18 APR 2018 CC/ 28 MAY 2018 UC

DEPARTMENT OF CHEMICAL ENGINEERING
College of Engineering
University of the Philippines Diliman, Quezon City

COURSE SYLLABUS
ChemE 105 Mathematical Methods in Chemical Engineering I

A. Course Catalogue Description

1. **Course Number:** ChemE 105
2. **Course Title:** Mathematical Methods in Chemical Engineering I
3. **Course Description:** Introduction to programming as a computational tool; matrix algebra; analytical and numerical solutions of systems of linear equations as applied to chemical engineering
4. **Prerequisite:** Math 21 Elementary Analysis I
5. **Corequisite:** ChemE 102 Chemical Engineering Process Analysis II
6. **Semester Offered:** Second Semester
7. **Course Credit:** 3u
8. **Number of Hours:** 2h lec, 3h lab
9. **Meeting Type:** lecture, laboratory
10. **Course Goals:** To introduce programming as a computational tool for solving chemical engineering problems; to introduce analytical and numerical methods for solving algebraic equations (both linear and nonlinear) and analyzing data plots based on chemical engineering processes

B. Rationale

This is the first course on mathematical methods in chemical engineering, which focuses on the numerical methods and their application to the analysis of chemical engineering systems. This course also covers the introduction of programming as a computational tool for performing mass and energy balance calculations, which is a key competency needed by chemical engineers in the analysis or design of any chemical system, whether it is a single equipment unit or an entire chemical plant.

C. Course Outline

1. Course Outcomes (CO)

Upon completion of the course, students must be able to:

- **CO 1.** apply programming knowledge to solve problems in mathematics and science, with applications in chemical engineering;
- **CO 2.** implement algorithms using computing programs;
- **CO 3.** develop computing programs to solve chemical engineering problems;
- **CO 4.** use linear algebra concepts in understanding systems of equations;
- **CO 5.** use computational tools to obtain numerical solutions to linear and non-linear equations; and
- **CO 6.** analyze the fit of models to data.

Course Outcomes and Relationship to Program Learning Objectives

Course Outcomes	Program Learning Objectives*				
	A	B	C	D	E
Apply programming knowledge to solve problems in mathematics and science, with applications in chemical engineering	■				
Implement algorithms using computing programs	■				
Develop computing programs to solve chemical engineering problems	■			■	
Use linear algebra concepts in understanding systems of equations	■				
Use computational tools to obtain numerical solutions to linear and non-linear equations	■				
Analyze the fit of models to data	■	■		■	

* **A** Equip students with strong technical education in chemical engineering necessary to succeed in their chosen careers and to become responsive citizens.
B Develop the students' ability to effectively communicate technical information to any audience.
C Train students to function in multidisciplinary teams, manage projects, and take leadership roles in their respective fields.
D Engage students in research, innovation, and life-long learning to identify opportunities, and address issues and challenges in their respective spheres of influence.
E Instill in students a strong commitment to the ethical practice of their profession; to health, safety, and environment; and to service to society.

2. Course Content

Lecture Topics	No. of Hours	
	Lec	Lab
Matrices and determinants 1. Matrices: definition, properties and operations 2. Determinants: definition and theorems 3. Adjoints and Inverses	6	9
Long Examination		
Introduction to MATLAB® 1. Built-in functions 2. Array operators 3. Plotting 4. Script files	2	3
Program control statements 1. User-defined functions 2. Recursion	4	6
Program functions 1. User-defined functions 2. Recursion	4	6
Machine Problem 1		

Lecture Topics	No. of Hours	
	Lec	Lab
Systems of linear equations 1. Direct methods 2. Iterative methods 3. Existence and uniqueness of solution 4. Applications in chemical engineering	8	12
Nonlinear equations in one variable 1. Bracketing methods 2. Open methods 3. Applications in chemical engineering	2	3
Systems of nonlinear equations 1. Newton-Raphson method 2. Applications in chemical engineering	2	3
Numerical integration 1. Integration 2. Newton-Cotes formulas 3. Gaussian quadrature 4. Applications in chemical engineering	2	3
Curve fitting and function approximation 1. Least squares regression 2. Interpolation 3. Applications in chemical engineering	2	3
Machine Problem 2		
Total number of hours	**32**	**48**

3. Course Coverage

Week	CO	TOPIC	ESSENTIAL/ KEY QUESTIONS	Suggested Teaching and Learning Activities	Suggested Assessment Tools
1-3	1,4	**Matrices and determinants** 1. Matrices: definition, properties and operations 2. Determinants: definition and theorems 3. Adjoints and Inverses	What is a matrix? How are determinants calculated from a given matrix?	lecture, classwork	seatwork
4	2,3	**Introduction to MATLAB®** 1. Built-in functions 2. Array operators 3. Plotting 4. Script files	What are the different programming functions in MATLAB® relevant in solving chemical engineering problems?	lecture, classwork	machine exercise
5-6	2,3	**Program control statements** 1. User-defined functions 2. Recursion	What is the proper way of writing program control statements?	lecture, classwork	machine exercise

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Week	CO	TOPIC	ESSENTIAL/ KEY QUESTIONS	Suggested Teaching and Learning Activities	Suggested Assessment Tools
7-8	2,3	**Program functions** 1. User-defined functions 2. Recursion	What is the proper syntax for scripts and functions? How are they used to perform chemical engineering calculations?	lecture, classwork	machine exercise
9-12	1,2,4, 5	**Systems of linear equations** 1. Direct methods 2. Iterative methods 3. Existence and uniqueness of solution 4. Applications in chemical engineering	How can systems of linear equations be derived from mass balance problems? What are the different methods of solving systems of linear equations?	lecture, classwork	seatwork, machine exercise
13	1,2,5	**Nonlinear equations in one variable** 1. Bracketing methods 2. Open methods 3. Applications in chemical engineering	What are the different methods of solving a nonlinear equation with one variable?	lecture, classwork	machine exercise
14	1,2,3, 4,5	**Systems of nonlinear equations** 1. Newton-Raphson method 2. Applications in chemical engineering	How can systems of nonlinear equations be derived from mass and energy balance problems? What are the different methods of solving systems of nonlinear equations?	lecture, classwork	machine exercise
15	2,3	**Numerical integration** 1. Integration 2. Newton-Cotes formulas 3. Gaussian quadrature 4. Applications in chemical engineering	What are the different methods of performing numerical integration? What is the application of numerical methods in chemical process and thermodynamic analysis?	lecture, classwork	machine exercise
16	2,3,5, 6	**Curve fitting and function approximation** 1. Least squares regression 2. Interpolation 3. Applications in chemical engineering	What are the different methods of curve fitting and interpolation? What is the application of numerical methods in chemical engineering data analysis?	lecture, classwork	machine exercise

4. Course Requirements

1. Long examination
2. Machine problem
3. Seatwork
4. Machine exercises

REFERENCES:

Chapra, S. C. and Canale, R. P. (2015). *Numerical Methods for Engineers* 7th Ed. NY: McGraw-Hill Education.

Cutlip, M. B. and Shacham, M. (2008). *Problem Solving in Chemical and Biochemical Engineering with POLYMATH™, Excel and MATLAB®* 2nd Ed. MA: Prentice Hall.

Gupta, S. K. (2003). *Mathematical Methods in Chemical and Environmental Engineering*. New Delhi, India: New Age International Publishers.

Kreyszig, E. O. (2011). *Advanced Engineering Mathematics* 10th Ed. NJ: John Wiley & Sons, Inc.

Rice, R. G. and Do, D. D. (2012). *Applied Mathematics and Modeling for Chemical Engineers* 2nd Ed. NJ: John Wiley & Sons.

Villa, R. P. (2014). Developing a predictive model for determining the mechanical properties of CFB fly ash thermoset composite (Master's thesis). University of the Philippines Diliman.