Department of Chemical Engineering
College of Engineering
University of the Philippines
Diliman, Quezon City

ChE 106

Mathematical Methods in Chemical Engineering

Course Description: Mathematical solution of problems in chemical engineering. Analytical and numerical solutions to ordinary and partial differential equations, Vector analysis.

Course Prerequisites: Math 55, ChE 26, ChE 101

Course Credit: 3.0 units (2 h lecture**,** 3 h laboratory)

Program Educational Objectives (BS Chemical Engineering)
The program aims to educate students such that three to five years from graduation, they:

1. take leadership roles in their respective fields and/or effectively work in or manage a team;
2. are equipped with the extensive knowledge and relevant skills necessary to succeed in their chosen careers and to become responsive citizens;
3. are able to demonstrate strong research & innovative capability as they recognize and address opportunities and challenges in their respective spheres of influence;
4. have shown strong commitment to the ethical practice of their profession; to health, safety and environment; and service to society.

Course Outcomes
At the end of the course, the students must be able to:

1. Apply knowledge of mathematics, science, and chemical engineering fundamentals in solving chemical engineering problems;
2. Identify, formulate, and analyze chemical engineering problems using fundamental principles in mathematics and chemical engineering;
3. Investigate a complex chemical engineering problem through models and provide conclusions by applying the knowledge in solving algebraic and differential equations;
4. Develop computer programs for the numerical solution of systems of linear and non-linear algebraic and differential equations; and
5. Write algorithms and documentation of solutions to Machine Problems including its background and applications

Student Outcomes Satisfied by Course Outcomes

[a] Ability to apply knowledge of mathematics and science to solve engineering problems
[e] Ability to identify, formulate, and solve engineering problems
[g] Ability to communicate effectively
[k] Ability to use the techniques, skills, and modern tools for engineering practice

Course Content

Topics	Outcomes	Mode of Assesment
I. Linear Algebra		
Matrices: Definitions	Identify a Matrix and its different forms	Quizzes Long Exam Home work
Elementary of Properties of Matrices and Matrix Operations	Increase Familiarity with Elementary Properties & Matrix Operations	
Determinants: Definition and Theorems	Determine the Determinant of a matrix and apply Theorems on Determinant	
Adjoints and Inverses	Learn the concept of Adjoints and Inverses of a Matrix	
Systems of Equations: Inverse Method, Cramer's Rule, and LU Decomposition method	Solve system of equations using Inverse Method, Cramer's Rule, LU Decomposition Method Gaussian Elimination and Gauss-Jordan Reduction	
Gaussian Elimination, Gauss-Jordan Reduction Method		
Rank of a Matrix and Systems of Equations	Determine Rank of a Matrix and Systems of Equations	
Application: Degree of freedom analysis for multi-component, multi-phase systems		
II. Numerical Solution of Algebraic Equations		
a. System of Nonlinear equations (optional)		Quizzes Machine Problem Home work
b. Numerical Root finding Methods	Determine the roots of functions using numerical root finding methods	
i. Bisection Method		
ii. False Position Method		
iii. Successive Substitution Method		
iv. Newton-Raphson Method		
v. Secant Method		
c. Curve-Fitting Techniques		
i. Regression	Perform linear regression and interpolation on a given data set	Quizzes Machine Problem Home work
ii. Interpolation		
d. Numerical Integration (Closed newton-cotes method)		
e. Numerical Differentiation		
III. Ordinary Differential Equations		
Introduction to Differential Equations		Quizzes Long Exam Home work
Determine the solution of First-Ordered Differential Equations	Identify various forms of differential equations and apply the appropriate method of solution.	
1. Separable Variables		
2. Homogeneous Differential Equations		
3. Exact Differential Equations		
4. Integrating Factors		
5. Linear Differential Equations and Bernoulli's Equation		
c. Applications	Solve differential equation problems in transport processes, unsteady mass balance and other chemical engineering applications	
IV. a. Higher Order Differential Equations		
Special Higher-Ordered Differential Equations		
a. The General nth – Ordered Linear Differential Equations with Constant Coefficients	Solve Nth order linear differential equations with constant coefficients	

Topics	Outcomes	Mode of Assesment
b. Non-Homogeneous Differential Equations		Quizzes Long Exam Home work
1. Method of Undetermined Coefficients (MUC)		
2. Method Of Variation of Parameters (MVP)		
c. Linear Differential Equations with Variable Coefficients	Solve Nth order linear differential equations with variable coefficients	
1. Cauchy-Euler Differential Equation		
2. Legendre Differential Equation		
d. Solutions to Systems of Linear Differential Equations	Determine the solution of systems of Linear differential equations	
IV. b. Laplace Transforms		
a. Definition of Laplace Transform	Apply Laplace transforms in the solution of differential equations	Quizzes Long Exam Home work
b. Transforms and Special Functions		
c. Inverse Laplace Transforms		
d. Laplace Transform of Derivatives		
e. Derivatives of Laplace Transforms		
f. Convolution		
g. Solution of Linear Differential Equations using Laplace Transforms		
h. Applications		
V. Numerical Methods		
Numerical Solutions to Differential Equations	Perform numerical integration, differentiation and solution of differential equations using numerical methods	Quizzes Machine Problem Home work
1. Euler Method		
2. Runge-Kutta Method		
3. Shooting Method		
4. Finite Difference Method		
Periodic Functions		
a. Fourier series Expansion		Quizzes Long Exam Home work
b. Half-Range Series Expansion (Even and Odd Functions)		
c. Applications		
Partial Differential Equations		
a. Analytical Solutions	Solve partial differential equations using analytical and numerical methods	Quizzes Machine Problem Home work

Course Assessment

Quizzes, Long Exams, and Machine Problems	90%
Homework	10%

Course Policies

1. **Long Examinations**
   a. There will be three long examinations.
   b. Answers and solutions should be written legibly in black or blue ink.
   c. A student who misses an exam with a valid excuse must approach his/her instructor to schedule a make-up exam. This should be done on or before the schedule of the next long exam; otherwise, a score of zero will be given for the missed exam. Only one excused missed long exam is allowed.

d. The students shall be given three working days after the release of exam results to seek corrections. Any grievance for whatever reason will not affect the grades if it is raised after the three-day grace period.
e. Cheating during the examinations will be penalized with a grade of 5.00 in the course or expulsion from the University.

2. **Machine Problems**
   a. There will be two sets of machine problems composed of three to four items each.
   b. Each set will be done by pair. The pairing will be decided by the instructor.
   c. Students can choose between Scilab or Matlab in writing the codes for their solution.
   d. The deadline for the submission of the machine problem will be announced in class. Failure to submit a machine problem on the deadline will result in a grade of zero. Late submissions will not be accepted for whatever reason.
   e. The students shall be given three working days after the release of machine problem results to seek corrections. Any grievance will not affect the grades if it is raised after the three-day grace period.
   f. Any form of cheating (e.g., plagiarism) will not be tolerated. If caught, the student involved shall be penalized with a grade of 5.00 for the course or expulsion from the University.
3. **Class Works**
   a. Class works, which may consist of seatwork and homework, are designed to enable the students to practice their problem-solving skills.
   b. There are no make-up activities for any seatworks missed in class.
   c. Homeworks are to be submitted on the designated deadline. No homework will be accepted beyond the deadline.
4. **Other Matters**
   a. University rules on absences, dropping and LOA shall apply.
   b. The instructor reserves the right to make changes in the class policies when deemed necessary.

Grading System

1.00	1.25	1.50	1.75	2.00	2.25	2.5	2.75	3.00	5.00
[92,100]	[88,92)	[84,88)	[80,84)	[76,80)	[72,76)	[68,72)	[64,68)	[60,64)	[0,60)

List of Instructors

Prof. Jonas Karl Christopher Agutaya
Prof. Charlimagne Montealegre
Prof. Miguel Francisco Remolona
Prof. Ralph Villa
Prof. Kristian July Yap
Prof. Karl Ezra Pilario

References

1. Davis, Mark E.: *Numerical Methods and Modeling for Chemical Engineers*
2. Ayres, F: *Schaum's Outline of Theory and Problems of Matrices*
3. Rainville, ED: *Elementary Differential Equations*
4. Spiegel, MR: *Applied Differential Equations*
5. Ray, Ajay K. & Santosh K. Gupta: *Mathematical methods in chemical engineering & environmental engineering*