ChBE 6500: Mathematical Models of Chemical Processes *(core course)*
Credit: 3-0-3

Suggested Prerequisites:
Linear algebra, multivariate calculus, ordinary differential equations

Catalog Description:
Formulation and solution of mathematical models of a range of chemical processes with an emphasis on differential balances and incorporation of uncertainty.

Textbook:
Numerical Methods for Chemical Engineering, Beers, K.J., Cambridge UP, 1st edition, 2006.

Course Objectives:
This course introduces a range of analytical and numerical methods for the solution of mathematical equations encountered in chemical engineering. Topics are motivated by and presented in the context of physical phenomena encountered in chemical engineering industrial and research problems. The accuracy and computational complexity of each approach, along with their potential modes of failure, are highlighted. Attention is also given to interpretation and handling of uncertainty in the context of different problems. MATLAB is used in the course as a vehicle for teaching basic programming technique and the use of commercial numerical packages.

Learning Outcomes:
By the end of this course, a student should be able to:
1. Formulate a chemical engineering problem as a mathematical model and select an appropriate solution method to solve the problem.
2. Assess the accuracy of a numerical solution method and identify alternate strategies and methods to achieve greater accuracy when it is needed.
3. Identify the computational requirements of various solution options.
4. Justify the selection of a given solution approach for a given problem.
5. Construct MATLAB code to represent the mathematical model of a chemical process, implement basic numerical solution approaches, and use built-in advanced numerical solution approaches.
6. Identify and explain relationships between different classes of mathematical modeling problems.
7. Apply these techniques to problems encountered in chemical engineering research settings.

Representative Topical Outline:
1. Vector spaces
    a. Spans and bases
    b. Inner products and projections
2. Linear algebra
    a. Solution of linear systems

    b. Eigenvalue analysis
3. Ordinary differential equations
    a. Numerical integration of initial value problems
    b. Stability
    c. Boundary value problems
4. Solutions to partial differential equations
5. Data interpretation and modeling
6. Statistics and probability
7. Nonlinear algebraic equations and optimization