1. **Course number and name - CHBE 2120 – Numerical Methods in Chemical Engineering *(required)***

2. **Credits and contact hours** - 3 credit hours, 3 lecture hours (3-0-0-3)

3. **Instructor's or course coordinator's name -** Dr. Mark Styczynski

4. **Textbook, title, author, and year**
   Chapra SC and Canale RP. "Numerical Methods for Engineers", seventh edition, McGraw-Hill, 2014.

5. **Specific course information**
   a. **Catalog Description -** Numerical methods are introduced and applied to the solution of chemical engineering problems. An introduction to chemical process simulation, and the appropriate software is provided.
   b. **Prerequisites or co-requisites** - CHBE 2100 Chemical Process Principles (minimum grade "C" or better); CS 1371 Computing for Engineers.
   c. **Required, elective, or selected elective course** (as per Table 5-1) – Required

6. **Specific goals for the course**
   a. **Specific outcomes of instruction**:
   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.
      2) Analyze the accuracy of the numerical solution and identify alternate strategies and methods to achieve greater accuracy when it is needed.
      3) Identify the computational requirements of various solution options and use this understanding in the selection of the solution method.
      4) Select the appropriate software package to perform the numerical solution to a chemical engineering problem.
      5) Design experiments using statistical methods, for the purpose of building models and designing chemical processes.
      6) Formulate and solve process design problems, based on economic analysis and using mathematical models of chemical processes.

   b. **Connection with Student Outcomes**

CHBE 2120							
	Student Outcomes						
Course Outcomes	(1)	(2)	(3)	(4)	(5)	(6)	(7)
Course Outcome 1	X						
Course Outcome 2	X						
Course Outcome 3	X						
Course Outcome 4	X	X					
Course Outcome 5	X	X				X	
Course Outcome 6	X	X				X	

Student Outcomes

(1) an ability to identify, formulate, and solve complex engineering problems by applying principles of engineering, science, and mathematics

(2) an ability to apply engineering design to produce solutions that meet specified needs with consideration of public health, safety, and welfare, as well as global, cultural, social, environmental, and economic factors

(3) an ability to communicate effectively with a range of audiences

(4) an ability to recognize ethical and professional responsibilities in engineering situations and make informed judgments, which must consider the impact of engineering solutions in global, economic, environmental, and societal contexts

(5) an ability to function effectively on a team whose members together provide leadership, create a collaborative and inclusive environment, establish goals, plan tasks, and meet objectives

(6) an ability to develop and conduct appropriate experimentation, analyze and interpret data, and use engineering judgment to draw conclusions

(7) an ability to acquire and apply new knowledge as needed, using appropriate learning strategies

7. **Brief list of topics to be covered**
    a. Solution of algebraic equations
        1) Application in mass and energy balances
        2) Numerical methods include:
            i. Linear equations: Gauss elimination
            ii. Nonlinear equations: Newton-Raphson
    b. Integrals and integration of differential equations
        1) Applications in chemical reaction and diffusion
        2) Numerical methods include:
            i. Initial value problems: Runge-Kutta methods
            ii. Boundary value problems: finite difference methods
            iii. Numerical integration: Newton-Cotes and Gaussian quadrature
    c. Optimization
        1) Applications to process design
            i. Plant economics
            ii. Equipment sizing
        2) Numerical methods include:
            i. Gradient steepest ascent
            ii. Newton's method
    d. Statistics and decision making
        1) Applications
            i. Curve fitting
            ii. Hypothesis testing
            iii. Design of experiments
        2) Numerical methods
            i. Linear models: least squares regression
            ii. Nonlinear models: minimize error by optimization methods
    e. Process modeling software
        1) Applications in material and energy balances
        2) Numerical methods
            i. AspenTech
            ii. Relationship to specific methods already learned