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. Course time will be divided about evenly between lectures and workshop activities.

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

Web: There is a simple class web page at http://icon.uiowa.edu/

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 - Making the Movie
- Common Chemical Methods of Parameterizing Chemical Systems
  - Equilibrium Methods
  - 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 in homework sets that 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 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.

A few homework sets will serve as a rudimentary demonstration of methods presented in lecture. Homework will be collected, but not 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 class; 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, E331 CB.

**Computer Access:** Please bring your laptop to class. Install Visual Basic if necessary.

**Exam Dates:** There will be no exams.

**Grading:** Grade will be determined by homework and class participation (20%), presentations and modeling efforts (50%), and final report (30%). A good grade does not rely on necessarily solving the research problem - modeling is not always successful.

**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 me before you begin.
From the College of Liberal Arts and Sciences: Teaching Policies & Procedures: Syllabus Content
(http://www.clas.uiowa.edu/faculty/teaching/policies.shtml)

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 Student Academic Handbook (http://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 (http://www.uiowa.edu/~our/opmanual/iii/15.htm#152). Scroll down to k.11.)

Accommodations for Disabilities: A student seeking academic accommodations should first register with Student Disability Services and then meet privately with the course instructor to make particular arrangements. See www.uiowa.edu/~sds/ for more information.

Academic Honesty: All CLAS students have, in essence, agreed to the College’s Code of Academic Honesty (http://clas.uiowa.edu/students/handbook/academic-fraud-honor-code): "I pledge to do my own academic work and to excel to the best of my abilities, upholding the IOWA Challenge (http://clas.uiowa.edu/students/handbook/academic-fraud-honor-code). 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, http://clas.uiowa.edu/students/handbook/academic-fraud-honor-code).

CLAS Final Examination Policies: The date and time of every final examination is announced during the fifth week of the semester; each CLAS student will receive an email from the Registrar stating the dates and times of the student’s final exams. 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.

Making a Suggestion or a Complaint: Students with a suggestion or complaint should first visit the instructor, then the course supervisor, and then the departmental DEO. Complaints must be made within six months of the incident. See the CLAS Student Academic Handbook (http://clas.uiowa.edu/students/handbook/student-rights-responsibilities#rights).

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 Comprehensive Guide on Sexual Harassment (http://www.uiowa.edu/~eod/policies/sexual-harassment-guide/index.html) 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 Public Safety web site (http://police.uiowa.edu/stay-informed/emergency-communication/).

*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.