

# Chemical and Biochemical Engineering

## Semester VI

S.N o	Course Code	Course Name	L	T	P	C
1	CL301T	<u>Introduction to Transport Phenomena</u>	3	0	0	6
2	CL301C	<u>Numerical Methods in Chemical Engineering</u>	3	0	0	6
3	CL302L	<u>Chemical Engineering Lab III</u>	0	0	3	3
4	CL306T	<u>AI in Chemical Engineering</u>	3	0	0	6
5	CL303L	<u>Chemical Engineering Lab IV</u>	0	0	3	3
6	CE301T	<u>Environmental studies</u>	3	0	0	6
7	--	Program Elective-I	3	0	0	6
		Total Credits				36

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1	<b>Title of the course (L-T-P-C)</b>	<b>Introduction to Transport Phenomena (3-0-0-6)</b>
2	<b>Pre-requisite courses(s)</b>	Nil
3	<b>Course content</b>	Introduction: Vectors/Tensors, Viscosity, Shell balance: Falling film, Circular tube; Equations of Change for isothermal systems: Continuity, Motion, Energy, Substantial derivatives; Unidirectional flows: Pipe flow, Variable viscosity falling film, Couette viscometer, Rotating Sphere; Unsteady flows: Startup Plate flow, Parallel plates, Oscillating plate; Thermal conductivity and mechanism of energy transport; Shell energy balances and temperature distributions in solids and laminar flow; The equations of change for nonisothermal systems; Diffusivity and the mechanisms of mass transport; Concentration distributions in solids and laminar flow; Equations of change for multicomponent systems; Introduction to the concept of heat and mass transfer coefficients.
4	<b>Texts/References</b>	1. R.B.Bird, W.E. Stewart and E.N. Lightfoot, Transport Phenomena, 2nd ed., Wiley, 2006

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1	<b>Title of the course (L-T-P-C)</b>	<b>Numerical Methods in Chemical Engineering</b> <b>3-0-0-6</b>
2	<b>Pre-requisite courses(s)</b>	--
3	<b>Course content</b>	Solution of simultaneous linear and non-linear equations; Eigenvalues and eigenvectors of matrixes; Statistical analysis of data; Curve fitting; Approximation of functions; Interpolation; Numerical integration and differentiation, solutions of cubic equations of state, P-x-y diagram using gamma-phi approach Solution of ordinary differential equations - initial and boundary value problems, Batch and stirred tank reactors, Chemical reaction and diffusion in pore problems, Tubular reactor with first and second order reactions, Chemical reaction and diffusion in a spherical catalyst pellet problem Solution of partial differential equations; Analysis of error and stability in numerical computing. One dimensional transient heat conduction, transient conduction rectangle/sphere/cylinder Implementation of numerical methods on computer through programming in FORTRAN/C++ and commercial software such as MATLAB.
4	<b>Texts/References</b>	<ol style="list-style-type: none"><li>1. S. C. Chapra and R. P. Canale, Numerical methods for engineers (8th ed), Tata McGraw- Hill, 2021.</li><li>2. S. K. Gupta, Numerical methods for engineers (3rd ed), New Age International, 2015</li><li>3. F. Gerald, and P. O. Wheatley, Applied numerical methods (7th ed), Pearson Education, 2022.</li><li>4. R. M. Somasundaram and R. M. Chandrasekaran, Numerical methods with C++ programming, Prentice-Hall of India, 2005.</li><li>5. Numerical Methods for Chemical Engineering, Applications in MATLAB, Kenneth J. Beers, Cambridge University Press, 2007</li></ol>

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1	<b>Title of the course (L-T-P-C)</b>	<b>Chemical Engineering Lab III (mass transfer and reaction engineering) (0-0-3-3)</b>
2	<b>Pre-requisite courses(s)</b>	--
3	<b>Course content</b>	<i>Mass transfer:</i> Experiments on hydrodynamics of a packed column, Differential distillation, drying, Cooling tower, gas liquid absorption <i>Reaction engineering:</i> Experiments on esterification kinetics, Batch reactive distillation, mi-cellular catalysis, homogeneous reaction, metal recovery from dilute solutions, reaction in CSTR, reaction in PFR
4	<b>Texts/References</b>	

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1	<b>Title of the course (L-T-P-C)</b>	<b>AI in Chemical Engineering</b> <b>1-2-0-6</b>
2	<b>Pre-requisite courses(s)</b>	CS101-Programming Languages, CS209- Artificial Intelligence, CS214- Artificial Intelligence Lab
3	<b>Course content</b>	<p><b>PART 1:</b> Programming Languages, Machine Learning Models, Software and Tools Overview of MATLAB and python, Different machine and deep learning models, concept of hybrid modeling, Overview of Pytorch, Keras, TensorFlow, Jupyter Notebook, and Google Colab</p> <p><b>PART 2:</b> Databases and Codes Open-source databases and codes, strategy for creating customized database from scratch, different file formats, overview of tools for database/descriptor generation, strategies for data cleaning and refinement</p> <p><b>PART 3:</b> Case Studies Thermophysical property prediction: aqueous solubility, liquid viscosity, polymer melting point and glass transition temperature, vapor liquid equilibrium (VLE)</p> <p><u>Catalyst and electrolyte design:</u> reaction yield prediction, optimization of catalyst property, battery electrolyte optimization</p> <p><u>Chemical process optimization:</u> process flow sheet synthesis, optimization of reactor performance, tuning of PID controller</p> <p><u>Applications in Biology:</u> Drug discovery- new molecule generation, binding affinity, and molecular toxicity prediction_Protein modeling and engineering- prediction of protein 3D structure, prediction of <u>thermostabilizing mutations</u></p>
4	<b>Texts/References</b>	<ol style="list-style-type: none"><li>1. José A. Romagnoli, Luis Briceño-Mena, Vidhyadhar Manee, "AI in Chemical Engineering: Unlocking the Power Within Data", 1st Edition, CRC Press, 2025, ISBN 9781032597003</li><li>2. Bharath Ramsundar, Peter Eastman, Pat Walters, and Vijay Pande. "Deep Learning for the Life Sciences", O'Reilly Media, Inc., 2019, ISBN: 9781492039839</li><li>3. Edgar I. S. Medina, Ehecatl A. D. R. Chanona, and Caroline Ganzer. "Machine Learning in Chemical Engineering (v1.0.0)", 2023, Zenodo. <a href="https://doi.org/10.5281/zenodo.7986905">https://doi.org/10.5281/zenodo.7986905</a></li><li>4. Fiammetta Caccaval, Carina L. Gargalo, Krist V. Gernaey, and Ulrich Krühne. "SPyCE: A structured and tailored series of Python</li><li>5. courses for (bio)chemical engineers", 2023, <a href="https://doi.org/10.1016/j.ece.2023.08.003">https://doi.org/10.1016/j.ece.2023.08.003</a></li><li>6. Thomas E. Quantrille, and Y. A. Liu. "Artificial Intelligence in Chemical Engineering" Academic Press Inc, 1992, ISBN:9780125695503.</li></ol>

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1	<b>Title of the course (L-T-P-C)</b>	<b>Environmental studies (3-0-0-6)</b>
2	<b>Pre-requisite courses(s)</b>	<b>Nill</b>
3	<b>Course content</b>	<p><b>Module A:</b> Natural Resources, Ecosystems, Biodiversity and its conservation: Natural resources and ecosystems, Forest, grassland, desert and aquatic ecosystems, biodiversity at global, national and local levels, conservation of biodiversity</p> <p><b>Module B:</b> Air Pollution Introduction to understanding air quality management, fundamental processes of meteorology, Air Pollutants – Gaseous and particulate, Criteria for pollutants, ambient and source standards, Aerosols: Characterisation of aerosols, size distributions, measurement methods; Transport behaviour: diffusion, sedimentation, inertia; Visibility; principles of particulate control systems.</p> <p><b>Module C:</b> Water Treatment Discussion of water quality constituents and introduction to the design and operation of water and wastewater treatment processes.</p> <p><b>Module D:</b> Solid Waste Management and Climate Change Different aspects of solid and hazardous waste management. Climate change and greenhouse gas emissions, technologies would reduce the greenhouse gas emissions. Climate change and its possible causes.</p> <p><b>Module E:</b> Sociology/Environmentalism Description: Environmentalism in sociological tradition, Sustainability, North-South divide, Political economy approaches in environmental studies, Debates over environmental issues.</p> <p><b>Module F:</b> Economics Energy economics and financial markets, Market dynamics, Energy derivatives, Energy Efficiency; Sustainable Development: Concept, Measurement &amp; Strategies, Interaction between Economic Development and the Environment</p> <p><b>Module G:</b> Philosophy Environmental ethics, Deep ecology, Practical ecology, Religion and attitude towards environmental ethics, Ecofeminism and its evolution.</p> <p><b>Module H:</b> Field work and project: visit to a local area to document environmental assets, case studies of a simple ecosystem and group discussions on current environmental issues.</p>
4	<b>Texts/References</b>	<ol style="list-style-type: none"><li>1. Cunningham W.P. and Cunningham M.A. (2002), Principles of Environmental Science, Tata McGraw-Hill Publishing Company, New Delhi.</li><li>2. Dasgupta, P. and Maler, G. (eds.), (1997), The Environment and Emerging Development Issues, Vol. I, Oxford University Press, New Delhi.</li><li>3. Jackson, A.R.W. and Jackson, J.M. (1996), Environmental Sciences: The Environment and Human Impact, Longman Publishers.</li><li>4. Nathanson, J.A., (2002), Basic Environmental Technology, Prentice Hall of India, New Delhi</li><li>5. Redclift, M. and Woodgate, G. (eds.), (1997), International Handbook of Environmental Sociology.</li><li>6. Srivastava, K.P. (2002), An Introduction to Environmental Study, Kalyani Publishers, Ludhiana.</li><li>7. Review articles from literature.</li></ol>

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