

Course Type	Course Code	Name of the Course	L	T	P	Credits
DC	CHC307	Process Modeling and Simulation	3	0	0	9

**Course Objective**

The objective of the course is to develop skills to build process models using the fundamental concepts and techniques of chemical engineering and to impart knowledge for numerical simulation of the developed models.

**Learning Outcomes**

At the end of the course, students are expected to be able to build a mathematical model of a chemical process and solve it using available computational tools.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	<b>Introduction:</b> Introduction to mathematical modelling and simulation, aims and objectives of process modelling and simulation, terminologies, classification of models, concept of degree of freedom analysis	07	Introduction to basic modelling and simulation and related terminologies
2	<b>NAE models:</b> Nonlinear algebraic equation (NAE) based models, steady state models of flash vessels, equilibrium staged processes distillation columns, absorbers, strippers, CSTR, etc., review of solution procedures and available numerical software libraries	12	Familiarity with NAE based model
3	<b>DAE models:</b> Differential algebraic equation (DAE) based models, rate-based approaches for staged processes, modelling of differential contactors distributed parameter models of packed beds, packed bed reactors, review of solution strategies for DAEs, partial differential equations (PDEs), and available numerical software libraries	14	Familiarity with DAE based model
4	<b>Flowsheeting:</b> Introduction to steady-state flowsheeting, approaches to flowsheeting systems, introduction to commercial process simulators	09	Will have basic knowledge of flow sheeting and application of commercial simulators.

**Textbooks:**

1. Ramirez, W. F. (1997). Computational Methods for Process Simulation. 2<sup>nd</sup> Ed., Butterworth Heinemann
2. Luyben, W.L. (1989). Process Modelling, Simulation and Control. 2<sup>nd</sup> Ed. McGraw Hill.
3. Bequette, B. W. (1998). Process Dynamics: Modeling, Analysis and Simulation. Prentice Hall International
4. Westerberg, A. W.; Hutchison, H. P.; Motard, R. L.; Winter, P. (1979). Process Flow sheeting. Cambridge University Press

**Reference Books:**

1. Frank, R. E. (1972). Modelling and Simulation in Chemical Engineering. John Wiley & Sons