Fall 2021

CHE 626-101: Math Methods in Chemical Engineering

Ecevit Bilgili

ChE 626 Mathematical Methods in Chemical Engineering
Fall 2021
Otto H. York Department of Chemical and Materials Engineering
New Jersey Institute of Technology, Newark, NJ, USA

Instructor: Dr. Ecevit Bilgili, Professor, Master Teacher, & Associate Chair for Undergrad Study
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Mode of Teaching: Face-to-face. All course materials and recorded office hours' discussion/workshop (if any) will be posted in Canvas, NJIT's Learning Management Platform. Both Webex and Canvas are freely available to NJIT students.

Course Requirements: Fri. office hours will be conducted via Webex; hence, students must have access to internet with reasonable speed, a laptop/desktop PC with audio/ microphone, and a webcam.

Students must strictly follow the NJIT policies regarding the Covid-19 pandemic.

Lectures: Monday, 6:00–8:50 PM (Central King Building Room 124, Face-to-Face)

Office Hours: Wed. 4:30–6:00 PM (**Face-to-Face, Tiernan Hall Rm. 373**) **and Fri. 5:00–6:30 PM** (**Webex**). The instructor will answer questions from students and solve many problems during **both office hours**. Hence, students are strongly recommended to attend both office hours. Instructor is available for questions at other times via e-mail. For personal matters, an appointment must be made a week in advance, which depends on instructor's availability.

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 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. <u>Electronic version is NOT acceptable.</u>

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. If available, IDR overrides the textbook on a given topic! 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. Also, any recorded office hours (F) via Webex will be uploaded to the respective Modules in Canvas whenever they are made available to the instructor by Webex.

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.

Strongly 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 626) 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 (HW) + Quizzes — 15% (A quiz has **<u>thrice</u>** the weighting of a HW)
Midterm Exam — 30%
Final Exam — 35%
Individual Term Project — 20%

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 for regular face-to-face lectures on Mondays and may affect your final grade, as described under Policies/Norms. **Attendance is strongly recommended for all lectures and both office hours on Wed. (Tier373) and Fri. (Webex).**

Score	**Grade**
90–100	A
80–89.9	B+
71–79.9	B
62–70.9	C+
55–61.9	C
<54.9	F

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]It is conceivable that slight changes to the above outline will 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 & lecture recordings. Ch: Chapter number refers to the textbook (Kreyszig) & associated slides in Canvas.

Pop Quizzes: Quizzes will not be announced. There will be no make-up quizzes. Hence, you must attend all lectures to avoid a 0 score. Questions will be about materials covered and HW.

HW Assignments: Once assigned (announced in class or via e-mail/Canvas), a HW is due the following week during class time and must be handed at the beginning of the lecture. Please do NOT submit HW via Canvas; you will get 0 score. HW will have two categories of questions. First category is *Questions for Potential Grading*. Hence, you must answer all questions fully in this category. Second category is *Additional Practice Questions* (odd-numbered questions in Kreyszig) that will not be graded. Nonetheless, you must solve all questions because both types of questions may appear in the quiz/exam. Quiz/exam questions may be similar in terms of style/concept/approach, but certainly not identical, to the HW questions. You can ask HW related questions as well as any questions regarding the class material and project during the office hours or by sending e-mails to the instructor. However, emails are largely reserved for questions that can be answered in a few minutes. Students are recommended to ask complex questions during the office hours–lectures.

Important Dates (***Please mark on your calendar, see Timetable document for details***)

Midterm Exam — Oct. 25; **Final Exam** — Dec. 15–21 (Day/time TBD by the registrar)

Project Report Due — Dec. 06 (Report via Canvas, computer codes via email to the instructor)

Pre-set Workshop on Matlab–NUMOL (Webex) — Nov. 06, Sat., 08:30–11:50 AM, US EDT

Last Day to Withdraw — Nov. 10 (Wed.), no special permission to withdraw thereafter.

Review Session — Face-to-face (Rm. TBA) or Webex (TBD), Dec. 13, Mon., 6:00–8:50 PM

Reading Days — Dec. 13 & 14

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 Chantonette Lyles, Associate Director of The Office of Accessibility Resources and Services, Fenster Hall Room 260 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 solving 1D transient problems (IVP–BVP) 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–office hours and watch the recorded videos in Canvas (if any). 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.
- 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.
- For any Webex meetings, normally mute your Webex. The instructor will allow for ample time for questions. To ask a question, you should unmute yourself and pose the question. You will participate when asked by the instructor.

- 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, JOIN all office hours, DO homework, READ the assigned material before each lecture, WATCH the recorded video of the office hours/Workshop etc., 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, E-mails & Office Hours

- The instructor highly encourages all students to show up to all official office hours (face-to-face on W and via Webex on F). You must make your best attempt to meet the instructor during these hours. The office hours are run in the studio mode so as to maximize efficiency. You will be with other students in Tiernan 373 or on a Webex call, and this will allow you to learn from the questions of other students. In addition, the professor will use the office hours to solve additional problems to clarify the concepts. The F office hours' discussion via Webex will be recorded & posted.
- Course notes, HW assignment, solutions to select questions, etc. will be posted on the Canvas course webpage. Critical announcements will be made through Canvas as well. 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 whole 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). **You are recommended to print and/or store all e-mails sent by the instructor in a separate folder.**

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 my

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 notes–books. ELECTRONIC SOURCES ARE NOT ALLOWED. You are required to bring notes, the required textbooks, and other books of your choosing.
- Use of laptop/PC/cell phone or any other electronic gadget during the exam/quiz is considered cheating.
- You have to write legibly while showing all work; otherwise, loss of points is likely. If two solutions are given for a problem including the correct and incorrect ones, you will be assigned 0 points. You are required to erase or cross out the incorrect solution.
- Students get 0 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–Project

- Once assigned, HW is due the following week during class time (US EDT), unless otherwise indicated. **Written HW must be handed in at the beginning of the lecture on the due date. HW submitted via email or Canvas will receive 0 score.**
- Late assignments will get 0 independent of the circumstances.
- You may discuss HW 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. The printed report must be handed in during the class and its electronic version must be submitted via Canvas. The relevant Matlab codes must be submitted via email (bilgece@njit.edu). If your computer codes do not work or worse yet they produce different results than those in your report, not only will you get a 0 score, but also you will be subjected to a misconduct investigation. Please check what you attach to the email.

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 forget 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 not succeed in 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. Although

I will cover these topics, I will mainly focus 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 webpage about the use of Matlab, which is required in the Project. The instructor will demonstrate how to use Matlab, but you must learn the basics yourself.

Reference Books

Mathematics

- Elementary Differential Equations, E.D. Rainville, P.E. Bedient, 7^{th} Ed., Maxwell-Macmillan, 1989.
- Boundary Value Problems of Heat Conduction, A.M. Ozisik, Dover, 2002.
- The Mathematics of Diffusion, J. Crank, 2^{nd} 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, 2^{nd} 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.