

## *Course Outline*

### **ChE 455: Mathematical Models in Chemical Engineering**

**INSTRUCTOR: DR. MD TANVIR SOWGATH**

#### **COURSE DESCRIPTION:**

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.

#### **Course Learning Outcomes:**

Upon completion of this course, the 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 able to use principles of engineering to develop equality and inequality constraints
- ✓ Be familiar with the preferred software packages and numerical techniques to solve problems.

#### **REFERENCES:**

Lecture notes and handouts will be found in the following link:

(<http://tanvirsowgath.com>)

1. “Applied Mathematics & Modelling for Chem.Eng.”, Wiley.1995 by Rice & Do,  
“Mathematical Modeling in Chemical Engineering”, Cambridge University Press.2014
2. “Optimization of Chemical Processes by Thomas F. Edgar, David. M. Himmelblau
3. Lecture Materials provided from different sources

#### **GRADING:**

- ✓ Attendance (10%)
- ✓ Assignments/Class Tests (20%)
- ✓ Final Exam (70%)

## TOPICS COVERED

TOPIC.	REFERENCES	LECTURES SCHEDULE
Fundamentals of model, Classification of models, Model formulation, Fundamental laws	Lecture Materials (Reference No:3) and Chapter 2 (Reference No:2)	<b>1-3</b>
Fundamentals of Optimization, Optimization Function and Numerical Methods, Basics of Linear Programming, Graphical Solution of Linear Programming and Nonlinear Programming	Chapter 1,4,5 and selected topics from Chapter 7-8 (Reference No:2)	<b>5-12</b>
<b>CLASS TEST 1</b>		
Simplex Method of Linear Programming Basics of Nonlinear Programming, Graphical Solution Penalty and Barrier Methods Method and other Methods (SLP, SQP, GRG)	Chapter 7 and Chapter 8 (Reference No:2)	<b>13-22</b>
<b>CLASS TEST 2</b>		
General analytical and numerical methods of solution for Chemical process models resulting in ODE equations for dynamic problem. Finite difference method of Staged process	Chapter 2, Chapter 3, Chapter 5 and Chapter 7 (Reference No:1)	<b>23-30</b>
<b>CLASS TEST 1</b>		
Solution Methods of linear system of Equations (Gauss Elimination, Gauss Jordan Elimination) Analytical Methods of Systems of Nonlinear Equations	Lecture Materials (Reference No:3)	<b>31-36</b>
<b>CLASS TEST 2</b>		
<b>REVISION CLASS</b>		<b>37-39</b>