Subject no: CH 62003

Subject name: Process modeling and simulation (LTP-3-1-0; CRD-4)

Revised Pre-requisites: Transport phenomena (CH 30012 or equivalent), Chemical Engineering Thermodynamics (CH 20004 or equivalent), Chemical Reaction Engineering (CH 300009 or equivalent)

Revised Syllabus:

Introduction: fundamentals of process modeling and simulations. Review of analytical and numerical techniques. Macroscopic mass, momentum and energy balances. Microscopic balances for mass, energy and momentum and associated constitutive relationships. Steady state modeling of chemical process equipments: flow systems, separators, reactors and heat exchangers. Modeling of unsteady state systems.

Modeling of disperse phase systems. Application of population balances in modeling particulate/disperse phase systems. Modeling of crystallizers, liquid-liquid extraction, polymerization reactors etc. Introduction to stochastic processes.Modeling of stochastic processes using Kinetic Monte Carlo simulation. Modeling of mixing. Effect of mixing on conversion and yield of reactions.

Empirical modeling techniques: principal component analysis (PCA), PLS (partial least square) and artificial neural network (ANN)

Revised Lecture-wise plan:

1. Introduction and fundamentals of process modeling and simulations. (1)

2. Review of analytical and numerical techniques,(2)

3. Macroscopic mass, momentum and energy balances (2)

4. Microscopic balances for mass, energy and momentum and associated constitutive relationships. (5)

5. Steady state modeling of chemical process equipments: flow systems, separation processes, reactive systems, thermal systems. (6)

6. Unsteady state systems. (6)

7. Modeling of disperse phase systems. Quantification of particulate systems: particle state vector, continuous phase vector and number density function. Formulation of population balance equations (PBE) for growth, breakage and aggregation. Batch and flow systems (6)

8. Applications of PBE in modeling of crystallizers, polymerization and colloidal systems. (6)

8. Introduction of stochastic modeling. Kinetic Monte Carlo simulation for stochastic systems. (6)

9. Modeling of mixing. Introduction to the process of turbulent mixing.Development of models towards studying effect of mixing on reaction conversion and yield. (6)

10. Empirical modeling techniques: principal component analysis (PCA), PLS and artificial neural network (ANN) (2)