THE OHIO STATE UNIVERSITY
COLLEGE OF ENGINEERING

Modeling and Simulation

CBE 5790

Credit Hours:
3.00 - 3.00

Course Levels:
Undergraduate (1000-5000 level)
Graduate (5000-8000 level)

Course Components:
Lecture

Course Description:
Application of chemical and biomolecular engineering principles to construct mathematical models of processes and perform simulations.

Prerequisites and Co-requisites:
Prereq: Jr, Sr, or Grad standing in CBE.

Course Goals / Objectives:
- Become familiar with the basic concepts of modeling and simulation
- Master programming fundamentals: flow control, loops, conditionals, functions, and subfunctions, input and output variables, working with numeric and character variables
- Learn how to derive the appropriate set of differential and/or algebraic equations to be solved for a particular problem of interest, and how to write a program in MATLAB to obtain a solution
- Understand modeling and simulation strategies for systems involving continuous and discrete variables
- Understand modeling and simulation strategies for systems involving deterministic and stochastic phenomena
- Demonstrate ability to write programs to model a wide variety of processes and phenomena relevant to chemical and biomolecular engineering

Course Topics:

- Overview of modeling and simulation; physical and mathematical models, phenomenological vs. mechanistic, continuous vs. discrete, deterministic vs. stochastic, algorithms
- Algorithms; programming fundamentals: flow control using loops and conditionals, nesting, writing efficient MATLAB code
- Primary functions, subfunctions, nested functions, variable scope, recursion, creating functions that take multiple inputs and return multiple outputs, troubleshooting and code debugging
- Working with string (character) data types; character arrays, structure variables, cell arrays
- MATLAB graphics, working with handle graphics, differential equation solvers, solving systems of ODEs, stiff ODEs
- Solving systems of linear algebraic equations and systems of nonlinear algebraic equations; application to modeling fluid behavior using thermodynamic equations of state
- Solving systems containing both differential and algebraic equations (DAEs); simulation examples: predator-prey, disease epidemics, chemical reactor design
- Stochastic simulation of chemical reactions, the Gillespie algorithm, application of this approach to model virus reproduction in a cell
- More examples of stochastic-discrete simulations: computing probabilities, modeling evolution, sequence analysis, replication, "mutation", and selection
- Introduction to game theory and Prisoner's Dilemma, class PD tournament, Monte Carlo simulations
- Graphical (visual) simulations: random walk simulations in2D, relation to polymers and proteins, boundary conditions, cellular automata
- Introduction to molecular simulation; intermolecular potential functions and energy minimizations

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Designation:
Elective