CH 5140: Process Analysis and Simulation

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Instructor

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Teaching Assistants

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Lectures

Lectures will be held in the B-Slot. There will be no lecture on Fridays.

Course Objectives

The objective of this course is to develop a fundamental understanding of steady state and dynamical behaviour of process systems using simulations and model analysis. A broad range of topics of interest to process engineers is covered in this course, relating to systems modelling, parameter estimation, linear and nonlinear systems analysis and some advanced topics in simulation. This course also attempts to acquaint the students to a variety of simulation software available in the market. While there is a large overlap in the topics covered in core chemical engineering curriculum, this course places a greater focus on simulation modules instead of theoretical aspects.

Since this is a Dual Degree core course, the intention is to get students ready for research work that follows in summer and next year. Naturally, there is a greater focus on projects and home assignments than quizzes and exams compared to a typical core course.

Software

This course will rely heavily on computer-based exercises to learn the practical aspects of implementing the theoretical concepts learnt in the lectures. The primary computational package used for simulation and analysis in this course will be MATLAB. Matlab is versatile and popular software, which was originally designed to handle matrix-based computations easily. Over years, its scope has grown and it touches nearly every aspect of Engineering.

SCILAB is an alternative software to Matlab. Scilab, available at http://www.scilab.org, is an open-source simulation package. Its capabilities for the purpose of this course are similar to those provided by Matlab. The students have a choice of using either SCILAB or MATLAB for this course.

Additionally / Optionally, students will be introduced to other software and/or simulation algorithms, including, CANTERA, FLUENT, etc.

Grading

Homeworks & Surprise tests	Projects	Quiz – 1	Quiz – 2	End-Semester
15%	2 × 15%	15%	15%	25%

Home Assignments and Surprise Tests

There will be home assignments and surprise tests throughout the course. All the assignments and projects will be posted on the course website. The assignments have to be turned in before or during the end of lecture on the due date; no late submissions will be entertained for any reason. The surprise tests will not be announced before-hand, and will cover material until the previous day. There will be a minimum of 10 such homework/tests. Final grade will be a weighted average of all except one assignment/test with least marks.

Students can work in groups of two for home assignments. In such a case, single assignment submission will be required. The grade assigned will be 0.8 times the actual marks received.

Course Projects

There will be two course projects, each accounting for 15% of the total credit. Students will work in groups of two for the project. Both project partners are expected to put almost equal amount of effort on the projects.

The first project will be due on Monday after Quiz-1 schedules. The project problem will be assigned and some marks will be reserved for writing style and communication with the instructor.

The second project will be due on the last day of classes. This will be an open-ended project, where students will have to develop their own problem statement for the project. Details will be revealed in due course.

Quizzes and Exams

The end-semester quiz will be comprehensive, i.e., based on the *entire syllabus* taught until the day of exam, including lectures, tutorials, assignments and supplementary reading material.

Code of Conduct

You are required to follow the honour code; copying other student's assignments or project (full or in part), plagiarism of any sort, dishonesty or copying during exams will not be tolerated.

Textbook and References

General Books for the Course

- Bequette, B.W., "Process Dynamics: Modelling, Analysis and Simulation," Prentice Hall (1998)
- Himmelblau D.M. and Bischoff K.B., *Process Analysis and Simulation*, Wiley, 1988
- Varma A. and Morbidelli M., *Mathematical Methods in Chemical Engineering*, Oxford University Press, 1997

Linear Algebra

- Strang G., *Introduction to Linear Algebra*, Cambridge Press, 4th edition, 2009
  (Indian edition of the book may be available)
- Golub G.H. and van Loan C.F., *Matrix Computations*, Johns Hopkins University Press, 3rd Edition, 1996

Process Modelling and Solutions

- Ogunnaike B. and W. Harmon Ray. *Process Dynamics, Modeling, and Control*, Oxford University Press, 1995
- Chapra S.C. and Canale R.P. *Numerical Methods for Engineers*, McGraw Hill, 2001
- Press W.H., Teukolsky S.A., Vetterling W.T. and Flannery B.P., *Numerical Recipes: The Art of Scientific Computing*, Cambridge University Press, 3rd Edition, 2007
  Also see online version at the Numerical Recipes website: http://www.nr.com/
- Netlib online repository for numerical and scientific computing: http://www.netlib.org/
- Patankar S.V., *Numerical Heat Transfer And Fluid Flow*, Hemisphere Publishing, 1980

Nonlinear Analysis

- Strogatz S.H., *Nonlinear Dynamics and Chaos: With Applications to Physics, Biology, Chemistry and Engineering*, Perseus Books Publishing, 1994
- Pushpavanam S., *Mathematical Methods in Chemical Engineering*, Prentice Hall – India, 2004.

Software Manuals

- FLUENT 6.1 User Manual, Fluent Inc. and ANSYS Inc., Nashua NY, 2004
- CANTERA, Object-Oriented Software for Reacting Flows: http://www.cantera.org/

Course Outline and Tentative Schedule

	Lecture Title	**Contents**	**Schedule**
Lecture 1	Introduction	What is process simulation? Where and how is simulation useful? A brief overview of topics covered in this course.	Day 1
Lecture 2	Linear Algebra	Matrix computation, Vector spaces, linear transformation, eigenvalue and singular value decomposition, linear operators	Weeks 1-2
Lecture 3	Theoretical Modelling of Processes	Phenomenological models, mass and energy balances, state space form	Week 3-4
Lecture 4	Numerical Techniques a. Algebraic Equations b. Differential Equations	Review of generation and solution of linear equations, algebraic equations and ordinary differential equations.	Week 4-5

Lecture 5	Semi-Empirical Modelling and Parameter Estimation	Black- and gray-box models, regression, neural networks, estimation of model parameters	Week 6-7
Lecture 6	Linear System Analysis	Stability, oscillations, saddle point, phase-plane approach, linearization and extension to nonlinear systems	Week 8
Lecture 7	Nonlinear Dynamics and Bifurcation	Introduction to nonlinear analysis, examination of multiple steady states	Week 9-10
Lecture 8	Chaos	Introduction to Chaos (Strange Attractor)	Week 11
Lecture 9	Partial Differential Equations	Types of PDEs, solution techniques, finite differences, finite element methods	Week 12-14
Lecture 10	Differential Algebraic Equations	Origin of DAEs, Index of DAEs, solution techniques	Week 14-15
Advanced Topics	a. Monte Carlo methods b. Combustion c. Thermal Radiation d. Chemical Vapour Deposition e. Computational Fluid Dynamics		
	These topics may be covered subject to availability of time and student interest. They will not be included in the End-Semester Exam.		