NATIONAL INSTITUTE OF TECHNOLOGY WARANGAL

Honors in

CHEMICAL ENGINEERING

SCHEME OF INSTRUCTION AND SYLLABI

(for students of B.Tech., Chemical Engineering)

(Effective from 2021-22)

DEPARTMENT OF CHEMICAL ENGINEERING

SCHEME OF INSTRUCTION

Honors Program* – Chemical Engineering

S. No.	Course Code	Course Title	L	T	P	Credits	Sem.
1	CH5102$	Advanced Reaction Engineering	3	0	0	3	V
2	CH5161	Molecular Thermodynamics	3	0	0	3	VI
3	CH5101$	Advanced Transport Phenomena	3	0	0	3	VII
4	CH5202$	Advanced Process Control	3	0	0	3	VII
5	CH5152	Steady State Process Simulation	3	0	0	3	VIII
6	CH5153	Computational Fluid Dynamics	3	0	0	3	VIII
7	CH5251	Intelligent Control	3	0	0	3	VIII
8	CH5167	Electrochemical Engineering	3	0	0	3	VIII
9	CHH01$	Project	0	0	6	3	VIII

* Out of the above, six courses (18 credits) should be completed by students for the award of Honor.

$ Mandatory courses: CH5102, CH5101, CH5202, CHH01

CH5102	ADVANCED REACTION ENGINEERING	3-0-0	3 Credits

Course Outcomes:

At the end of the course, the student will be able to

CO1	Evaluate heterogeneous reactor performance considering mass transfer.
CO2	Determine the concentration profiles in multiphase reactors.
CO3	Estimate the performance of multiphase reactors under non-isothermal conditions.
CO4	Evaluate the role of modern reactor technologies for mitigation of global warming.

Syllabus:

Non-Isothermal reaction modelling in CSTR & Batch, Semi-Batch reactor: Energy Balance equations for CSTR, PFR and Batch reactors. Unsteady state non isothermal reactor design, adiabatic operation in batch, Heat effects in semi-batch. Auto thermal reactors.

Catalyst preparation and characterization: Catalysis - Nature of catalyses, methods of evaluation of catalysis, factors affecting the choice of catalysts, promoters, inhibitors, and supports, catalyst specifications, preparation and characterization of catalysts, surface area measurement by BET method, pore size distribution, catalyst, poison, mechanism and kinetics of catalyst, deactivation.

Heterogeneous Reactors: Catalytic wall reactor, monolithic reactors, limiting steps reactions and mass transfer limiting Porous catalyst on tube wall reactors Design of packed bed porous catalytic reactors: Mass transfer limited reactions in Packed bed packed beds : Transport and Reactions, Gradients in the reactors : temperature. Fluidized bed reactor modelling: Class III Modelling the Bubbling Fluidized Bed Reactor, BFB, The Kunii-Levenspiel bubbling bed model, Gas Flow Around and Within a Rising Gas Bubble in a Fine particle BFB, Reactor performance of BFB.CVD, trickle bed reactors. Polymerization techniques and reactors.

Application of Population Balance Equations for reactor modelling: Particle size distribution, Distribution Functions in Particle Measuring Techniques, Particle distribution model in colloidal particle synthesis in batch reactor, Moments of Distribution, Nucleation rate based on volumetric holdup versus crystal growth rate.

Reaction engineering and mitigation of Global warming CO_2 absorption, different techniques of mitigation of CO_2, Recent advancements, automotive monolith catalytic converter example, removal and utilization of CO_2 for thermal power plants.

Learning Resources:

Text Books:

1. Elements of Chemical Reaction Engineering, Fogler H.S., Prentice Hall of India, 2008.
2. Chemical Reaction Engineering, Levenspiel O., John Wiley & Sons, 1999, Third Edition.
3. Chemical Reactor Analysis and Design, Fromment G.F. and Bischoff K.B., John Wiley, 2010.

Reference Books:

1. The Engineering of Chemical Reactions, Schmidt L. D, Oxford, 2007.
2. Chemical Reactor Design, Harriott P., CRC Press, 2002
3. Chemical and catalytic reaction engineering, James J. Carberry, Dover Publications, 2001.

Online Resources:

https://nptel.ac.in/courses/103/101/103101001

CH 5161	MOLECULAR THERMODYNAMICS	3-0-0	3 Credits

Course Outcomes:

At the end of the course, the student will be able to

CO1	Determine thermodynamic properties using intermolecular forces.
CO2	Apply activity coefficient models for non-ideal systems.
CO3	Solve multiphase equilibrium problems.
CO4	Analyse molecular simulation trajectories.

Syllabus:

Classical Thermodynamics: First and Second laws, Property relationships, Ideal and Non-ideal gases, equation of state, Fugacity in Gas and Liquid Mixtures.

Intermolecular forces theory: Potential Energy functions, Electrostatic forces, Polarizability & Induced dipoles, Mie's potential-energy function for non-polar molecules, Structural effects, Chemical Forces.

Statistical thermodynamics: Partition function, Partition function for ideal gases, Ensembles (NVE, NVT, NPT and μVT), Equation of state, Virial equation of state for non-ideal gases.

Monte Carlo Simulations: Metropolis Algorithm, Basic Monte Carlo Algorithm, Different Trial Moves, Free Energy Calculation using Thermodynamic Integration.

Molecular dynamics simulations: Newton's Equation of Motion, Bonded and Non-bonded interactions, Sampling and averaging, Analysis of simulation using a simulation trajectory.

Application: A Case Study for Molecular System using Water Molecules.

Learning Resources:

Text Books:

1. Molecular Thermodynamics of Fluid-Phase Equilibria, Prausnitz J. M., Lichtenthaler R. N., Azevedo E. G., Prentice-Hall, 1999, 3rd Edition.
2. An Introduction to Applied Statistical Thermodynamics, Sandler S. I., Wiley, 2011.
3. Statistical Mechanics, Donald A. McQuarrie., Published by Longman Education, 2000.
4. Understanding molecular simulation: from algorithms to applications, Frenkel, Daan, and Berend Smit., Elsevier, 2001, Vol. 1.
5. Introduction to Chemical Engineering Thermodynamics, Smith J. M., Van Ness H. C., Abbott M.M., McGraw Hill, 2001, 5th Edition.

Reference Books:

1. Thermodynamics and its Applications, Modell M., Reid R. C, Prentice-Hall, 1983.
2. Thermodynamics and its Applications, Tester J. W., Modell M., Prentice-Hall, 1997, 3rd Edition.

Online Resources:

1. https://nptel.ac.in/courses/103/107/103107208/
2. https://nptel.ac.in/courses/103/103/103103162/
3. https://nptel.ac.in/courses/103/101/103101004/
4. https://nptel.ac.in/courses/103/103/103103144/
5. https://nptel.ac.in/courses/103/104/103104151/

CH 5101	ADVANCED TRANSPORT PHENOMENA	3-0-0	3 Credits

Course Outcomes:

At the end of the course, the student will be able to:

CO1	Perform momentum, energy and mass balances for a given system at macroscopic and microscopic scale.
CO2	Solve the governing equations to obtain velocity, temperature and concentration profiles
CO3	Model the momentum, heat and mass transport under turbulent conditions.
CO4	Develop analogies among momentum, energy and mass transport.

Syllabus:

Equations of Change for Isothermal Systems: Equation of Continuity, Equation of Motion, Equation of Mechanical Energy, Equations of Change in terms of the Substantial Derivative, Use of the Equations to solve Flow Problems, Dimensional Analysis of the Equations of Change.

Velocity Distributions with more than one Independent Variable: Time Dependent Flow of Newtonian Fluids. Velocity Distributions in Turbulent Flow -Comparisons of Laminar and Turbulent Flows, Time Smoothed Equations of Change for Incompressible Fluids, Time Smoothed Velocity Profile near a wall, Empirical Expressions for the Turbulent Momentum Flux, Turbulent Flow in Ducts.

Macroscopic Balances for Isothermal Systems: The Macroscopic Mass Balance, The Macroscopic Momentum Balance, The Macroscopic Mechanical Energy Balance, Estimation of the Viscous loss, Use of the Macroscopic Balances for Steady-State Problems, Derivation of the Macroscopic Mechanical Energy Balance.

Equations of Change for Non-Isothermal Systems: The Energy Equation, Special forms of the Energy Equation, The Boussinesq Equation of Motion for Forced and Free Convection, Use of the Equations of change to Solve Steady-State Problems, Dimensional Analysis of the Equations of Change for Non-Isothermal Systems.

Temperature Distributions in Solids and in Laminar Flow: Heat Conduction with an Electrical Heat Source, Heat Conduction with a Viscous Heat Source. Temperature Distributions with more than One Independent Variable - Unsteady Heat Conduction in Solids, Temperature Distributions in Turbulent Flow - Time-Smoothed Equations of Change for Incompressible Non-Isothermal Flow, Time-Smoothed Temperature Profile near a Wall, Empirical Expressions for the Turbulent Heat Flux Temperature Distribution for Turbulent Flow in Tubes.

Macroscopic Balances For Non-Isothermal Systems: Macroscopic Energy Balance, Macroscopic Mechanical Energy Balance, Use Of The Macroscopic Balances To Solve Steady State Problems With Flat Velocity Profiles.

Concentration Distributions in Solids and in Laminar Flow: Shell Mass Balances Boundary Conditions, Diffusion through a Stagnant Gas Film, Diffusion with a Heterogeneous Chemical Reaction. Concentration Distributions with more than One Independent Variable: Time-Dependent Diffusion. Concentration Distributions in Turbulent Flow - Concentration Fluctuations and the Time-Smoothed Concentration, Time-Smoothing of the Equation of Continuity of A, Semi-Empirical Expressions for the Turbulent Mass Flux.

Interphase Transport in Multi-Component Systems: Definition of Transfer Coefficients in One Phase, Analytical Expressions for Mass Transfer Coefficients, Correlation of Binary Transfer Coefficients in One Phase, Definition of Transfer Coefficients in Two Phases, Mass Transfer and Chemical Reactions.

Macroscopic Balances For Multi-Component Systems: Macroscopic Mass Balances, Macroscopic Momentum, Use of the Macroscopic Balances to solve Steady-State Problems.

Learning Resources:

Text Books:

1. Transport Phenomena, Bird R. B., Stewart W. E. and Light Foot E. N., John Wiley & Sons, 2007, Revised 2nd Edition.
2. Transport Processes and Unit Operations, Geankopolis C. J., Prentice Hall (India) Pvt. Ltd., New Delhi., 2004, 4th Edition.
3. Transport Phenomena in Multiphase Flows, Mauri Robert., Springer International Publishing, Switzerland, 2015.

ReferenceBooks:

1. Mass Transfer: From Fundamentals to Modern Industrial Applications, Koichi Asano, Wiley-VCH VerlagGmbh& Co, KGaA, Weinheim, Germany, 2006.
2. Transport Phenomena, Thomson W. J., Pearson education, Asia, 2001.
3. Analysis of Transport Phenomena, W.M. Deen, Oxford University Press, 2013, 2nd Edition.

OnlineResources:

1. https://nptel.ac.in/courses/103/106/103106068/#
2. https://ocw.tudelft.nl/courses/advanced-transport-phenomena/?view=lectures&paging=1

CH 5202	ADVANCED PROCESS CONTROL	3-0-0	3 Credits

Course Outcomes:

At the end of the course, the student will be able to

CO1	Identify controlled and manipulated variables.
CO2	Design regulatory control scheme for a given process.
CO3	Analyse the controlled and manipulated variables in multivariable processes.
CO4	Apply linear and nonlinear model predictive control.

Syllabus:

Introduction to control; Hierarchy of control layers, review of basics. Selection of controlled and manipulated variables. System linearization; state space and transfer function models.

Advanced regulatory control schemes - Cascade control, feed-forward control, ratio control, split-range control, time delay compensator, and inverse response compensator.

Multivariable control - Challenges; Control pairing; Interactions in closed-loop systems; Relative Gain Array (RGA) and variants. Centralized, decentralized, decoupled control schemes. Directionality.

Model Predictive Control (MPC) - Concepts; Theory and implementation; Relation with LQ-control. Implementation of MPC, State update and model prediction. Receding Horizon implementation; Issues and Challenges.

Economic MPC, Nonlinear Model Predictive Control (NMPC) – Theory and implementation.

Introduction to controller performance assessment and diagnosis – minimum variance benchmark.

Learning Resources:

Text Books:

1. Process Dynamics and Control, Seborg, D. E., Edgar, T. F., Millechamp, D. A., Doyle III, F. J., Wiley, 2014, 3rd Edition.
2. Process Control Fundamentals: Analysis, Design, Assessment, and Diagnosis, RaghunathanRengaswamy, Babji Srinivasan, NiravPravinbhai Bhatt, CRC Press, 2020.
3. Model Predictive Control System Design and Implementation using MATLAB, Liuping Wang, Springer, 2009.

Reference Books:

1. Predictive Control for Linear and Hybrid Systems, Francesco Borrelli, Alberto Bemporad, Manfred Morari, Cambridge University Press, 2017.
2. Process Control: Theory and Applications, Jean-Pierre Corriou, Springer, 2018, 2nd Edition.
3. Process Dynamics and Control: Modeling for Control and Prediction, B. Roffel and B. Betlem, Wiley, 2006.

4. Advanced Process Control: Beyond single loop control, Cecil L. Smith, Wiley, 2010.
5. Process Control: Principles and Applications, SurekhaBhanot, Oxford, 2008.

Online Resources:

https://onlinecourses.nptel.ac.in/noc21_ge01/preview

CH5152	STEADY STATE PROCESS SIMULATION	3-0-0	3 Credits

Course Outcomes:

At the end of the course, the student will be able to

CO1	Analyse the role and importance of property estimation methods in process simulation.
CO2	Determine the degrees of freedom for a given stream, process unit and flowsheet.
CO3	Apply suitable mathematical methods for solving sparse sets of equations, partitioning & precedence ordering and tear stream sets.
CO4	Carry out steady state process simulation using sequential modular approach and equation-oriented approach.
CO5	Apply convergence promotion techniques for both sequential and simultaneous convergence loops.

Syllabus:

Introduction: Steady-state flow sheeting and the design process, the total design project.

Flowsheeting on the computer: Motivation for development, Developing a simulation model, Approaches to flowsheeting systems-examples.

Solving linear and nonlinear algebraic equations: Solving one equation in one unknown, Solution methods for linear equations, General approaches to solving sets of nonlinear equations, Solving sets of sparse nonlinear equations.

Physical property service facilities: The data cycle, Computerized physical property systems, Physical property calculations.

Degrees of freedom in a flowsheet: Degrees of freedom, Independent stream variables, Degrees of freedom for a stream and a unit, Degrees of freedom for a flowsheet.

The sequential modular approach to flowsheeting: The solution of an example flowsheeting problem, Other features: Handling design specifications, information streams and control blocks.

Convergence of tear streams: Sequential convergence and simultaneous convergence, Partitioning and precedence ordering set of equations and a flowsheet, tearing a flowsheet, Finding the best tear set family or tear set with minimum number of tears.

Flowsheeting by equation solving methods based on tearing: An example system based on equation solving, A complex example of selecting decision and tear variables for a flowsheet, Handling the iterated variables.

Simulation by linear methods: Introduction to linear simulation, Application to staged operations, Application to management problem.

Learning Resources:

Text Books:

1. Process Flowsheeting, Westerberg A. W., Hutchison H. P., Motard R. L. and Winter P., Cambridge University Press, 2011.

Reference Books:

1. Process Analysis and Simulation in Chemical Engineering, Ivan Dano Gill Chaves, Javier Ricardo Guevara Lopez, Jpose Luis Garcia Zapata, Alexander LeguizamonRobayo and Gerardo Rodrigue Nino, Springer, 2016.
2. Process Plant Simulation, Babu B. V., Oxford University Press, 2004.
3. Introduction to Software for Chemical Engineers, Mariano Martin Martin, CRC Press, 2015.

CH 5153	COMPUTATIONAL FLUID DYNAMICS	3-0-0	3 Credits

Course Outcomes:

At the end of the course, the student will be able to

CO1	Write governing equations of fluid flow and heat transfer.
CO2	Discretise the equations using finite difference and finite volume formulation.
CO3	Solve the discretized equations.
CO4	Implement pressure velocity coupling algorithms.
CO5	Generate grid for a given geometry.

Syllabus:

Introduction: CFD approach, Need for CFD.

Governing equations of fluid flow and heat transfer: Introduction to Laws of conservation: Mass, Momentum, Energy equations; Initial and boundary conditions; Conservative form – Differential and Integral forms of general transport equations; Application of Navier-Stokes equations; Classification of physical behaviours – Classification of fluid flow equations.

Discretization of equations: Finite difference / volume methods – 1D, 2D and 3D Diffusion problems, Convection and diffusion problems; Properties of discretisation schemes-Central, upwind, hybrid and higher order differencing schemes.

Solution methods of discretised equations: Tridiagonal matrix algorithm (TDMA); Application of TDMA for 2D and 3D problems; Iterative methods.

Pressure – velocity coupling algorithms in steady flows: Staggered grid; SIMPLE, SIMPLEC and PISO

Unsteady flows: Explicit scheme, Crank Nicholson scheme, fully implicit scheme, Pressure-velocity coupling algorithms in unsteady flows

Turbulence modelling: Prandtl mixing length mode - One equation model, k - ε model.
Grid generation: Structured and unstructured grids, Grid generation methods.

Learning Resources:

Text Books:

1. An Introduction to Computational Fluid Dynamics – The Finite Volume Method, H.K. Versteeg, W. Malalasekera, Prentice Hall, 2007 and 2nd Edition.
2. Computational Fluid Dynamics – The Basics with Applications, John D. Anderson, Jr., McGraw Hill Education, 2017.

Reference Books:

1. Numerical Computation of Internal and External Flows: The Fundamentals of Computational Fluid Dynamics: 1, C. Hirsch, Wiley, 2007 and 2nd Edition

2. Computational Methods for Fluid Dynamics, J.H. Ferziger, M. Peric, R.L. Street, Springer, 2019 and 4th Edition.
3. Computational Fluid Dynamics for Engineers and Scientists, SreenivasJayanti, Springer, 2018 and 1st Edition.

Online Resources:

1. https://nptel.ac.in/courses/103/106/103106119/
2. https://www.cfd-online.com

CH5251	INTELLIGENT CONTROL	3-0-0	3 Credits

Course Outcomes:

At the end of the course, the student will be able to

CO1	Understand the concept of neural networks.
CO2	Apply neural networks to control the process plants.
CO3	Develop fuzzy logic based controllers.
CO4	Design controllers using genetic algorithms.

Syllabus:

Introduction to Neural Networks: Artificial Neural Networks: Basic properties of Neurons, Neuron Models, Feed forward networks. Computational complexity of ANNs.

Neural Networks Based Control: ANN based control: Introduction: Representation and identification, Modelling the plant, control structures – supervised control, Model reference control, Internal model control, Predictive control.

Introduction to reinforcement learning and deep learning.

Introduction to Fuzzy Logic: Fuzzy Controllers: Preliminaries – Fuzzy sets and Basic notions – Fuzzy relation calculations – Fuzzy members – Indices of Fuzziness – comparison of Fuzzy quantities – Methods of determination of membership functions.

Fuzzy Logic Based Control: Fuzzy Controllers: Preliminaries – Fuzzy sets in commercial products – basic construction of fuzzy controller – Analysis of static and dynamic properties of fuzzy controller.

Neuro – Fuzzy and Fuzzy – Neural Controllers: Neuro – fuzzy systems: A unified approximate reasoning approach – Construction of role bases by self-learning: System structure and learning.

Genetic algorithms: Introduction, Controller design using genetic algorithms.
Applications to different engineering systems

Learning Resources:

Text Books:

1. Artificial Neural Networks, Bose and Liang, Tata McGraw Hill, 1996.
2. Fuzzy Modelling and Fuzzy Control, Huaguang Zhang, Derong Liu, Birkhauser Publishers, 2006.
3. Principles of Soft Computing, S. N. Sivanandam and S. N. Deepa, John Wiley & Sons, 2007.

Reference Books:

1. Neural Networks for Modelling and Control of Dynamic Systems, M. Nørgaard, O. Ravn, N. K. Poulsen, L. K. Hansen, Springer-Verlag, 2000.

2. Intelligent Systems and Control, LaxmidharBehera and IndraniKar, Oxford, 2009.
3. Neural Networks and Fuzzy Systems: A Dynamic Approach to Machine Intelligence, Kosco B, Prentice Hall of India, New Delhi, 1992.
4. Fusion of Neural Networks, Fuzzy Systems and Genetic Algorithms: Industrial Applications, Lakshmi C. Jain, N. M. Martin, CRC Press, 1998.
5. Fuzzy Controller Design, ZdenkoKovacic and Stjepan Bogdan, Taylor & Francis, 2006.

Online Resources:

http://eewww.eng.ohio-state.edu/~passino/ICbook/ic_code.html

CH5167	ELECTROCHEMICAL ENGINEERING	3-0-0	3 Credits

Course Outcomes:

At the end of the course, the student will be able to

CO1	Understand thermodynamics and kinetics of electrochemical processes.
CO2	Characterize electrochemical systems using analytical instruments.
CO3	Evaluate unit operations involving electrochemical applications.
CO4	Explain the principles of electrochemical energy systems.

Syllabus:

Electrode Potentials and Thermodynamics of Cells: Basic electrochemical thermodynamics, free energy, cell emf and Nernst equation, half-cell reactions and redox potentials, reference electrodes.

Electrode Kinetics: Arrhenius equation and potential energy surfaces, transition state theory, Butler-Volmer model of electrode kinetics, current-over potentials, Tafel plots.

Electroplating: Electrochemistry fundamentals, anode-cathode reactions, Faraday's law of electrolysis, current efficiency, current density, current distribution, voltage-current relationship, over potential and over voltage, surface preparation, electrolytic metal deposition, Electrolyte, types of electroplating processes and coatings Anodizing: Aluminium anodizing, nanopores in anodized alumina, Electropolishing: Types of metals and electrolytes, characteristics of electropolished surfaces, electropolishing vs mechanical polishing, applications.

Batteries: Basic concepts, battery characteristics, classification of batteries– primary, secondary and reserve batteries, modern batteries - construction, working and applications of zinc–air, nickel-metal hydride and Li-MnO2 batteries.

Fuel cells: Introduction, types of fuel cells - alkaline, phosphoric acid, molten carbonate, solid polymer electrolyte and solid oxide fuel cells, construction and working of methanol-oxygen fuel cell.

Corrosion Protection: Sacrificial anodes, impressed current techniques, polarization characteristics, galvanic series, coatings.

Learning Resources:

Text Books:

1. Electrochemical Methods: Fundamentals and Applications, Bard A. J., Faulkner L. R., Wiley 2010, 2nd Edition.
2. Corrosion Engineering, Fontana M. G., McGraw-Hill, 2008, 3rd Edition.
3. Electrochemical Power Sources: Batteries, Fuel Cells, and Supercapacitors (The ECS Series of Texts and Monographs) 2015.

Reference Books:

1. Solar Photovoltaics – Fundamentals, Technologies and Applications, Solanki C. S., PHI Publishers, 2015.
2. Electrochemistry and Electrochemical Engineering: An Introduction, West, Alan C., Columbia University, 2013.
3. Electrochemistry and Electrochemical Engineering, Hart, Lenny, Larsen and Keller, 2017

Online Resources:

https://nptel.ac.in/courses/113/105/113105102/

CHH01	PROJECT	3-0-0	3 Credits

Course Outcomes:

At the end of the course, the student will be able to

CO1	Understand thermodynamics and kinetics of electrochemical processes.
CO2	Characterize electrochemical systems using analytical instruments.
CO3	Evaluate unit operations involving electrochemical applications.
CO4	Explain the principles of electrochemical energy systems.

Syllabus:

The student is required to choose any one of the following:

Project involving experimentation/modelling/simulation/Design/optimization in chemical engineering related toresearch/industry/society

Attheendofthesemester,thestudentisrequiredtopresent(i)Literaturesurvey,(ii)Problem formulation, (iii) Methodology, (iv) Results and Discussion, (v) Conclusions (vi) Futurework, (vii) References. Project involving manufacture of any chemical product on industrialscale

Learning Resources:

1. Handbooks,
2. Journals andmagazines
3. Martyn S. Ray and Martin G. Sneesby, Chemical Engineering Design Project: A Case Study Approach, Gordon and Breach Science Publishers, Second Edition,1989.