GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Master of Engineering

Level: PG

Branch: Computer Aided Process Design

Subject Code: ME02072051

Subject Name: Computational Tools in Chemical Engineering

w. e. f. Academic Year:	2024-25
Semester:	2
Category of the Course:	Professional Elective Course

Prerequisite:	Strong foundation in core chemical engineering principles like thermodynamics, reaction kinetics, transport phenomena (fluid mechanics, heat transfer, mass transfer), and process design principles. Familiarity with scientific computing libraries would be beneficial but not mandatory.
Rationale:	The field of chemical engineering is increasingly reliant on computational tools for process design, simulation, and optimization. This course equips M.E. students specializing in Computer Aided Process Design with the necessary skills to leverage these tools effectively. Focus will be laid on problem solving and industry relevance.

Course Outcome:

After Completion of the Course, Student will able to:

No	Course Outcomes
01	Demonstrate knowledge of computational languages in chemical engineering
02	Apply basic programming techniques in MATLAB/Scilab, Python and Excel to solve chemical engineering problems
03	Analyze results obtained from MATLAB/Scilab, Python and Excel
04	Explain the potential applications of Artificial Intelligence and Machine Learning in chemical engineering
05	Simulate chemical processes using DWSIM/Aspen Plus

Teaching and Examination Scheme:

Teaching Scheme (in Hours)			Total Credits L+T+ (PR/2)	Assessment Pattern and Marks				Total Marks
				Theory		Tutorial / Practical		
L	T	PR	C	ESE (E)	PA / CA (M)	PA/CA (I)	ESE (V)	
3	0	2	4	70	30	20	30	150

Course Content:

Unit No.	Content	No. of Hours	% of Weightage
1.	**Introduction to Computational Tools:** Overview of computational tools in chemical engineering, Introduction to MATLAB/Scilab, Excel, Python and DWSIM for chemical engineering applications.	2	4
2.	**Basics of MATLAB/Scilab and Excel:** Basic features, writing codes, plotting and presentation of results, goal seek, solver, curve fitting etc.	6	13
3.	**Application of MATLAB/Scilab and Excel to chemical engineering problems:** Analysis of frictional losses in pipe flows, steady-state analysis of diabatic operation of a CSTR, analysis of multicomponent distillation, analysis of steady-state heat conduction in a one-dimensional rod etc.	8	18
4.	**Basics of Python language:** Basic syntax, variables, data types, and control structures, Introduction to the Python Standard Library etc.	8	18
5.	**Application of Python to chemical engineering problems:** Python for stoichiometry and thermodynamics calculations, problems of reaction kinetics, heat transfer and mass transfer operations.	9	20
6.	**Fundamentals of Artificial Intelligence (AI) and Machine Learning (ML) in Chemical Engineering:** Introduction to AI and ML; supervised, unsupervised, semi-supervised learning; Overview of software tools used in AI & ML for solving problems in chemical engineering.	4	9
7	**Simulation in DWSIM/Aspen Plus:** Introduction to DWSIM/Aspen Plus, Flowsheeting, Shortcut and Rigorous Distillation, Simulation of reactors (CSTR, PFR, Gibbs, Equilibrium),Shell and Tube Heat Exchanger, Binary Phase Envelope (Txy, Pxy, xy plots), Calculation of Dew points and Bubble points, Sensitivity Analysis.	8	18
	Total	**45**	**100**

Suggested Specification Table with Marks (Theory):

Distribution of Theory Marks					
R Level	**U Level**	**A Level**	**N Level**	**E Level**	**C Level**
10	10	10	10	5	5

Where R: Remember; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create (as per Revised Bloom's Taxonomy)

References/Suggested Learning Resources:

(a) Books:

1. Problem Solving in Chemical and Biochemical Engineering with POLYMATH, Excel, and MATLAB, M. B. Cutlip and M. Shacham, Pearson Education Inc, 2nd edition, 2008.
2. Computational techniques for process simulations and analysis using MATLAB, N. S. Kaisare, CRC Press, 2018.
3. Introduction to Chemical Engineering Computing, Finlayson, Bruce A, Wiley, 3rd Edition, 2012.

(b) Open source software and website:

1. https://in.mathworks.com/products/matlab-online/matlab-online-versions.html
2. https://www.python.org/downloads/
3. https://diveintopython3.net/
4. https://www.scilab.org/download/scilab-2024.1.0
5. https://sourceforge.net/projects/dwsim/files/DWSIM/

Suggested Activities for Students: MATLAB On-Ramp certification course (free)**,** Online NPTEL courses on Python and DWSIM.

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