ChE 626 Mathematical Methods in Chemical Engineering
Fall 2023
Otto H. York Department of Chemical and Materials Engineering
New Jersey Institute of Technology, Newark, NJ, USA

Fall 2023 Academic Calendar

Sept	4	Labor Day. University Closed
Sept	5	First Day of Classes
Sept	11	Last Day to Add/Drop a Class
Sept	11	Last Day for 100% Refund, Full or Partial Withdrawal
Sept	12	W Grades Posted for Course Withdrawals
Sept	18	Last Day for 90% Refund, Full or Partial Withdrawal - No Refund for Partial Withdrawal after this date
Oct	2	Last Day for 50% Refund, Full Withdrawal
Oct	23	Last Day for 25% Refund, Full Withdrawal
Nov	13	Last Day to Withdraw from Classes
Nov	21	Thursday Classes Meet
Nov	22	Friday Classes Meet
Nov	23	Thanksgiving Recess Begins. No Classes
Nov	26	Thanksgiving Recess Ends
Dec	13	Last Day of Classes
Dec	14	Reading Day 1
Dec	15	Reading Day 2
Dec	16	Saturday Classes Meet
Dec	17	Final Exams Begin

Instructor: Dr. Boris Khusid, Professor
Faculty Memorial Hall Room 215 (office); 973-596-3316 (phone); khusid@njit.edu (e-mail)
http://chemicaleng.njit.edu/people/khusid.php (website)

Mode of Teaching: Face-to-face. All course materials will be posted in Canvas, NJIT's Learning Management Platform. Students are responsible for all materials posted in Canvas.
Lectures: Tuesday, 6:00–8:50 PM CULM 110, Face-to-Face)
Office Hours: Faculty Memorial Hall Room 215, Tuesday, 8:30 am-11:30 am by arrangement to ensure proper social distancing.
Note: You can always schedule an appointment or a WebEx session by email if the office hour time conflicts with your classes.

Course Description and Prerequisites

ChE 626 Mathematical Methods in Chemical Engineering (3,0,0), 3 credits, 3 contact hours. 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.

Required Textbooks

Advanced Engineering Mathematics, E. Kreyszig, 10th Edition, Wiley, ISBN: 9781119505402. Electronic version is NOT acceptable. Only hardcover/paperback; loose-leaf version is not acceptable unless it perfectly matches the hardcover/paperback version.
Schaum's Outline of Mathematical Handbook of Formulas and Tables, 5th Edition, By S. Lipschutz, M.R. Spiegel, J. Liu, McGrow Hill, ISBN: 97812600105341 Electronic version is NOT acceptable.

Other Learning Materials/Tools

Instructor-Developed Resources (IDR): Instructor will post class notes to the Canvas course webpage as the semester progresses. Please print them and use them along with your book. You may take additional notes on them during the lectures. You are responsible for all the materials covered in the class, not just in the notes.
Required Software: MS Office, Matlab, 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.

Recommended Textbooks (Not Required)

- Applied Mathematics and Modeling for Chemical Engineers, 2nd Edition, R.G. Rice and D.D. Do, Wiley. Available freely from Knovel Database (access from NJIT Library).
- Applied Partial Differential Equations with Fourier Series and Boundary Value Problems, 5th Edition, Pearson.

- Applied Mathematical Methods for Chemical Engineers, N. Loney, 3rd Edition, CRC Press, Boca Raton.
- Transport Phenomena, R. B. Bird, W. E. Stewart, E. N. Lightfoot, 2nd Edition, John Wiley and Sons, New York.

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.

Assessment/Grading

Homework + Quizzes (individual)	15%
Project/group activities	30%
Midterm exam (individual)	25%
Final exam (individual)	30%

Your performance will be evaluated on an absolute scale and not relative to the performance of other students in the class. Final letter grades will be awarded based on your weighted composite average score (see weighting above) and the following table of composite score vs. letter grade. Attendance will be taken at the beginning of each lecture and may affect your final grade, as described under Policies/Norms.

Score	Grade
90–100	A (Excellent)
80–89.9	B+ (Good)
71–79.9	B (Acceptable)
62–70.9	C+ (Marginal Performance)e
55–61.9	C (Minimum Performance)
<54.9	F (Failure)

Course Outline

Week[a]	Topic	Resource
1–2	Introduction: classification of models, formulation of mathematical models for chemical engineering systems, & field–constitutive eqns.	IDR[b]
2	First-order ordinary differential equations (ODEs): separable ODEs, exact ODEs, linear ODEs, and applications to ChE systems	IDR & Ch. 1
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	IDR, Ch. 2, & Ch. 3
5-6	Systems of ODEs: Wronskian, constant-coefficient systems, non-homogeneous linear systems of ODEs, and their applications in ChE	IDR & Ch. 4
6-7	Laplace Transforms: shifting theorems, transforms of derivatives and integrals, partial fractions, convolution, differentiation and integration of transforms, systems of ODEs, applications to ChE problems	IDR & Ch. 6

8	**Midterm Exam**	
9	Finite difference discretization of ODE/PDEs, explicit/implicit integration of ODEs, errors, numerical method of lines for PDEs	IDR & Ch. 21
10-11	Fourier Analysis: Fourier series, Sturm–Liouville problems, orthogonal functions and series, Fourier integrals and transforms, generalized Fourier Series.	IDR & Ch. 11
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	IDR & Ch. 12
14	Solution of PDEs via Laplace transform and similarity transformation	IDR & Ch. 12
15	**Final Exam**	

[a]Slight changes to the above outline may occur, depending on the overall performance of the class and the time required to cover the most important concepts and approaches.
[b]IDR: instructor-developed resources including notes–supplementary materials to be posted to Canvas & Ch: Chapter number refers to the textbook (Kreyszig) & associated slides in Canvas.

Quizzes: Quizzes will not be announced. There will be no make-up quizzes. Hence, you must attend all lectures to avoid a zero score. Questions will be about materials covered and HW.
HW assignments will be posted on Canvas and must be uploaded into Canvas in DOC or PDF format by the due date. Do not email HW solutions. Do not upload images taking with cell phone! Late HW will not be accepted for grading without an excuse authorized by the NJIT Dean of Students Office. All HW assignments will be individual. HW solutions will be posted after the due date.

Academic Integrity

Academic Integrity is the cornerstone of higher education and is central to the ideals of this course and the university. Cheating is strictly prohibited and devalues the degree that you are working on. As a member of the NJIT community, it is your responsibility to protect your educational investment by knowing and following the academic code of integrity policy that is found at:

http://www5.njit.edu/policies/sites/policies/files/academic-integrity-code.pdf .

Please note that it is my professional obligation and responsibility to report any academic misconduct to the Dean of Students Office. Any student found in violation of the code by cheating, plagiarizing or using any online software inappropriately will result in disciplinary action. This may include a failing grade of F, and/or suspension or dismissal from the university. If you have any questions about the code of Academic Integrity, please contact the Dean of Students Office at dos@njit.edu

Specific Accommodations

If you need accommodations due to a disability, please contact The Office of Accessibility Resources and Services https://www.njit.edu/accessibility/ to discuss your specific needs. A Letter of Accommodation Eligibility from The Office of Accessibility Resources and Services authorizing your accommodations will be required.

Contact Dean of Students and provide evidence for any extenuating circumstance regarding absence from an exam, accessibility issues regarding remote learning, etc.

Student Learning Outcomes

After completing this course, the student will be able to

1. classify models into various categories
2. explain the terms in macroscopic (global) balance equations and differential (local) balance equations/field equations
3. explain and express the three molecular fluxes and explain the difference between convective and molecular fluxes
4. express Drichlet, Neumann, and Robin boundary conditions commonly used in transport of mass, momentum, and energy
5. 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
6. recognize different types of first-order ODEs, solve them analytically, and apply them to chemical engineering systems
7. recognize different types of second-order and higher-order linear ODEs (homogeneous, non-homogeneous, constant coefficients, etc.), solve them analytically using various methods, and apply them to chemical engineering systems
8. solve homogenous and non-homogeneous linear systems of ODEs and apply them to chemical engineering systems
9. describe and define properties of Laplace transform and use them to solve a linear ODE or systems of ODEs, which are of major interest to chemical engineering practice
10. derive finite difference approximations, discretize ODEs and PDEs toward a numerical solution, explain numerical errors associated with various discretization methods associated with finite differencing, and explain pros/cons of explicit vs. implicit ODE integration
11. derive numerical method lines (NUMOL) equations as a general approach to solve 1D transient problems or 2D steady-state problems of parabolic PDE type
12. 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
13. describe different types of partial differential equations (PDEs)
14. formulate mathematical models (PDEs) for various types of transport phenomena problems and solve them via separation of variables, Laplace transforms, and similarity transformation

General Policies, Rules, and Expectations during the Lectures/Course

- You are strongly recommended to attend all lectures. As the lectures cover many abstract/complex concepts and derivations, even missing a single lecture would cause you to spend enormous time to recover. The instructor's experience is that there exists a significant **correlation between absenteeism and non-satisfactory performance: W-F grades.**
- Please attend the lecture 5 min before the lecture starts or at least ON TIME. Under no circumstances, you should distract your peers and the instructor. Attendance will be taken at each lecture.
- You are responsible for all information given in the lectures/Canvas (oral, written, posted notes, audiovisual materials), whether you are present or not during the lectures.
- You are expected to behave, communicate, and interact with the instructor and peers with respect and dignity as a professional chemical engineer.
- **Expectations:** ATTEND all lectures, ASK questions, DO homework, READ the assigned material before each lecture, REVIEW/WORK ON/SOLVE the material already covered prior to subsequent lecture. You are expected to READ the class/posted notes and covered sections of Kreyszig and IDR, BRING the printed notes to class along with your book, and TAKE additional notes on them during the lectures.

- For success, you have to WORK OUT all derivations and examples in the notes/in-class examples on your own after each lecture. In case of questions, please communicate to the instructor during the office hours or raise questions during the lectures. Do not delay questions to the exam week.

Rules, Policies and Expectations about Course Materials

- Course notes, HW assignment, solutions to select questions, etc. will be posted on the Canvas course webpage. You are required to visit Canvas CHE626 webpage daily to get recent homework assignments and other relevant announcements. You will bring the relevant notes and the required textbooks to each lecture and take additional notes on them.
- E-mail is usually intended for quick clarification questions, not for asking about the solution of complex problems. You are first encouraged to check Canvas for information. Then, you should discuss the problems among your peers or study group. In the end, you are welcome to use the Office Hours fully. It is best for students to engage with the instructor during the lectures/office hours; use e-mail for clarifying questions preferably.
- The instructor reserves the right not to respond to e-mails. Improperly written e-mails with lax attitude will not be replied. If e-mailed questions require more than 5 min to respond, students will be asked to contact the instructor during the office hours. Sometimes, instructor will share student questions with the whole class, keeping the anonymity of the student intact. This will help all class to benefit from such inquiries.
- Instructor-originated information is communicated via e-mail or posted on Canvas (check daily).

Policies and Expectations about Grades–Exams/Quizzes

- Letter grade will be assigned automatically by an Excel code (no emotions attached). The assigned letter grade is FINAL without subject to negotiation!
- You must plan, study, and do well in exams, quizzes, HWs, and project if you want to get a good grade in this class. Instructor will NOT change letter grades to accommodate any special circumstances of students. The student will get the letter grade he/she deserves.
- You can dispute the exam scores within a week following the announcement of the score. You cannot dispute your prior exams or HWs after one week or at the end of the semester! After first review of the dispute, if the score is not modified, but you are unconvinced and ask for an additional review, then you assume the possibility of reviewing the whole exam paper and removing points as well as giving points.
- No extra credit will be allowed (no need to ask) under any circumstances. The project is intended to give you the opportunity to raise your letter grade; use it well.
- Exams are open HARDCOPY lecture and in-class notes as well as the official textbooks.
- Students get zero for no-show to exams. Make-up exams (**no make-up quizzes**) may only be given under extreme circumstances (e.g., major close-family emergency, accident or acute medical problem) at the sole discretion of the instructor. Students bear the responsibility of due proof and documentation to the Dean of Students. It is the student's responsibility to inform the instructor and Dean of Students ASAP.
- Show all work, otherwise no partial credit means you cannot simply skip fundamental equations and important intermediate steps during a derivation. You will lose significant points even if the final answer is correct.

Policies and Expectations about Homework, Exam and Project

- **Homework format:** Failure to observe the following HW conventions will result in a downgrade of the HW score.
- **File name** should include student's first and last names, HW assignment No.
- **Header:** The top of each sheet of a HW assignment must contain the following information from left to right:

Student's first & last names	Course No	HW assignment No	Date due	Page No/total pages

- **Writing**: Homework and exam papers must be written legibly in an organized, structured fashion. You are responsible for potential loss of points due to sloppy, unclear, or illegible work. **If it can't be read, it can't be graded!**
- **Problem-solution format**: Problems should be clearly labeled and include the HW problem number, brief problem statement and present basic steps and calculations.
- **Calculations -** Homework should include complete calculations for every calculation presented to demonstrate how results were obtained.
- Feedback on the homework will be provided during lectures, solutions will be posted on the class website.
- Each problem will be graded individually (**up to 5 points**). You may and should discuss HW problems with your peers but cannot copy/use even a small portion of their solution. This will be considered cheating!
- Homework and exam papers must be written legibly in an organized, structured fashion. You are responsible for potential loss of points due to sloppy, unclear, or illegible work.
- All information about **the Project will be communicated via Canvas. You must read the project document once the project is assigned**; follow the instructions therein, and prepare a report.

Expectations for Pre-requisites

- This is a graduate course in chemical engineering; fundamental knowledge of chemical engineering principles regarding mass–energy balances, fluid mechanics and heat–mass transfer is assumed. You must review your fundamentals if you have forgotten them before or during the progress of this course.
- Mathematics is the language of engineers, and the course will heavily rely on Calculus and Differential Equations. It is assumed that **you have a good, operating PREREQUISITE knowledge of Calculus and Differential Equations**. If this is not the case, you will likely fail this course. Hence, you must REVIEW basic calculus, differentiation/integration rules–transformations, solution of first and second-order differential equations as well as Laplace transforms before the semester starts. While these topics will be covered, the course focuses on more advanced materials and applications commensurate with the graduate level education, assuming you know the basics.
- You are recommended to use online resources as well as documents posted on the CHE626 Canvas.

Reference Books

Mathematics

- Elementary Differential Equations, E.D. Rainville, P.E. Bedient, 7th Ed., Maxwell-Macmillan, 1989.
- Boundary Value Problems of Heat Conduction, A.M. Ozisik, Dover, 2002.
- The Mathematics of Diffusion, J. Crank, 2nd Ed., Clarendon Press.
- Schaum's Outline of Advanced Mathematics for Engineers and Scientists, M.R. Spiegel, McGraw-Hill.

Numerical Methods

- Numerical Methods for Chemical Engineers with MATLAB Applications, Constantinides, A. and Mostoufi, N., Pearson.
- Problem Solving in Chemical and Biochemical Engineering with POLYMATH, Excel, and MATLAB Cutlip, M.B. and Shacham, M., Pearson, 2nd Ed.
- Fundamentals of Engineering Numerical Analysis, P. Moin, Cambridge Univ. Press, 2001.
- Solving ODEs with MATLAB, L.F. Shampine, G.S. Thompson, Cambridge Univ. Press, 2003.

- Introduction to Chemical Engineering Computing, B.A. Finlayson, Wiley, 2006.

Transport Phenomena

- Advanced Transport Phenomena, J.C. Slattery, Cambridge Univ. Press, 1999.
- Transport Phenomena Fundamentals, J. Plawsky, CRC Press, 2009.
- Analysis of Transport Phenomena, W.M. Deen, Oxford Univ. Press, 1998.