CHE 626 Mathematical Methods in Chemical Engineering – Fall 2025

**Instructor:** Dr. Richard T. Cimino, Senior Lecturer

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**Class: Tuesday** 6-8:50 PM; Face-To-Face; CKB 226

**Office Hours:**

Office hours this semester are offered online **by arrangement only -** please sign up online at https://drcimino.youcanbook.me.  Office hours will take place using my personal Zoom meeting room.  Additional meeting times/days/locations can be arranged as needed and pending my availability.

**Course Description and Requirements**

This course aims to provide students with advanced knowledge–skills to formulate mathematical models, derive analytical solutions, and find numerical solutions of steady and unsteady-state problems encountered in chemical engineering systems. First-order and higher-order ordinary differential equations as well as their systems are presented along with applications to dynamic systems. Sturm-Liouville eigenvalue problems, eigenfunction expansion, orthogonality of functions, and Fourier and generalized Fourier series are presented with the dual purpose of solving boundary-value problems and building the foundation needed for solving partial differential equations. Separation of variables is used to solve partial differential equations in 2D-3D steady-state and 1D-3D transient problems that arise in Cartesian, cylindrical, and spherical coordinates. Laplace transform and similarity transformation are used to solve semi-infinite domain problems. Numerical methods based on finite differences, full or semi-discretization of partial differential equations, accuracy, and error estimates are covered.

**Prerequisites:** MATH 222 or equivalent undergraduate degree in Chemical Engineering.

**Prerequisites by Topics:** Calculus, Differential Equations, Material–Energy Balances, Fluid Mechanics, Heat and Mass Transfer, and Chemical Reaction Engineering. Students will not be successful in this course without fundamental knowledge of chemical engineering and differential equations.

## Course Objectives

1. Provide students with the advanced knowledge–skills of mathematical methods, both analytical and numerical, required for solving mathematical models, which naturally arise in the practice of chemical engineering as well as students' graduate coursework, e.g., *Transport Phenomena* (CHE 624) and/or students' research.
2. Enable students to formulate basic mathematical models based on either macroscopic balance equations or differential (local) balance equations derived via a shell balance approach or reduction from the general field equations coupled with relevant constitutive equations as well as initial/boundary conditions.
3. Through application of these models to various chemical engineering systems, enable students to assess the models' accuracy, precision, robustness, generality, and fruitfulness.

## Student Learning Outcomes

1. Develop a methodical approach to model building: recognizing the physico-chemical aspects, geometry, etc. of the system, making realistic assumptions, derive simplified models based on field equations incorporating proper initial and boundary conditions
2. Express Drichlet, Neumann, and Robin boundary conditions commonly used in transport of mass, momentum, and energy
3. Identify different types of first-order ODEs, solve them analytically, using computational software, and apply them to chemical engineering systems
4. Identify different types of second-order and higher-order linear ODEs (homogeneous, non-homogeneous, constant coefficients, etc.), solve them analytically using various methods, using computational software, and apply them to chemical engineering systems
5. Solve homogenous and non-homogeneous linear systems of ODEs analytically and using computational software, and apply them to chemical engineering systems
6. Use Laplace Transforms to solve a linear ODE or systems of ODEs, which are of major interest to chemical engineering practice
7. Perform Fourier analysis via Fourier series, Fourier integrals and transforms, and generalized Fourier Series; express and explain the properties of orthogonal functions and series, while solving Sturm–Liouville problems
8. Formulate mathematical models (PDEs) for various types of transport phenomena problems and solve them via separation of variables and using computational

software.

**Learning Materials**

**Textbooks (Required)**

Advanced Engineering Mathematics, E. Kreyszig, 10th Edition, Wiley, ISBN: 9781119505402. All versions and editions acceptable. Hard copy preferred, electronic copy acceptable.

Schaum's Mathematical Handbook of Formulas and Tables, M.R. Spiegel (with J.S. Lipschutz, J.L. Liu), 3rd Edition, McGraw-Hill. Newer editions/other co-authors are acceptable. MUST HAVE HARD COPY.

Additional materials will be posted on Canvas.

**Calculator:** A graphing calculator (TI-83, TI-84 or TI-84SE) is required for solving numerical problems.

**Required Hardware:**

A working computer equipped with Windows is necessary to run MATLAB on your own computer.

**Required Software:** MS Office, Matlab (especially Symbolic Math Toolbox, PDE Toolbox), Adobe Reader. All software can be downloaded from NJIT IST webpage. Students will have access to/accounts in Webex and Canvas via NJIT directly. If you do not have access for any reason, please contact NJIT Help Desk as soon as possible.

**Internet Access:** You must have a reliable internet connection for your device.

**Course Outline**

| Week | Topic |
|---|---|
| 1 | Introduction: classification of models, formulation of mathematical models for chemical engineering systems, & field–constitutive eqns. |
| 2 | First-order ordinary differential equations (ODEs): separable ODEs, exact ODEs, linear ODEs, and applications to ChE systems |

| | |
|---|---|
| 3-4 | Second-order linear ODEs: ODEs with constant coefficients, differential operators, Euler–Cauchy equations, non-homogeneous ODEs, undetermined coefficients, variation of parameters; higher-order linear ODEs; and applications to chemical engineering systems |
| 5 | Systems of ODEs: Wronskian, constant-coefficient systems, non-homogeneous linear systems of ODEs, and their applications in ChE |
| 6 & 8 | Laplace Transforms: shifting theorems, transforms of derivatives and integrals, partial fractions, convolution, differentiation and integration of transforms, systems of ODEs, applications to ChE problems |
| 7 | **MIDTERM EXAM** |
| 9-10 | Fourier Analysis: Fourier series, Sturm–Liouville problems, orthogonal functions and series, Fourier integrals and transforms, generalized Fourier Series. |
| 11-13 | Partial Differential Eqs. (PDEs): Solutions of various transport phenomena problems by separation of variables (Fourier series, integrals/transforms) in Cartesian, cylindrical, & spherical coordinates |
| 14 | Project Wrap Up |
| 15 | **FINAL EXAM** |

**Assessment and Grading**

**Homework:** There is no formal "homework" in this course. However, there are ample home practice problems provided each week to help prepare you for the weekly quizzes.

**Quizzes:** These will occur at the beginning of the period each week and will consist of a single problem related to the practice problems from the prior week. Note: the LOWEST quiz grade will be dropped from your average at the end of the semester.

**Term Project:** There will be one Term Project in this course, to be completed individually. This project is research-based and will have several deliverables throughout the semester.

**Exams:** There will be one midterm exams and one final exam, each lasting the full class period.

**Grading:** Your final course grade will be calculated by weighted average, using the following weights:

| Category | Weight |
|---|---|
| **Quizzes** | **20%** |
| **Project** | **20%** |
| **Midterm** | **30%** |
| **Final Exam** | **30%** |
| **Total** | **100%** |

**Final course grades will be assigned according to the following rubric:**

| Lower Bound | Letter Grade | Upper Bound |
|---|---|---|
| **90** | **A** | **100** |
| **80** | **B+** | **89** |
| **70** | **B** | **79** |
| **60** | **C+** | **69** |
| **50** | **C** | **59** |
| **0** | **F** | **49** |

**Policies**

**NJIT Honor Code:** The NJIT Honor Code will be upheld and any violations will be brought to the immediate attention of the Dean of Students.

**Special Needs:** If you need accommodations due to a disability please contact OARS to discuss your specific needs. A Letter of Accommodation Eligibility from the Disability Support Services office authorizing your accommodations will be required.

**Lectures**

This course is a face-to-face course. This means that each lecture will take place in-person during the class hours. Failure to attend the sessions may result in a negative impact on your course grade, because there are numerous in-class activities and quizzes. Additionally, the examples discussed in the class are not necessarily from the main textbook and therefore missing a class will have consequences for your preparation for exams. ***Note, if at any point the course is forced to go into a virtual modality, you will be provided with additional information on how to access the course lectures electronically.***

Students are expected to be in the classroom at the starting time of the class period. Being late to class may have consequences for your final course grade.

No audio or video recording is allowed. Detailed lecture notes for all sessions will be provided for you to review at a later date.

Cellphones should be silenced during lectures and turned off during exams.

**Course materials, office hours and correspondence**

The course Canvas page is the main platform for delivering information about the course. All relevant course materials and assignments will be posted on Canvas, so a student should check it regularly.

Students must upload a professional-looking head shot for their Canvas profile.

Students are strongly encouraged to attend Office Hours. Long questions which require derivations will be discussed only during the Office Hours and will not be answered by email. Questions regarding grades can be discussed only during the Office Hours.

E-mail and Canvas correspondence is intended only for quick questions. Questions which require a detailed discussion should be discussed in person during the Office Hours.

All correspondence should be conducted in a professional style, using formal English.

To assure a quick response to your emails, please add "CHE626" in the subject of your emails.

The instructor reserves the right not to respond to emails at his personal discretion.

**Exams, Quizzes, Homework and Grades**

A letter grade is based on the final score, calculated using Canvas in accordance with the Tables given in this syllabus. The assigned letter grade is final and cannot be negotiated.

A student can dispute the exam scores within a week after the announcement of the score. Exam scores can only be disputed during the official Office Hours, not during class time or via email.

Students will get zero for not coming to exams or any other course activity. If students miss an exam due to extreme circumstances (such as a medical problem), they need to notify the instructor via email before the beginning of the exam, and bring proof of the circumstance to the Dean of Student's office. Only in the case of official approval from the Dean of Student's office may a make-up be given at the discretion of the instructor.

A student must show full details when solving a problem during an exam. Not showing the work will cause the loss of points even if the final answer is correct.

Partial credit can be given for solving the exam and quiz problems, though no partial credit will be given if there are not enough details to follow.

The final answer should be always evaluated with respect to its reasonability. No partial credit will be given if the final answer is wrong and unreasonable if the student does not acknowledge this explicitly on the exam problem.

Student handwriting must be legible in order to receive points.