Modeling, Dynamics and Control of Chemical and Biological Systems
ChemBE 540.409 — Fall 2010

Instructor:	Professor Jeffrey J. Gray 208 Maryland Hall, jgray@jhu.edu, 410-516-5313
Office Hours:	MW 11-12, or by appointment
Lectures:	MWF 10-11 a.m., Shaffer 303
Recitations:	MTW 1-2 p.m. or T 12-1 p.m. (choose one)
TAs:	Brian Weitzner, Maryland 305, brian.weitzner@jhu.edu Krishna Kilambi, Maryland 303, kkpraneeth@jhu.edu
TA Office Hours:	W 2-3 (Weitzner), Tu 2-3 (Kilambi) or by appointment
Graders:	Tommy Harrelson (tharrel4@jhu.edu), John Huang (shuang31@jhu.edu), Mike Keung (mkeung@jhu.edu)
Office Hours:	Th 12-1 (Harrelson) NEB 39 or F 12-1 (Huang), NEB 39; M 3-4 (Keung) HAC lab
Course Website:	*http://graylab.jhu.edu/courses/540.409*
Required Texts:	*Process Control: Modeling, Design, and Simulation* B. Wayne Bequette, Prentice Hall 2003, ISBN 0133536408, ~$70-144
	An Introduction to Systems Biology: Design Principles of Biological Circuits Uri Alon, Chapman & Hall/CRC 2007, ISBN 1584886420,~ $40-50

Recommended Software and Text:

MATLAB and Simulink, Student Version ($99; available at the Krieger lab)
Octave (free, *www.gnu.org/software/octave*) is a suitable alternative for the first two weeks of class.

Essential MATLAB for Engineers and Scientists, Fourth Edition
Brian D. Hahn & Daniel T. Valentine, Newnes 2010 (~$25)

Supplementary Texts: (on reserve at the MSEL)

- *Process Dynamics and Control*, Third Edition, D.E. Seborg, T.F. Edgar, D.A. Mellichamp & F.J. Doyle, Wiley 2011
- *Process Dynamics, Modeling and Control*, B.A. Ogunnaike & W.H. Ray, Oxford 1994
- *Mathematics for Dynamic Modeling*, E. Beltrami, Academic Press, 2nd Ed. 1998
- *Dynamics: The Geometry of Behavior*, R.H. Abraham and C.D. Shaw, 2nd Ed., Addison-Wesley 1992
- *Biochemistry*, J.M. Berg, J.L. Tymoczko, and L. Stryer, 5th Ed., Freeman 2002

- *A Guide to MATLAB for Beginners and Experienced Users*, B.R. Hunt, R.L. Lipsman, J.M. Rosenberg, Cambridge University Press, 2nd Ed., 2006
- Additional literature readings will be assigned for special topics.

Overview: In this class you will learn to model and control chemical and biological processes. Previous ChemBE courses have usually focused on mathematical models of *steady-state* behavior; here, you will learn to model *dynamics*, that is, responses over time. In particular, you will model the transient response around a steady-state solution, and you will design appropriate control systems to maintain desired process behavior. In the chemical process industries, correct process control is essential for safety, environmental security, and economic optimality. In biological systems, complex control loops already exist to maintain homeostasis and enable interesting function. It is necessary to create models for these existing biological systems and then to identify appropriate means to judiciously interrupt the circuits to change the system's behavior, for example by using a drug to combat a disease.

Specific Objectives: (numbers/letters indicate alignment with department/ABET objectives)

1. Create dynamic models for chemical and biological processes, including single-variable and multivariable systems, and linear and nonlinear systems. (2ae)
2. Integrate dynamic models to determine system behavior over time using Laplace methods, state space methods, or numerical methods. (23abe)
3. Design control schemes to control system behavior. (23c)
4. Analyze dynamics and control with frequency approaches. (24ak)
5. Meet environmental and safety objectives through process control. (7fhj)
6. Use computational tools for system analysis. (4k)
7. Operate an industrial control system on a lab-scale process. (346abdk)
8. Collaborate in small working teams on research, analysis, and design. (2347bcdek)

Prerequisites:

110.302 or 500.303 or equivalent differential equations course. You should be able to integrate ODEs using several different methods. Knowledge of linear algebra and eigenvalues helpful but not required.

540.203 (Engin. Thermo), 540.301 (Kinetics), 540.303 (Transport I). Many examples are drawn from chemical and biomolecular engineering applications, and therefore it will be necessary to recall mass and energy balances, constitutive laws, and design equations.

020.305 (Biochemistry), 020.306 (Cell Biology) – recommended. Biological examples and the project may require familiarity with biomolecules and cells. Students should be able to read literature and extract the relevant stories and appropriate parameters.

An enthusiastic student might be able to excel in this course without all of the prerequisites, but he or she will have to do additional background work to complete homework problems when knowledge is required from the prerequisite courses. For example, in the past, BME majors have

succeeded without first taking Kinetics. I recommend that students form homework study groups with others with a diversity of knowledge of engineering experiences and biological phenomena.

Grading: Grades will be determined from an *absolute* scale: 85% = A-; 75% = B-; 65% = C- etc. I reserve the right to shift these percentages down (but not up). For example, if a particular exam is more difficult than I originally planned, an A- may be achieved with an 83. It is not advisable to rely on a grade shift, however.

Your course grade will be computed as follows:

Midterm I	20%
Midterm II	20%
Final Exam	20%
Homework	25%
Lab	10%
Resume & Interview	5%
Total	100%

Homework: Homework will be assigned regularly and will be due after approximately one week. Half of the homework grade will be awarded simply for completing the problem; the other half will be awarded based on the correctness of the result and approach. Homework not received by five minutes after the start of class on the due date will be penalized 25%; an additional 25% penalty will be incurred for every additional day late. Late homework should be turned in to the graders' mailbox in 226 Maryland Hall.

Exams: Mid-term exams will be given in the evenings to allow ample time for completion. Exams will include both a closed-book portion of mostly short-answer problems and an open-book portion with more complex analytical problems.

Regrades: Any regrade requests (exam or homework) must be submitted in writing within one week of the return of the exam or assignment. Homework regrades will be performed by the grader, with review by the professor. Exam regrades will be performed by Prof. Gray. Note that in the event of a regrade, the entire submission (not just the item of contention) is subject to regarding, at the discretion of the reviewer.

Lab: To gain hands-on experience with an industrial feedback control system, there will be one short lab experience integrated with a homework problem on feedback control. The process control laboratory is in the basement of Maryland Hall and is composed of a mixing tank, temperature and level sensors, flow valves, and a computer control system. The lab will involve the modeling of the process and the comparison of several control strategies. Labs will be completed in groups of three people. After the first mid-term, each group will need to schedule a two-hour period to perform the experiments.

Teamwork on Lab Assignment: I encourage teamwork and collaboration to improve your leadership abilities and to increase your learning. The lab assignment is explicitly designed to allow you practice interpersonal as well as technical skills. I expect each member of the team to

contribute significantly to group projects. It is the responsibility of the team to resolve internal conflicts and balance the workload between team members.

Collaboration on Homework: Homework is provided as practice of your individual problem solving skills, and exam problems will primarily test skills developed through the homework. Therefore, you are expected to attempt to solve the problems individually, and each student must submit his or her own work. However, the test of whether one truly understands something is the ability to explain it to others. Therefore, you may consult with your colleagues if you have difficulty with a problem, and you may also act as a consultant. For example, legitimate consulting questions might be, "How do you take the Laplace transform of this equation?" or "Does this block diagram look correct to you?" However, copying of another person's homework ("I don't understand problem 3.1, can I see yours?") or giving a colleague a copy of your results are strictly forbidden. Violations will be dealt with in accordance to the university's policies on academic ethics. If you consult another member of the class on a particular homework assignment, please put the name of that person (or persons) under your name at the top of your homework. The number of consultants will not alter your homework grade.

Class Participation: I will use a variety of individual and small-group active learning exercises in class, therefore you are expected to participate. I will frequently call on students for answers and examples. Thinking time will be provided, but answers of "I don't know" are not allowed. Finally, you are encouraged to ask questions during lecture.

Resume and Mock Interview: As part of your professional preparation, the department strongly encourages you to make use of all of the resources in the Career Center. There are two formal requirements for the resume & interview portion of the grade for this course. First, students must have their resume critiqued and stamped at the Career Center, and the marked-up and a revised resume should be submitted for grading. Second, students must participate in a mock interview arranged through the Career Center. This requirement must be fulfilled by November 30 (with submission of homework 8), but it is best to complete this requirement as early in the semester as possible, since the Career Center has only limited times available for the critiques and the mock interviews. Resumes should be submitted along with another homework assignment (but not attached); graders will track submissions.

Ethics: Cheating is wrong. Cheating hurts our community by undermining academic integrity, creating mistrust, and fostering unfair competition. The university will punish cheaters with failure on an assignment, failure in a course, permanent transcript notation, suspension, and/or expulsion. Offenses may be reported to medical, law or other professional or graduate schools when a cheater applies.

Violations can include cheating on exams, plagiarism, reuse of assignments without permission, improper use of the Internet and electronic devices, unauthorized collaboration, alteration of graded assignments, forgery and falsification, lying, facilitating academic dishonesty, and unfair competition. Ignorance of these rules is not an excuse.

You may collaborate with other students in this course, but only on homework, the literature review and the lab as detailed above. If you have questions about this policy, please ask the instructor.

On every exam, you will sign the following pledge: "I agree to complete this exam without unauthorized assistance from any person, materials or device. [Signed and dated]"

Old exams from this course may be found at http://graylab.jhu.edu/courses/540.409.

For more information, see the guide on "Academic Ethics for Undergraduates" and the Ethics Board web site (http://ethics.jhu.edu).

Topics: Tentative material to be covered:

1. Incentives for Process Control
2. Modeling & system representations
3. State space models
4. Introduction to MATLAB
5. Linearization
6. Pharmacokinetic modeling, biomolecular modeling, and the Central Dogma
7. Laplace functions
8. Transfer functions
9. First, second, and higher-order systems
10. Poles and zeros, time delay
11. Empirical model formulation
12. Feedback control
13. PID controllers
14. Closed-loop transfer function
15. Frequency response
16. Bode and Nyquist approaches
17. Biological network motifs (FFLs)
18. Temporal programs
19. Bi-fans, kinase cascades, and multi-layer perceptrons
20. Introduction to nonlinear dynamics

Special Dates and Times:

M	Aug 30	First day of class
M	Sep 6	No class—Labor Day
W	Oct 6	Exam I, 7-10 p.m. (tentative)
Tu	Oct 12	Class held according to Monday schedule (fall break)
Tu	Nov 9	Exam II, 7-10 p.m. (tentative)
W	Nov 24	No class—Thanksgiving weekend
F	Dec 3	Last day of class, course evaluations
Tu	Dec 14	Final Exam, 2-5 p.m.