

Course Code: CHE 455 **Course Title:** - Mathematical Models in Chemical Engineering
Term: January 2019

1. Instructor: [Dr. Md Tanvir Sowgath]
[mstanvir@che.buet.ac.bd]
[<https://tanvirsowgath.com/current-course-taught>]

2. Class meets: Sunday 09:00-09:50, Room 255, OAB
Tuesday 10:00-10:50, Room 255, OAB
Wednesday 11:00-11:50, Room 255, OAB

3. Course Learning Outcomes:

The first part of the course provides coverage of chemical engineering model formulation and solution strategy as well as a review to different mathematical techniques. The second part of the course is intended to teach students how to use optimization algorithms to improve the design and operation of chemical processes. The students of this study are equipped with theoretical knowledge of both Process Model base Techniques and Optimizations Techniques. Upon completion of the course, students will be able to:

-Be able to formulate the chemical process model
-Be able to use analytical and numerical techniques in solving the associated algebraic as well as differential equations
-Be able to use economics to derive an objective function
-Be familiar with the software packages and numerical techniques to solve problems.

4. Course Description:

- Introduction to Chemical Process Modeling(*Week 1-2*)
 - Fundamentals of model, Classification of models, Model formulation, Fundamental laws.
- Basics of Optimisation (*Week 3-4, Class Test # 1*)
 - Fundamentals of Optimization, Optimization Function and Numerical Methods, Basics of Linear Programming, Graphical Solution of Linear Programming and Nonlinear Programming
- Solution Strategy of Linear and Nonlinear Optimisation (*Week 5-8, Class Test # 2*)
 - Simplex Method of Linear Programming, Basics of Nonlinear Programming, Numerical Solution Strategy Penalty and Barrier Methods Method, SLP, SQP, GRG and other methods.
- Analytical and Numerical Solution Strategy of Steady state Process(*Week 9-11 Class Test # 3*)
 - Chemical process models resulting in ODE and DAE equations for dynamic problem.

- Numerical Solution Strategy of Dynamic Process(*Week 12-13, Class Test # 4*)
 - Chemical process models resulting in ODE and DAE equations for dynamic problem

5. Knowledge Required: Basic knowledge in Mathematics Course and Fundamental Course of Chemical Engineering offered by ChE Department

6. Recommended books:

1. Applied Mathematics & Modelling for Chem.Eng., Wiley.1995 by Rice & Do,
2. Optimization of Chemical Processes by Thomas F. Edgar, David. M. Himmelblau
3. Mathematical Modeling Approaches For Optimization Of Chemical Processes, Nova Science Publishers, Inc. by Gabriela Corsano, Jorge M. Montagna, Oscar A. Iribarren And Pío A. Aguirre
4. Process Modeling, Simulation, And Control For Chemical Engineers, McGraw-Hill Publishing Company by William L. Luyben
5. Lecture Notes on Computer Aided Process Engineering by Prof. I. M. Mujtaba
6. Supplementary Lecture notes and handouts will be published by instructor in the following link: (<http://tanvirsowgath.com>)

7. Grading: Attendance: 10% of total grade
Class test/Assignment (minimum 4): 20% of total grade
Final Exam (comprehensive): 70% of total grade