Registrar generally by the fifth week of classes. Final exams are offered only during the official final examination period. No exams of any kind are allowed during the last week of classes. All students should plan on being at the UI through the final examination period. Once the Registrar has announced the date, time, and location of each final exam, the complete schedule will be published on the Registrar's web site and will be shared with instructors and students. It is the student's responsibility to know the date, time, and place of a final exam.

Making a Suggestion or a Complaint: Students with a suggestion or complaint should first visit with the instructor (and the course supervisor), and then with the departmental DEO. Complaints must be made within six months of the incident (CLAS Academic Policies Handbook).

Understanding Sexual Harassment: Sexual harassment subverts the mission of the University and threatens the well-being of students, faculty, and staff. All members of the UI community have a responsibility to uphold this mission and to contribute to a safe environment that enhances learning. Incidents of sexual harassment should be reported immediately. See the UI Office of the Sexual Misconduct Response Coordinator for assistance, definitions, and the full University policy.

Reacting Safely to Severe Weather: In severe weather, class members should seek appropriate shelter immediately, leaving the classroom if necessary. The class will continue if possible when the event is over. For more information on Hawk Alert and the siren warning system, visit the Department of Public Safety website.

*These CLAS policy and procedural statements have been summarized from the web pages of the College of Liberal Arts and Sciences and The University of Iowa Operations Manual.