INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/CENTRE/SCHOOL: Department of Chemical Engineering

Subject Code: CHC-501 **Course Title:** Mathematical Methods in Chemical Engineering

L-T-P: 3-0-2 **Credits:** 4 **Subject Area:** PCC

Course Outlines: Vectors, Tensor, Tensor Algebra and Calculus, Matrix Algebra, Eigenvalue And Eigenvectors, Solution of Set of Algebraic Equations, Solution of Set of Ordinary Differential Equations, Solution of Set of Non-Homogeneous First Order Ordinary Differential Equations, Partial Differential Equations, Second Order Linear ODEs, Second Order Linear Partial Differential Equations (PDEs): Solution Methods for Hyperbolic, Elliptic and Parabolic Equations: Eigen Function Expansion, Separation of Variables, Transform Methods, Applications from Heat and Mass Transfer, Reaction Engineering, Numerical Solution of Linear and Nonlinear Algebraic Equations, Gauss Elimination Methods, LU Decomposition, Newton-Raphson Method; Finite Difference Method for Solving ODEs and PDEs. Spectral Methods for Solving Differential Equations, Chemical Engineering Applications from Separation Processes, Reaction Engineering, Fluid Mechanics etc.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/CENTRE/SCHOOL: Department of Chemical Engineering

Subject Code: CHC-503 **Course Title:** Advanced Transport Phenomena

L-T-P: 3-0-2 **Credits:** 4 **Subject Area:** PCC

Course Outlines: Introduction to transport mechanisms: diffusive and convective fluxes, Conservation equations for scalar quantity (heat and mass) transport, Solution methods of conservation equation: similarity solutions, separation of variables, asymptotic methods etc., Conservation equations for momentum transport, Solution of momentum conservation equation: unidirectional and nearly unidirectional flows, low and high Reynolds number flows, Forced convection heat and mass transport

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/CENTRE/SCHOOL: Department of Chemical Engineering

Subject Code: CHC-505 **Course Title:** Advanced Reaction Engineering

L-T-P: 3-0-2 **Credits:** 4 **Subject Area:** PCC

Course Outlines: Introduction of various reactors (BR, CSTR, PFR), Pressure drops in reactor design (PBR); Catalyst deactivation, types of deactivations, deactivation rate laws; Catalysis and Catalytic reactors, Surface reaction mechanism and model studies; Steady state non-isothermal reactor design, Energy Balance, various RTD Models; Diffusion, and Reaction; Catalyst synthesis and Catalyst characterization.

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT/CENTRE/SCHOOL: Department of Chemical Engineering

Subject Code: CHC-507 **Course Title:** Advanced Thermodynamics and Molecular Simulations

L-T-P: 3-1-0 **Credits:** 4 **Subject Area:** PCC

Course Outlines: Probability, Distributions, and Thermodynamic Equilibrium. Laws of Thermodynamics, Partition Function, Thermodynamic Functions and Thermodynamic Ensembles, Maxwell Relations, Phase Space, Averages and Fluctuations, Boltzmann Approximation, Gibbs Phase Rule and Phase Equilibrium, Equations of State, Solution Thermodynamics, Phase equilibrium, Osmotic Pressure, Chemical Potential, Mixing and Phase Separation, Theory of electrolytes, Molecular Dynamics Simulations in Various Ensembles: Numerical Integration of Equations of Motion, Temperature and Pressure Control, Force-Fields, Analysis and Interpretation of Results, Efficiency and Parallelization, Methods of Free Energy Calculations, Monte Carlo Simulations, Non-equilibrium Simulations

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPARTMENT: Department of Chemical Engineering

Subject Code: CHL-541 **Course Title:** Biomass Conversion and Biofuels

L-T-P: 3-1-0 **Credits:** 4 **Subject Area:** PEC

Course Outlines: Different biomass types, distribution, and availabilities; Biomass Characterization, Different thermochemical biomass conversion techniques such as Torrefaction, Pyrolysis, Gasification, Liquefaction, etc.; Biochemical conversion of biomass; Details on the process, product distribution, separation strategies, reaction kinetics, types of reactors, challenges and status; Product upgradation & utilization.