DEPARTMENT OF CHEMICAL ENGINEERING, MIT Manipal

M.TECH. CHEMICAL EGINEERING

Program Structure (Applicable to 2023 admission onwards)

YEAR	FIRST SEMESTER						SECOND SEMESTER					
	SUB CODE	**SUBJECT NAME**	**L**	**T**	**P**	**C**	**SUB CODE**	**SUBJECT NAME**	**L**	**T**	**P**	**C**
I	CHE ****	COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING	3	1	0	4	CHE ****	OPTIMIZATION OF CHEMICAL PROCESSES	3	1	0	4
	CHE ****	ADVANCED CONTROL THEORY	3	1	0	4	CHE ****	PROCESS MODELING, ANALYSIS AND SIMULATION	3	1	0	4
	CHE ****	ADVANCED REACTION ENGINEERING	3	1	0	4	CHE ****	PROGRAM ELECTIVE I	3	1	0	4
	CHE ****	ADVANCED TRANSPORT PHENOMENA	3	1	0	4	CHE ****	PROGRAM ELECTIVE II	3	1	0	4
	CHE ****	PROCESS DESIGN OF CHEMICAL EQUIPMENT	3	1	0	4	CHE ****	PROGRAM ELECTIVE III	3	1	0	4
	HUM ****	RESEARCH METHODOLOGY & TECHNICAL COMMUNICATION*	1	0	3	-	CHE ****	OPEN ELECTIVE	3	0	0	3
	CHE ****	ADVANCED CHEMICAL ENGINEERING LAB	0	0	3	1	HUM ****	RESEARCH METHODOLOGY & TECHNICAL COMMUNICATION*	1	0	3	2
	CHE ****	COMPUTATIONAL METHODS FOR CHEMICAL ENGINEERING LAB	0	0	6	2	CHE ****	ADVANCED PROCESS CONTROL LAB	0	0	3	1
							CHE ****	PROCESS SIMULATION LAB	0	0	3	1
	Total					**23**						**27**
	THIRD AND FOURTH SEMESTER											
II	CHE ****	PROJECT WORK & INDUSTRIAL TRAINING							**0**	**0**	**0**	**25**

*TAUGHT IN BOTH SEMESTERS AND EVALUATED AND CREDITED IN THE SECOND SEMESTER

PROGRAM ELECTIVES			
COURSE CODE	COURSE TITLE	COURSE CODE	COURSE TITLE
CHE ****	AIR POLLUTION MONITORING AND CONTROL	CHE ****	METABOLIC ENGINEERING
CHE ****	BIOPROCESS ENGINEERING	CHE ****	NANOSCIENCE & TECHNOLOGY
CHE ****	ENVIRONMENTAL MANAGEMENT SYSTEM	CHE ****	PINCH TECHNOLOGY
CHE ****	FUEL CELL & HYDROGEN ENERGY	CHE ****	PROCESS DATA ANALYSIS
CHE ****	INDUSTRIAL WASTE WATER ENGINEERING	CHE ****	SOLID WASTE MANAGEMENT
CHE ****	INTERFACIAL SCIENCE & ENGINEERING	CHE ****	UPSTREAM AND DOWNSTREAM BIOPROCESSING
CHE ****	MEMBRANE SCIENCE & TECHNOLOGY	CHE ****	ARTIFICIAL INTELLIGENCE & MACHINE LEARNING
CHE ****	RISK AND SAFETY MANAGEMENT IN PROCESS INDUSTRIES	CHE ****	MULTISCALE MOLECULAR SIMULATIONS

OPEN ELECTIVES			
COURSE CODE	COURSE TITLE	COURSE CODE	COURSE TITLE
CHE ****	SUSTAINABLE ENGINEERING	CHE ****	GREEN PROCESSES

M.TECH. CHEMICAL EGINEERING
FIRST YEAR - FIRST SEMESTER

CHE ****: COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING [3 1 0 4]

Matrix Algebra, solvability conditions for systems of linear algebraic equations, vector algebra, Linear independence, Norm and Inner Product, linear and nonlinear algebraic equations, Gauss elimination methods, LU decomposition, Newton-Raphson method. Types of models in Chemical Engineering, Systems of first-order ordinary differential equations (ODEs). Stability analysis, Second-order linear ODEs, second-order linear partial differential equations (PDEs): classification, canonical forms. Chemical engineering applications for separation processes, reaction engineering, fluid mechanics, and process control. Hyperbolic, elliptic and parabolic equations: Eigenfunction expansion, separation of variables, transform methods, finite difference method for solving ODEs and PDEs. Model parameter estimation, Multivariate linear regression. Least square formulation for linear in parameter models, Solution of linear least square problem.

References:

1. Pushpavanam S., *Mathematical methods in Chemical engineering,* (1e), PH Learning Pvt.Ltd.,2004.
2. Canale R.P. and Chapra S.C , *Numerical Methods for Engineers*, , (7e), McGraw Hill, 2015
3. Ray, A. K., Gupta, S. K. Mathematical Methods in Chemical and Environmental Engineering, Cengage Learning Asia; 2 nd edition (2003).
4. Hoffman, J. D. Numerical Methods for Engineers and Scientists, Taylor and Francis (2001).
5. Computational and Statistical methods for chemical Engineering, (1e) Taylor & Francis Ltd;, Emst C. Wit and Wim P. Krijnen, 2022.

HUM***: RESEARCH METHODOLOGY & TECHNICAL COMMUNICATION

Research Methodology: Basic concepts: Types of research, Significance of research, Research framework. Sources of data, Methods of data collection. Research formulation: Components, selection and formulation of a research problem, Objectives of formulation, and Criteria of a good research problem. Research hypothesis: Criterion for hypothesis construction, Nature of hypothesis, Characteristics and Types of hypotheses, Elements of research design, Introduction to various sampling methods Sources of data, Collection of data, Research reports, references styles, Effective Presentation techniques, Research Ethics.

References:

1. Sekaran, U., & Bougie, R. (2016). *Research methods for business: A skill building approach*. John Wiley & Sons.

2. Zikmund, W. G., Babin, B. J., Carr, J. C., & Griffin, M. (2013). *Business research methods*. Cengage Learning.

3. Creswell, J. W., & Creswell, J. D. (2017). *Research design: Qualitative, quantitative, and mixed methods approaches*. Sage Publications.
4. Donald R Cooper & Pamela S Schindler, *Business Research Methods*, McGraw Hill International, 2018.

CHE ****: ADVANCED CONTROL THEORY [3 1 0 4]

Review of linear control theory and its application, SISO and MIMO systems, Enhancement of SISO loop control performance and its applications. Case studies for MIMO system, control relevant models. Introduction to discrete time system and analysis using Z-transform. Discrete state space representation. Stability of linear discrete systems. Models for computer control from input-output data. Discrete dynamic models, Parameter estimation problem. Prediction error methods, Parameter estimation of Black box models (i.e. ARX, ARMAX Models). State Estimator & model predictive control.

References:

1. Seborg D.E., Edgar T.F., Mellichamp, *Process dynamics and control*, (2e), John Wiley & sons, 2004
2. Harmon Ray W., Babatunde Ogunnaike. *Process dynamics, modeling and control*, (1e), Oxford University press. 1994
3. Wayne Bequette B., *Process control, Modelling, analysis and simulation*, (2e), Prentice Hall Int. Series. 2003.
4. Arun K. Tangirala, *Principles of System Identification: Theory and Practice*, CRC Press, 2014.
5. Ogata K., Discrete *Time Control systems*, (2e),Pearson Education, 2005.
6. Astrom K.J., and Wittermark B., *Computer-Controlled Systems: Theory and Design*, (3e), Prentice Hall, 1996

CHE *** : ADVANCED REACTION ENGINEERING [3 1 0 4]

Non-ideal flow in reactors: RTD and the models. Non-isothermal and non-adiabatic systems and their balance equations. Theory of Mass transfer with chemical reaction, model contactors. Kinetics of solid-catalysed and other heterogeneous reactions: Diffusion with reaction in porous catalyst, Mechanism of catalytic reactions. Development of rate equations for solid catalysed fluid phase reactions. Muti-phase reactors: Hydrodynamic characteristics of different reactors, slurry reactors, Fluidized bed, etc. Design aspects of multiphase reactors: pressure drop, fractional phase hold-up, mass and heat transfer coefficient, extent of mixing, etc.

References:

1. Scott Fogler, H, Elements of Chemical Reaction Engg – PH- 6th Edition- 2020.
2. Octave Levenspiel, Chemical Reaction Engineering, Wiley & Sons - 3rd *Edition*, 2003.
3. Rawlings J.B. and Ekerd, J.G., Chemical Reactor Analysis and Design Fundamentals Nole. Hill 2002.

4. Smith, J.M, Chemical Engineering Kinetics, 3rd edition, McGrawl-Hill, International student edition
5. Mark E Davis, Robert E Davis, Fundamentals of Chemical Reaction Engineering, 1st edition, McGrawl-Hill, 2003
6. Ronald W. Missen, Charles A. Mims, Bradley A. Saville; Introduction to chemical reaction engineering and kinetics, John Wiley & Sons, Inc.

CHE **** : ADVANCED TRANSPORT PHENOMENA [3 1 0 4]

Review of fundamental of momentum, mass and energy transfer. Equation of change in momentum, mass and energy –steady state solutions- velocity, temperature, concentration distribution in more than one independent variable in viscous and turbulent flow. Integral averaging in momentum, mass and energy transfer. Interphase transport in isothermal, non-isothermal and multicomponent systems. Microscopic balance for isothermal, non isothermal and multicomponent systems.

References:

1. R. Byron Bird, Warren E. Stewart and Edwin N. Lightfoot, Transport Phenomena, Revised second Edition, John Wiley & Sons, 2007.
2. John C Slattery, Advanced Transport Phenomena(2e), Cambridge University Press, 1999.
3. J.R.Welty, C. E. Wicks and R. E. Wilson, G. L Rorrer, Fundamentals of Momentum, Heat and Mass transfer, 5th Edition, 2008.
4. C. O. Bennet and J. O. Meyers, Momentum, Heat and Mass transfer, McGraw Hill, 1995.
5. H. Schlichting and K. Gersten, Boundary-Layer Theory, 8th edition, Springer, 2004.

CHE **** : PROCESS DESIGN OF CHEMICAL EQUIPMENT [3 1 0 4]

Prediction of physical properties needed for design calculations: Density, thermal conductivity, specific heat capacity, viscosity, diffusivity, surface tension, latent heat, phase equilibrium data, enthalpy. PID diagram, piping design, pipe size selection, pumps and compressors, Process design of Heat Transfer equipment: Heat exchangers, condensers, reboilers, vaporisers. Process design of Mass Transfer equipment: Distillation column, absorption column, liquid-liquid extraction column. Process design of simultaneous heat and mass transfer equipment: Evaporator, dryer, cooling tower.

References:

1. Gavin T. & Ray S., Chemical engineering design-Principles, Practice and Economics of Plant and Process Design, Butterworth and Heinemann (Elsevier), Third Edition, 2021.
2. Stanley W., Chemical Process equipment- Selection and Design, Butterworth and Heinemann, 2010.
3. Don G. and Robert P., Chemical Engineers Handbook, McGraw Hill, 9th edition, 2019
4. R. Sinnott and G. Towler, Coulson & Richardson's Chemical Engineering Series, Vol.6: Chemical Engineering Design, 5th Ed., Elsevier, 1993.

CHE ***: ADVANCED CHEMICAL ENGINEERING LAB [0 0 3 1]

Experiments involving reaction engineering, process dynamics & control and analytical instruments.

References:

Lab manual with instructions.

CHE ***: COMPUTATIONAL METHODS FOR CHEMICAL ENGINEERING LAB [0 0 6 2]

Introduction to MATLAB, Coding using MATLAB for simple system analysis, Solution of non-linear algebraic equation, Regression and Optimization, Solution of linear differential equation. Regression and Optimization, Solution of partial differential equations, steady state and dynamic simulation of a chemical process. Design of experiments and ANOVA study on experimental data.

References:

6. Gupta S.K., *Numerical methods for Engineer*, Wiley Eastern Ltd, 1995
7. Pushpavanam S., *Mathematical methods in Chemical engineering*, (1e), PH Learning Pvt.Ltd.,2005.
8. Canale R.P. and Chapra S.C, *Numerical Methods for Engineers*, , (7e),McGraw Hill, 2015
9. Montgomery D.C., *Design and Analysis of Experiments*, (8e), Wiley, 2012.
10. Lab manual

CHEMICAL ENGINEERING
FIRST YEAR – SECOND SEMESTER

CHE **** : OPTIMIZATION OF CHEMICAL PROCESSES [3 1 0 4]

Introduction to Optimization: Optimal problem formulation, essential features of optimization problems. Optimization theory and methods. Optimization of un-constrained functions: Single variable and multivariable. Optimality criteria, necessary and sufficient condition for optimality of constrained Optimization. Linear programming and applications, Simplex Algorithm. Direct and gradient based methods for constrained optimization problem. Nonlinear programming with constraints, application of optimization in chemical engineering systems. Introduction non-traditional optimization algorithms. MATLAB software for problem solving.

References:

1. Edgar T.F, Himmelblau D.M., Ladson L.S., *Optimization of chemical processes*, (2e), Mc Graw Hill international Editions, 2003
2. Rao S.S, *Engg. Optimization-theory and practice*, (4e), John wile and sons, 2009.
3. Joshi M.C. and Moudagalya K. M., *Optimizations, Theory and practice*, (1e), Narosa Pub, New Delhi, 2008.
4. Kalyanmoy D., *Optimization for Engineering design; Algorithm and Examples*, PHI, New Delhi, 2009.

CHE****: PROCESS MODELING, ANALYSIS AND SIMULATION [3 1 0 4]

Fundamental principles and process model development. Systematic approach to model building, Conservation principles, Constitutive relations, Dynamic models- Lumped parameters and distributed parameter systems and their solution strategies. Introduction to Process model hierarchies and basic tools for process model analysis, Introduction to data acquisition and analysis, Modelling discrete event systems, Modelling hybrid systems, Empirical model building.

References:

1. Hangos K. M.,Cameron I. T., *Process modelling and analysis* (1e), Academic press. 2007
2. Ramirez, W, *Computational methods in process simulation* (2e), Butterworths, NY 2000
3. Ingham J., Dunn I.J., Heinzle E., Peensoil J.E., *Chemical Engineering Dynamics, Modelling and Computer Simulation*, (3e), Wiley VCH, Verlog, GMbH & LOKGaA-2007

CHE ***: AIR POLLUTION MONITORING AND CONTROL [3 1 0 4]

The earth's atmosphere, structure and composition, air pollution history, sources and emissions, meteorology and instruments, gas sampling, atmospheric motion and pollutant transport, , atmospheric stability, gas phase chemistry and photochemical smog, air pollution monitoring, air pollution monitoring networks, aerosols and particulate matter, SO_x, NO_x, VOCs, CO_2, CO, particulate matter and their reduction, exposure and health effects, climate change, air pollution modelling, fixed box, gaussian plume models. Control Of Gaseous Pollutants: Process and equipment for the removal by chemical methods - Design and operation of absorption and adsorption equipment -

References:

1. Air Pollution, M N Rao and H V N Rao, McGraw Hill Education Pvt Ltd 2013
2. Colls, J., Air Pollution: Measurement, Modeling and Mitigation, CRC Press, 2009
3. Noel, D. N., Air Pollution Control Engineering, Tata McGraw Hill Publishers, 1999

CHE **** BIOPROCESS ENGINEERING [3 1 0 4]

Fundamentals of microbiology and biochemistry; Bioprocess principles: Kinetics of biomass, substrate and product; Batch, continuous and fed-batch cultures; Fermentation processes: General requirements, aerobic and anaerobic fermentations; Types of media and design of commercial media; Thermal death kinetics, heat sterilization and filter sterilization; Enzyme technology: enzymes classification and properties, kinetics of enzyme catalytic reaction; Bioreactor design and scale up; Mass transfer and heat transfer processes in biological systems; Recovery and purification of products.

References:

1. Shuler M. L., Kargi F., DeLisa M.P., *Bioprocess Engineering: Basic Concepts*, (3e), Pearson, 2017.
2. Stanbury P.F., Whitaker A., Hall S.J., *Principles of Fermentation Technology*, Elsevier Publishers, (3e), 2016.
3. Pauline M. D., *Bioprocess engineering principles*, (2e), Academic press. 2013

CHE **** ENVIRONMENTAL MANAGEMENT SYSTEM [3 1 0 4]

Introduction to air, water and air pollutants, Introduction and need for Impact assessment, legislation and pollution control acts and notifications, Environmental Impact assessment report, environmental management plan, Environmental audits, Life cycle analysis, sustainable development parameters, sampling and analysis techniques. Case studies clean technology options. Environmental management, Environmental audit, introduction to ISO and ISO 14000, Life cycle assessment; Triple bottom line approach, Carbon trading, Sustainable development, Environmental Management systems, case studies.

References:

1. L. W. Canter, Environmental Impact Assessment, (2e), McGraw-Hill, 1997
2. Environmental Impact Assessment Methodologies, by Y. Anjaneyulu, B.S. Publication, Sultan Bazar, Hyderabad (2006).
3. G. Burke, B. R. Singh, L. Theodore, Handbook of Environmental Management and Technology, (2e), John Wiley & Sons, 2000

CHE ***: FUEL CELL & HYDROGEN ENERGY [3 1 0 4]

Fuel cell Basics, Fuel cell thermodynamics, Fuel cell types, Fuel Cell Performance, Activation, Ohmic and Concentration over potential, Fuel cell design and components, Overview of intermediate/high temperature fuel cells, Current issues in fuel cells, Hydrogen energy, Hydrogen production methods, reaction kinetics studies on various methods,

References:

1. J. Larminie and A.Dicks, *Fuel Cell Systems Explained*, 2nd Edition, Wiley (2003)
2. Xianguo Li, *Principles of Fuel Cells*, Taylor and Francis (2005)
3. S. Srinivasan, *Fuel Cells: From fundamentals to Applications*, Springer (2006)
4. ‘O’Hayre, S.W.Cha, W.Colella and F.B.Prinz, *Fuel Cell Fundamentals*, Wiley (2005)
5. A.J. Bard and L.R.Faulkner, *Electrochemical Methods: Fundamentals and Applications*, 2nd Edition, Wiley 2000.
6. A.Faghri and Y.Zhang, *Transport Phenomena in Multiphase Systems*, Elsevier 2006.

CHE *** : INDUSTRIAL WASTE WATER ENGINEERING [3 1 0 4]

Water Quality- Primary, Secondary and tertiary treatment-Unit operations-Unit processes- Design of wastewater treatment systems-Primary, secondary and tertiary treatments- Evaluation of Biokinetic Parameters -Activated Sludge and its process- Modifications. Anaerobic filters. Expanded /fluidized bed reactors-Upflow anaerobic sludge blanket reactors, Membrane Technologies

References:

1. Weber, W.J., *Physicochemical processes for water quality control*, John Wiley and sons, New York, 1983.
2. Peavy, H.S., Rowe, D.R., Tchobanoglous, G., *Environmental Engineering*, McGraw Hills, New York 1985.
3. Metcalf and Eddy, *Wastewater engineering, Treatment and Reuse*, Tata McGraw-Hill, New Delhi, 2003.
4. Benefield, L.D. and Randall C.W., *Biological Processes Design for wastewaters*, Prentice-Hall, Inc. Eaglewood Cliffs, 1982.
5. Eckenfelder, W.W., *Industrial Water Pollution Control*, McGraw-Hill, 1999.
6. Arceivala, S.J., *Wastewater Treatment for Pollution Control*, McGraw-Hill, 1998.
7. Frank Woodard, *Industrial waste treatment Handbook*, Butterworth Heinemann, 2001
8. Grady Jr. C.P.L and Lin H.C., *Biological wastewater treatment: Theory and Applications*,Marcel Dekker, Inc New York, 1980

CHE **** : INTERFACIAL SCIENCE & ENGINEERING [3 1 0 4]

Introduction to the interface engineering; Occurrence of liquid-liquid & liquid-solid interfaces, Colloidal systems and their stability, Intermolecular and surface forces; electrostatic and steric interactions, DLVO theory, surface/interfacial tension; theoretical and experimental techniques for their determination, properties and characterization of colloidal systems, Adsorption at liquid-liquid & liquid-solid interfaces; Self –assembly of Amphiphiles, the hydrophobic effect, effect of counter ions, Interfacial engineering applications; fabrication of novel nano-colloidal systems, latest trends and innovation in interfacial science.

References:

1. Hiemenz, P. C, Rajagopalan, R., Principles of Colloid and Surface Chemistry, (3e), Marcel Dekker, New York, 1997.
2. Jacob N. Israelachvili, Intermolecular & Surface Forces, (3e), Academic Press, Elsevier, 2011
3. Milton J. Rosen, Joy T. Kunjappu, Surfactants and Interfacial Phenomena, (4e), Wiley-Interscience Publication, New York, 2012.
4. Adamson, A. W. Gast, A. P., Physical Chemistry of Surfaces, (1e), Wiley-Interscience, New York, 1997.
5. Fennell D. E., Wennerstrom K., The Colloidal Domain: Where Physics, Chemistry, Biology, and Technology Meet (Advances in Interfacial Engineering), Wiley-VCH, 1999

CHE **** : MEMBRANE SCIENCE & TECHNOLOGY [3 1 0 4]

Membrane preparation and structure, membrane permeability, flow pattern and classification: micro filtration, ultrafiltration, nano filtration, reverse osmosis, electro dialysis, dialysis, membrane modules and plant configuration, liquid separation: pervaporation, vacuum membrane distillation, transport through membrane, solution diffusion model and pore diffusion models. Gas separation: complete mixing model (binary and multi component) for gas separation, cross flow model, counter current flow model, single stage membrane separation, multistage membrane separation. Membrane reactor: perovskite type, bio catalytic membrane reactor, Transport through bio membrane like kidney.

References:

1. Mulder M.H.V., *Membrane Separation*, (1e), Springer Publ. 2007.
2. Scott K.S., Hughes R. (Editors), *Industrial Membrane Separation Technology*, (1e), Blackie Academic & Professional Chapmann & Hall, Glasgaw, 1996
3. Nath Kaushik, *Membrane Separation Processes*, (2e) PHI 2016.
4. Takeshi Matsuura *Synthetic Membranes and Membrane Separation Processes*, (1e, e book) Taylor and Francis 2020

CHE ****: RISK AND SAFETY MANAGEMENT IN PROCESS INDUSTRIES [3 1 0 4]

Introduction to Safety and Risk Management; Material hazard - GHS MSD - physical hazard, toxic hazard and eco-toxicity; PSM elements; Hazard Evaluation Techniques – What-If, Checklist, HAZOP, FEMA; Hazard identification and assessment (Process safety, thermal safety, dust explosion); Flammability and fire safety-extinguishers; SHE regulations in India-Factories act, water and environment act; Human elements in safety-behaviour safety; Laboratory safety; OSH; Compliance to statutory safety audits; Biosafety. Plant layout based on process safety & fire safety-fire hydrant system design; Management Practice in SHE in Plant Operation; Safety in utilities; Storage, handling and transportation of hazardous substances; Environmental Impact Assessment; Emergency response plan.

References:

1. Willie Hammer, Dennis Price, Occupational Safety Management and Engineering, Prentice Hall, fifth edition
2. Roland P. Blake, Industrial safety, (2e), Prentice Hall Inc, New York, 1953
3. Muir G.D, Hazards in Chemical Laboratory, (2e), The Chemical Society, London, 1980
4. Judson and Brown, Occupational Accident Prevention, John Wiley, New York, 1980
5. Handley W., Industrial Safety Hand Book, McGraw Hill, London, 1969

CHE *** : METABOLIC ENGINEERING [3 1 0 4]

Review of cellular metabolism. Transport processes: passive and active transport, facilitated diffusion. Models for cellular reactions: Material balances and data consistency. Regulation of metabolic pathways, enhancement of product yield and productivity. Metabolic pathway synthesis. Metabolic flux analysis: experimental determination and applications. Metabolic control analysis: analysis of structure and metabolic networks, extension and control analysis, consistency tests and experimental validation, thermodynamics of cellular processes, Determination of $\Delta G°$ by various methods, applications of thermo kinetics to MCA.

References:

1. Stephanopoulos G.N, Aristose A. A., Nielsen J., *Metabolic engineering principles and Methodologies*, (1e), Academic press,1998.
2. Sang Y. L., Eleftherios T., Papoutsakis T., *Metabolic Engg.*, (2e), CRC Press, 1999.
3. Khdoderko B.N., Thomas and Westerhoft B H.W., *Metabolic engg in Post Genomic Era*, (1e), Horizon Bio Science, Amsterdam, The Netherlands, 2004.
4. Carbonell, P., *Metabolic Pathway Design*, (1e), Springer International Publishing, 2019.

CHE ****: NANOSCIENCE & TECHNOLOGY [4 0 0 4]

Basic concepts and definitions: material science, nanoscience. Unusual and useful properties of nanomaterials. Applications of nanomaterials. Applications of Nano materials in energy and environmental engineering. Challenges and opportunities in the synthesis and applications of nanomaterials. Methods of synthesis of nanomaterials "Top-down" vs. "Bottom-up" approaches. Physical, Chemical and Biological methods of synthesis of nanomaterials. Inorganic and organic nanomaterials, Carbon nanomaterials – fullerene, CNT, graphene, carbon nanofiber. Semiconductor nanomaterials- Functionalized nanomaterials. Supported nanomaterials. Core-shell nanoparticles. Nano fluids, Characterization of nanoparticles.

References:

1. Pradeep T, Nano: The Essentials Understanding Nanoscience McGraw Hill, first Ed, 2017.
2. Robert Kelsall, Ian W. Hamley, Mark Geoghegan Nanoscale Science and technology John Wiley 2005
3. Poole C. P., Owens Jr., F. J., Introduction to Nanotechnology, Wiley, 2003
4. Stuart Lindsay, Introduction to Nanoscience Oxford University Press 2010
5. Michael R., Nano-Engineering in Science and Technology: An Introduction to the World of Nano design", World Scientific, 2003
6. Ventra M. Di, Evoy S. and Heflin J. R., Introduction to Nanoscale Science and Technology, Springer, 2004.
7. Chattopadhyay K K; Banerjee A N, Introduction to Nanoscience and Nanotechnology, Prentice Hall India, 2009

CHE **** : PINCH TECHNOLOGY [3 1 0 4]

Definition of Process Integration (PI), Techniques available for PI, onion diagram. Introduction, key steps of Pinch Technology: Data extraction, Targeting, Designing, Optimization- Super targeting. Essential elements of Pinch Technology: Grid diagram, Composite curve, Problem table algorithm, Grand composite curve. Targeting of Heat Exchanger Network (HEN): Energy targeting, Area targeting, Number of units targeting, Shell targeting, cost targeting. Designing of HEN: Pinch design methods, heuristic rules, stream splitting, design of maximum energy recovery (MER), design of multiple utilities and pinches, Heat Integration of equipment.

References:

1. Uday S. V., *Heat Exchanger network synthesis*, (1e), Gulf Publishing Co, USA, 1995
2. Douglas J. M., *Conceptual Design of Chemical Processes*, (1e), McGraw Hill, New York, 1988.
3. Linnhoff, B. Townseod D.W., Boland D., Hewitt G.F., Thomas, B.E.A., Guy, A.R. and Marsland, R.H., *A User's guide on process integration for the efficient use of energy*, (1e), Inst. Of Chemical Engineers, London (1982).
4. Smith, R., *Chemical Process Design*, (1e), McGraw Hill (1995).

CHE **** : PROCESS DATA ANALYSIS [3 1 0 4]

Fundamental statistical analysis, Simple regression analysis, Multiple regression analysis, Parameter estimation, Statistical inferences based on multivariate linear regression models, weighted least squares Nonlinear Regression Analysis, determine model adequacy, Statistical inferences based on nonlinear regression models. Design of Experiments: Strategies for experimentation, Single factor experiments, Two-level factorial experiments, Fractional factorial design, multiple level factorial experiments, Analysis of variance, Interpretation of results from experiments. Response surface methods for optimal experimentation decision making, Statistical quality Control, Introduction to control monitoring charts.

References:

1. Montgomery D.C., *Design and Analysis of Experiments*, 8th edition, Wiley, 2012.
2. Montgomery D.C. and Runger G.C., *Applied Statistics and Probability for Engineers*.1994.
3. Box G.E.P., Hunter W.G. and Hunter J.S., *Statistics for Experimenters*, John Wiley & Sons, 1978.
4. An electronic textbook on Statistics is available at the following website. This site is an excellent source of information and learning aids in basic statistics: http://www.statsoft.com/textbook/stathome.html

CHE ***: SOLID WASTE MANAGEMENT [3 1 0 4]

Solid Waste – A consequence of life, evolution of solid waste management, engineering principles, generation of solid waste, onsite handling, storage and processing, collection of solid waste, transfer and transport, processing techniques and equipment, recovery of resources, conversion products and energy, disposal of solid waste including sanitary land fill, biogasification, composting, incineration and pyrolysis, hazardous wastes, management issues, planning, choices in onsite handling storage and processing, collection alternatives, transfer and transport options, dispersal options, planning, development, selection and implementation, Land fill design exercises.

References:

1. Tchobanoglous, G., *Integrated Solid Waste Management*, (Indian edition), McGraw Hill, 2014.
2. Tchobanoglous, G., Kreith, F., *Handbook of Solid Waste Management*, (2e), McGraw Hill, 2002.
3. LaGrega, Mi, Buckingham P., and Evans, J., Hazardous Waste Management, (2e), Waveland Press, Inc., 2010
4. McBean E., Rovers F. and Farquhar G., Solid Waste landfill Engineering and Design (1e), Prentice Hall, 2002

CHE ****: UPSTREAM AND DOWNSTREAM BIOPROCESSING [3 1 0 4]

Substrates for bioconversion processes and design of media, Sterilization of air and medium, development of inocula for industrial fermentation and the aseptic inoculation. Role, importance and economics of downstream processing in biotechnological processes, Removal of insolubles: Filtration and micro filtration, Sedimentation, Centrifugation, Cell disruption methods. Isolation: Extraction, batch, staged operation, differential extractions and fractional extractions, Precipitation, Adsorption. Product purification: Chromatography, scale-up of chromatography, precipitation, ultrafiltration and electrophoresis. Polishing: crystallization and drying.

References:

1. Belter P. A., Cussler E. L and Hu W-S, Bioseparations, Downstream processing for biotechnology, (1e), John Wiley and Sons. 1988
2. Pauline M. D., Bioprocess engineering principles, (1e), Academic press. 1995
3. Rehm H.J. and Reed G., Stephanopoulos G., Biotechnology, (2e), Bio Processing, Vol. 3, John Wiley, 1993.
4. Stanbury P.F., Whitakar A. and Hall S.J., Principles of Fermentation Technology, Elsevier Publishers, (2e), 2005

CHE ****: ARTIFICIAL INTELLIGENCE & MACHINE LEARNING [3 1 0 4]

Introduction to AI & ML supervised and unsupervised learning. Linear regression, Cost/ Objective function. Gradient descent algorithms, Linear regression with multiple variables-gradient descent algorithm. Classification, the concept of regularization. Neural networks. Bias-Variance trade-off, Support vector machines, Clustering algorithm. ANN, Deep learning, Orthogonal projection, PCA, PLS. An algorithm developed and analyzed in MATLAB / PYTHON software, application in process system engineering.

References:

1. Stephen Marsland, “Machine Learning” , Second edition CRC Press, 2014

2. Steven L. Brunton and J. Nathan Kutz, “Data-Driven Science and Engineering: Machine Learning, Dynamical Systems, and Control” Edn., 2, Cambridge University Press; 2022.
3. Alpaydin Ethem, “Introduction to Machine Learning”, Edn. 2, PHI, New Delhi.
4. Shalev-Shwartz Shai;Ben-David Shai, “Understanding machine learning”, Cambridge Univerwity Press, 2017.
5. Saikat Dutt, Subramanian Chandramouli and Amit Kumar Das, “Machine Learning” 1st edition, Pearson, 2018.

CHE ****: MULTISCALE MOLECULAR SIMULATIONS [3 1 0 4]

Intermolecular forces, force fields, potential energy surfaces, structural properties molecular orbital theory, introduction to density functional theory, molecular mechanics, introduction to programming methods and algorithms used in the course, molecular dynamics simulations, ensembles NVE, NVT & NPT, periodic boundaries, Monte Carlo simulations, free energy calculations, phase equilibria calculations, interfacial properties, rare events.

References:

1. Computer Simulation of Liquids, M. P. Allen & D. J. Tildesley, 1987
2. Understanding Molecular Simulation, 2nd Ed., Daan Frenkel & Berend Smit, 2002
3. The Theory of Intermolecular Forces, 2nd Ed., Anthony Stone, 2013
4. Molecular Modeling – Principles and Applications, 2nd Ed., Andrew Leach, 2001
5. The Art of Molecular Dynamics Simulations, D C Rappaport, Cambridge University Press, Second Edition, 2003

OPEN ELECTIVES:

CHE **** : SUSTAINABLE ENGINEERING [3 0 0 3]

Sustainable Development and Role of Engineers , Sustainable Engineering Concepts, Goals of sustainability, System Thinking, Life Cycle Thinking and Circular Economy, Green Economy and Low Carbon Economy, Eco Efficiency, Triple bottom Line, Guiding principles of sustainable engineering, Frameworks for sustainable Engineering, Tools for sustainability Assessment, Fundamentals of Life Cycle Assessment, Environmental Life Cycle Costing, Social Life Cycle Assessment, and Life Cycle Sustainability Assessment, Introduction to Environmental Economics, Integrating Sustainability in Engineering Design, Case Studies.

References:

1. Introduction to Sustainability for Engineers, Toolseeram Ramjeawon, CRC Press, 1st Edn., 2020
2. Sustainability Engineering: Concepts, Design and Case studies, David Allen, David R. Shonnard, Pearson, 1st Edn, 2011

3. System Analysis for sustainable Engineering: Theory and applications, Ni-bin Chang, McGraw Hill Publications, 1st Edn. 2010
4. Engineering for Sustainable development: Delivery a sustainable development goals, UNESCO, International Centre for Engineering Education, France, 1st Edn., 2021

CHE **** : GREEN PROCESSES [3 0 0 3]

Introduction: Definition, the twelve basic principles of green chemistry. Green synthetic methods: Microwave synthesis, electro-organic synthesis, The design and development of environmentally friendly chemical pathways: challenges and opportunities. High-yield and zero-waste chemical processes. Representative processes. Materials for green chemistry and technology: Catalysis, environmental friendly catalysts, Bio-catalysis, biodegradable polymers, alternative solvents, ionic liquids Bio-energy: Thermo-chemical conversion: direct combustion, gasification, pyrolysis and liquefaction; Biochemical conversion: anaerobic digestion, alcohol production from biomass; Chemical conversion process: hydrolysis and hydrogenation; Biophotolysis: Hydrogen generation from algae biological pathways; Storage and transportation; Applications

References:

1. Mikami K., Green Reaction Media in Organic Synthesis, Wiley-Blackwell 2005.
2. Koichi T., Solvent-free Organic Synthesis Green chemistry, Wiley-VCH; 2003
3. Maartje F. K. and Thierry M., Supercritical Carbon Dioxide: in Polymer Reaction Engineering Green Chemistry, Wiley VCH 2005
4. Alvise P., Fulvio Z., and Pietro T., Methods and Reagents for Green Chemistry: An Introduction, Wiley Inter science 2007
5. Lancaster M,Green Chemistry, RSC 2002
6. Stanely E. Manahan, Green Chemistry and the Ten Commandments of Sustainability, ChemChar 2005
7. David T. A. and David R. S., Green Engineering: Environmentally conscious Design of Chemical Processes, Prentice Hall PTR 2001
8. Roger A. S., Isabel A., and Hanefeld U., Green Chemistry and Catalysis, Wiley VCH, 2007 9. James V. B., Heat Conduction Using Green's Function (Series in Computational and Physical Processes in Mechanics and Thermal Sciences) Taylor & Francis, 1992

CHE **** : ADVANCED PROCESS CONTROL LAB [0 0 3 1]

Data driven model development, Design of conventional controller for SISO system, Data driven model development using system identification toolbox for MIMO system. Design and validation of decoupler for MIMO system. Design of P/PI/PID controller for SISO and MIMO system. Design of model-based controller for SISO and MIMO system.

References:

1. Seborg D.E., Edgar T.F., Mellichamp, *Process dynamics and control*, (2e), John Wiley & sons, 2004

2. Astrom K. J. and Wittermark B., *Computer-Controlled Systems: Theory and Design*, Prentice Hall; 3rd edition, 1996
3. Tangirala A. K., *Principles of System Identification: Theory and Practice*, CRC Press, 2014.
4. Lab Manual

CHE****: PROCESS SIMULATION LAB [0 0 3 1]

Introduction to simulation software packages, Aspen Plus. Steady state and Dynamic simulation practice sessions with ASPEN for single equipment and chemical process plants.

References:

1. Amiya K Jana , *Process simulation and control using ASPEN*, (2e), Prentice Hall India,2012
2. Bruce A Finlayson, *Introduction to chemical engineering computing*, John Wiley & sons, 2006

CHE **** : PROJECT WORK & INDUSTRIAL TRAINING

Guidelines for Second year M Tech Project work & Industrial Training

1. A student of M Tech shall carry out a Project Work during the second year of the programme, in the institution/ industry/ research laboratory or any other institution of higher learning where facilities exist, with approval from the parent Department.

Any one of the following options is permitted for undertaking the project work:

1.1 A single project at the parent institute/industry/research laboratory/any other institution of higher learning.

1.1.1 If the project work is undertaken at the industry/research laboratory/any other institute of higher learning, the minimum duration of the work will be 36 weeks.

1.1.2 If it is undertaken at the parent institute of the student, the minimum duration for the project work will be 32 weeks and in addition to this, the student has to undergo a mandatory industrial training for 4 weeks.

1.2 A project work for a minimum duration of 16 to 24 weeks at an industry/research laboratory/institution of higher learning and another project work at the parent institute for a minimum duration of 12 to 20 weeks so that the total duration of the two projects together will be a minimum of 36 weeks.

2. There will be a mid-term evaluation of the work after about 18 weeks by the department concerned if it is a single project. This evaluation will be out of 100 marks.

3. If the student undertakes two projects, one in an industry/research organization/institution of higher learning and the other one in the parent institute, there will be a mid-term evaluation of the work by the department for each of them. The evaluation will be out of 50 marks each.

4. In case of external projects, the feedback of the external guide shall be considered during evaluation.

5. If the student has undertaken more than one project work, a single report has to be submitted at the end of the second year that includes the relevant contents of both the projects in the form such as PART A and PART B.

6. The final evaluation will be conducted after the completion of the project work and submission of the report, by a panel of examiners including the internal/institute guide. The final evaluation will be out of 300 marks.

7. The grade awarded to the student will be on the basis of total marks obtained out of 400 marks.