CML 302: CHEMICAL PROCESS MODELING AND SIMULATION

Course No. : CML 302  
Course Title: Chemical Process Modeling and Simulation  
Course Type: Core  
Course Credits: 3

Course description:

The core subject CML 302 Chemical Process Modelling and Simulation covers fundamental Laws, principles, and uses as well as the formulation of the mathematical model. It also covers various mathematical models related to chemical engineering systems. The subject covers practical knowledge of simulation examples of core chemical engineering systems formulated by FORTRAN

Pre-requisites: Maths, Thermodynamics, Heat Transfer, Mass Transfer, CRE, Fluid Mechanics

Objectives:

1) To understand knowledge of fundamental principles and basic laws of modeling  
2) To understand the approach for mass/heat transfer & CRE  
3) To apply the knowledge of differential equations  
4) To understand the approach to modeling  
5) Formulation of a mathematical model for various chemical Engg. system

Outcomes:

Students are able to model every Chemical Engineering system assigned to them. Moreover, they could make the program of the model equation to get output results and analyzed the performance of the system

Expanded Course description:
INTRODUCTION TO PROCESS MODELING AND SIMULATION

MATHEMATICAL MODELING OF CHEMICAL ENGINEERING SYSTEM

MODELING OF CHEMICAL KINETICS AND REACTOR DESIGN
Modeling for different reaction scheme
Introduction to Reactor Design Fundamentals for Ideal Systems
A General Approach
Ideal Isothermal Reactors
Numerical Methods for Reactor Systems Design
Reversible Series Reactions
The Semibatch Reactor
Continuous Flow Stirred Tank Reactor (CFSTR)
Multi-Stage Continuous Flow Stirred Tank Reactor
Equal Size CFSTR In Series

APPLICATIONS IN CHEMICAL ENGINEERING SYSTEMS
Series of isothermal, constant holdup CSTR’S, CSTR’S with variable Holdups, two heated tanks, Gas- Phase pressurized CSTS, NON-ISOTHERMAL CSTS, single component vaporizer, Multicomponent flash Drum, Batch Reactor, Reactor with mass Transfer, idial binary distillation column, multicomponent Nonidial distillation column, batch distillation with holdup

TREATMENT OF EXPERIMENTAL RESULTS
Solve above developed modeling equations using polymath/matlab/c++

Class Schedule: Three lectures of 60 minutes each per week.

Textbooks:

1. Mickley H. S., Sherwood T. S., Reed C. E., Application of Mathematical Modeling in
4. A. Kayode Coker, Modelling of Chemical Kinetics and Reactor Design, Gulf professional publication