M Tech in Chemical Engineering
(Specialization: Computer Aided Process Engineering, CAPE)

Preamble: The fourth industrial revolution, Industry 4.0 emphasises upon accelerated decision making, optimising processes, maximising profits while minimising risks in a sustainable manner through digital transformation. This requires proficiency of human resources skilled in terms of development of new computer models and utilisation of existing computational tools. The models in the chemical industry vary over a range of time and length scales. While the design of a new process or optimisation of an existing process may require the use of atomistic modelling at the molecular scale, the design and analysis of the equipment require continuum modelling of mass, heat and momentum transport simultaneously. Further, the efficient process design, operation and control requires a system-level modelling approach. Needless to convey, tools such as artificial intelligence (AI) and machine learning (ML) along with statistical pedagogies provide newer horizons to tackle and solve complex problems. The proposed postgraduate programme aims to train students in the development of physics-based mathematical models, computational methods to solve the models, data analysis, and exposure to the industry-standard modelling tools through a blend of theoretical and practical relevant soft skills and project-based curriculum.

Eligibility Criteria: Same as for PST/MST

Semester wise course structure:

Semester I						Semester II					
Course	**Course Name**	**L**	**T**	**P**	**C**	**Course**	**Course Name**	**L**	**T**	**P**	**C**
CL501	Advanced Transport Phenomena	3	0	0	6	CL503	Advanced Thermodynamics	3	0	0	6
CL502	Computer Aided Numerical Methods	2	1	2	8	CL504	Advanced Reaction Engineering	3	0	0	6
CL645	Applied Statistics for Chemical Engineers	3	0	0	6	CL6xx	Applications of Artificial Intelligence and Machine Learning in Chemical Engineering*	2	0	2	6
CL6xx	Process Modelling & Simulation Laboratory*	0	0	3	3	CL6xx	Multiscale Modelling and Simulation*	2	0	2	6
CL6xx	Elective – I	3	0	0	6	CL6xx	Elective – II	3	0	0	6
						CL599	Scientific Communications	0	0	2	2
	Total Credits	11	1	5	**29**		**Total Credits**	13	0	6	**32**
Semester III						**Semester IV**					
CL698	Project – I	0	0	24	**24**	CL699	Project – II	0	0	24	**24**

Note: Elective – I and II can be taken from the existing elective courses along with the additional electives proposed (see below).

*Newly Proposed Electives Courses. Details are given below.

Elective Courses

Course Number & Title: CL6xx Applications of Artificial Intelligence and Machine Learning in Chemical Engineering
L-T-P-C: 2-0-2-6
Type of Letter Grading (Regular Letter Grades / PP or NP Letter Grades): Regular
Kind of Proposal (New Course / Revision of Existing Course): New Course
Offered as (Compulsory / Elective): Compulsory for M.Tech (Specialization Computational Chemical Engineering), Elective for B.Tech, M.Tech., and Ph.D.
Offered to: B.Tech., M.Tech., Ph.D.,
Offered in (Odd/ Even / Any): Even
Offered by (Name of Department/ Center): Chemical Engineering
Pre-Requisite: Nil
Course Content/Syllabus: Introduction to Artificial Intelligence (AI) and Machine Learning (ML); Types of learning problems: Supervised, Unsupervised, Semi-supervised; Overview of optimization techniques; Introduction to software tools used in AI & ML; Solving problems in Chemical Engineering (like decision support system, process control, modeling and simulation) applying rule-based AI & ML tools and lifecycle: (i) Data preprocessing: Data visualization, Outlier detection, & Smoothing techniques, Data scaling (Need for Scaling – Scale invariance, Standardization, Normalization), Dimensionality reduction, Feature extraction, selection (ii) Model Evaluation & identification: Performance metrics, analysis, Model selection, Hybrid cross-Validation methods (iii) Model development: (a) Classification – (Logistic regression, Naïve Bayes classifier, K-nearest neighbors, Support vector machines, Decision trees, Random forests, Boosting), (b) Regression - (Linear regression – simple, multiple, Kernel, Regression analysis, Box-Jenkins models (ARMA, ARIMA), Neural Network).
References: (Format: Authors, *Book Title in Italics font,* Volume/Series, Edition Number, Publisher, Year.)

1	Hastie, T., Tibshirani, R., Friedman, J.H., The Elements of Statistical Learning Data Mining, Inference, and Prediction, Second Edition, Springer, 2009
2	Abu-Mostafa, Y.S., Magdon-Ismail, M., Hsuan-Tein, L., Learning from Data. AMLBook, 2012
3	Bishop, C., Pattern Recognition and Machine Learning. Springer-Verlag, 2006
4	Gareth, J., Witten, D., Hastie. T., Tibshirani, R., An Introduction to Statistical Learning with Applications in R, Springer-Verlag, 2013
5	Müller, A. C., Gudio, S., Introduction to Machine Learning with Python, O'Reilly Media, Inc., 2016
6.	Shalev-Shwartz, S. and Ben-David, S., Understanding Machine Learning: From Theory to Algorithms, Cambridge University Press., 2014

New Course

Course Number & Title: CL 6XX: Process Modelling & Simulation Laboratory
L-T-P-C: 0-0-3-3
Type of Letter Grading (Regular Letter Grades / PP or NP Letter Grades): Regular
Kind of Proposal (New Course / Revision of Existing Course): New Course
Offered as (Compulsory / Elective): Compulsory for M.Tech (Specialization: Computational Chemical Engineering), Elective for B.Tech, M.Tech., and Ph.D.
Offered to: B.Tech., M.Tech., Ph.D.
Offered in (Odd/ Even / Any): Odd
Offered by (Name of Department / Center): Chemical Engineering
Pre-Requisite: Nil
Preamble: Chemical Processes often has complex model structure with various units working in tandem and hence synchronized. Therefore, a large equation set becomes invariable owing to both the nature and number of components. Further the operating conditions such as temperature and pressure becomes a challenging task due to the involvement of several complex processes in an industrial plant. To address these challenges, process flow sheet simulators are necessary in the gambit of chemical engineering. The current laboratory course shall demonstrate and offer a step by step tutorial with respect to simulation, optimization and dynamics of such processes in commercial or generic simulators.
Course Content/Syllabus: Fundamental concepts of mathematical models in chemical processes; Dynamic Simulation of chemical units including flash drum, binary distillation, continuous stirred tank reactor, plug flow reactor, petroleum refining column, heat exchanger, absorption tower and reactive distillation etc; Pipeline system design; Economic and sensitivity analysis; Design of various chemical processes.

References: (Format: Authors, *Book Title in Italics font,* Volume/Series, Edition Number, Publisher, Year.)	
1	Kamal I. M., Al-Malah. Aspen Plus: Chemical Engineering Applications, Wiley, 2016
2	Amiya K. J., Process Simulation and Control Using Aspen, Second Edition, Prentice Hall India, 2012
3	Bequette, B., Process Dynamics: Modeling, Analysis and Simulation, Second Edition, Prentice Hall, 2003
4	Foo, D. C. Y., Chemical Engineering Process Simulation, First Edition, Elsevier, 2017
5	Luyben, W., Process Modelling, Simulation and Control for Chemical Engineers, Second Edition, McGraw-Hill, 1989

New Course

Course Number & Title: CL 6XX: Multiscale Modelling and Simulation	
L-T-P-C: 2-0-2-6	
Type of Letter Grading (Regular Letter Grades / PP or NP Letter Grades): Regular	
Kind of Proposal (New Course / Revision of Existing Course): New Course	
Offered as (Compulsory / Elective): Compulsory to M.Tech (Specialization: Computational Chemical Engineering), Elective for B.Tech., M.Tech and Ph.D.	
Offered to: B.Tech., M.Tech., Ph.D.	
Offered in (Odd/ Even / Any): Even	
Offered by (Name of Department / Center): Chemical Engineering	
Pre-Requisite: Nil	
Preamble: With a rapid rise in the computational power and therefore in computational techniques, it has now become possible to model the transport processes in process equipment for their design, analysis and troubleshooting. In this course, the students will learn the use of computational fluid dynamics to understand flow, heat and mass transport in process equipment. The students will also learn to apply molecular simulation techniques to study systems at an atomistic level and calculate thermodynamic and transport properties.	
Course Content/Syllabus: Governing equations and boundary conditions: Mass, momentum, and energy transport, Introduction to typical CFD workflow: geometry creation/cleaning, generating structured and unstructured mesh, grid independence, discretization techniques (finite volume method), solution techniques, post processing to calculate variables of engineering interest. CFD in Chemical engineering applications. Introduction to turbulence modelling, introduction to models for multiphase and reacting flows. Basic statistical mechanics, ensembles, interactions and force fields, periodic boundary condition and minimum image convention, molecular visualization, geometry optimization, Monte Carlo method, Monte Carlo simulation in various ensembles, molecular dynamics simulations, equations of motion and integration algorithms, calculation of thermodynamic, structural and transport properties. Applications in gas adsorption and separation, phase equilibria and other applications in energy and environmental sciences.	
References: (Format: Authors, *Book Title in Italics font,* Volume/Series, Edition Number, Publisher, Year.)	
1	Patankar, S. V., Numerical Fluid Flow and Heat Transfer, CRC Press, 1980
2	Ranade, V., Computational Flow Modeling for Chemical Reactor Engineering, First Edition, Academic Press, 2001.
3	Frenkel, D., Smit, B., Understanding Molecular Simulation: From Algorithms to Applications, Second Edition, Academic Press, 2001.
4	Leach, A.R., Molecular Modelling: Principles and Applications, Second Edition, Pearson, 2001.
5	Versteeg, H. K., and Malalasekara, W., An Introduction to Computational Fluid Dynamics: The Finite Volume Method, Second Edition, Pearson, 2007
6	Allen, M. P., and Tildesley, D. J., Computer Simulation of Liquids, Second Edition, Oxford, 2017