Process Modelling and Simulation - Web course

COURSE OUTLINE

The Process Modeling and Simulation of Chemical engineering processes has attracted the attention of scientists and engineers for many decades and is still a subject of major importance for the knowledge of unitary processes of transport and kinetics.

Basically it deals with three aspects, namely; Modeling of chemical engineering processes, parameter estimations and application of numerical methods for solution of models.

In this course first chapter is devoted to introduction of the course and discusses the simulation and need of simulation.

Subsequently it follows the parameter estimation, tools of simulation, development of models, classification of models, unit models of unit process, models of heat transfer equipment, separation processes and reactors, and application of numerical methods for solutions of models.

Contents:

Process simulation, tools of simulation, parameter estimation, models and classification of models, alternate classification of models, mathematical modeling based on transport phenomena, population balance, principles of probability and experimental data.

Unit models of unit processes, detailed mathematical models of heat transfer equipment, separation processes, reactors, numerical methods for solution of mathematical models in the form of partial differential equations.

COURSE DETAIL

S.No	Topics	No. of Hours
1	**Introduction :**	3

NP-TEL

NPTEL

http://nptel.ac.in

Chemical Engineering

Pre-requisites:

Basic knowledge of Courses on Material & Energy Balance; Transport Phenomena and Numerical methods.

Additional Reading:

Standards software of simulation.

Coordinators:

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	Introduction to process modeling and simulation, tools of simulation, approaches of simulation, planning of calculation in a plant simulation.	
2	**Parameter Estimation:** Parameter estimation techniques in theoretical as well as numerical models.	3
3	**Models:** Models, need of models and their classification, models based on transport phenomena principles, alternate classification of models, population balance, stochastic, and empirical models, unit models.	8
4	**Models of Heat Transfer Equipment:** Development of detailed mathematical models of evaporators, use of Newton-Raphson method for solving evaporator problems.	4
5	**Models of Separation Processes:** Separation of multicomponents mixtures by use of a single equilibrium stage, flash calculation under isothermal and adiabatic conditions. Tridigonal formulation of component-material balances and equilibrium relationships for distillation, absorption and extraction of multicomponents. Thiele and Geddes method plus θ - method and Kb method, models of absorbers , strippers and extractors.	12
6	**Models of Reactors:** Classification of fixed bed reactor models, one dimensional and two dimensional fixed bed reactor models, fluidized bed reactor models, bioreactor models.	4

7	**Numerical Methods:** Classification of partial differential equations (PDE's), solution of PDEs by Finite difference techniques, method of weighted residuals. Orthogonal collocation to solve PDEs with their application to chemical engineering systems models.	6
	Total	40

References:

1. Denn M. M., "Process Modeling", Longman, 1986.
2. Holland C. D., "Fundamentals and Modeling of Separation Processes", Prentice Hall., 1975.
3. Luyben W. L., "Process Modeling Simulation and Control for Chemical Engineers", 2nd Ed., McGraw Hill, 1990.
4. Najim K., "Process Modeling and Control in Chemical Engineering", CRC, 1990.
5. Aris R., "Mathematical Modeling, Vol. 1: A Chemical Engineering Perspective (Process System Engineering)", Academic Press, 1999.