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| **B.Tech. I (Chemical Engineering) Semester – II PROGRAMMING FOR CHEMICAL ENGINEERS**  **CH-108** | **Scheme** | **L** | **T** | **P** | **Credit** |
| **3** | **0** | **2** | **04** |

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| **1.** | **Course Outcomes (COs):**  **At the end of the course, students will be able to** |
| CO1 | Acquire knowledge about computer architecture and algorithm development. |
| CO2 | Identify the suitable software tools for the given chemical engineering problem. |
| CO3 | Analyze the given problem and develop the suitable algorithm. |
| CO4 | Evaluate programming solutions with different aspects. |
| CO5 | Design and develop solution for given problems. |

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| **2.** | **Syllabus** | |  |
|  | **INTRODUCTION TO COMPUTER AND ITS ARCHITECTURE** | | **(02 Hours)** |
|  | Introduction and Characteristics, Computer Architecture, Generations, Classifications, Applications, Central Processing Unit and Memory, Communication between various Units, Processor Speed, Multiprocessor System, Peripheral Buses, Motherboard Demonstration. | | |
|  | **INTRODUCTION TO PROGRAMMING LANGUAGES** | | **(11 Hours)** |
|  | Introduction and Classification of Computer Languages, Programming basics: variables, constants, data types; Input/output operations in SCILAB & python; Operators: arithmetic, relational, logical; Flowcharts, pseudocode, problem solving approach  Loops, Nested Loops, Break, Continue & Pause commands in SCILAB/python. | | |
|  | **PROGRAMMING USING ‘SCILAB/Python’ LANGUAGE – ARRAYS** | | **(6 Hours)** |
|  | Arrays in SCILAB; lists in Python, Matrices and vectorized operations (SCILAB emphasis), Python NumPy arrays introduction, One Dimensional Array of Numbers and Characters, Two-Dimensional Array, Solving linear equations (material balance of mixing problem), Matrix operations: transpose, determinant, inverse (SCILAB & Python), Case studies on chemical process mass balance. | | |
|  | **PROGRAMMING USING ‘SCILAB/Python’ LANGUAGE – Function Writing & Numeric Computation of Non-Linear Equations** | | **(6 Hours)** |
|  | Writing functions in SCILAB, Writing functions in Python (arguments, return values), Chemical engineering examples: enthalpy calculation using functions, Function for Raoult’s Law (bubble point & dew point), Root-finding methods: Bisection in SCILAB & Python, Newton–Raphson method (equilibrium constant calculation) | | |
|  | **PROGRAMMING USING ‘SCILAB/Python’ LANGUAGE- Data Visualization** | | **(6 Hours)** |
|  | Plotting in SCILAB: 2D plots (Least Square Regression Method), Plotting in Python: Matplotlib basics (Least Square Regression Method), Comparative plotting, Various libraries and tools used for the data visualization. 3D graphs, bar plot, histogram, scatter plot, pie chart. Libraries like pandas for Data manipulation | | |
|  | **PROGRAMMING USING ‘SCILAB/Python’ LANGUAGE –Numeric integration & Differentiation** | **(5 Hours)** | |
|  | Numerical integration: trapezoidal rule & Simpson’s rule, Numerical differentiation: forward, backward newtons difference method, ODE solving in SCILAB: ode function, ODE solving in Python: scipy.integrate.odeint | | |
|  | **CASE STUDIES AND APPLICATION OF PROGRAMMING FOR CHEMICAL ENGINEERING PROGRAMMING** | **(9 Hours)** | |
|  | Cooling of a hot sphere (unsteady heat transfer), Chemical reactor kinetics simulation (1st order), Fluid flow problems: pressure drop in pipes, Heat exchanger performance calculations | | |
|  | **PRACTICALS WILL BE BASED ON THE COVERAGE OF THE ABOVE TOPICS SEPARATELY.** | | **(30 Hours)** |
|  | **(Total Contact Time: 45 Hours + 30 Hours = 75 Hours)** | | |

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| **3. Practicals:** | |
| 1 | To develop algorithm for simple unit conversion problems (temperature, pressure, energy etc). |
| 2 | To develop algorithm in SCILAB and python for Antoine equation |
| 3 | Algorithm development using SCILAB and python for interpolation |
| 4 | Algorithm development using SCILAB and python for solution of system of linear equations (Direct Methods) |
| 5 | Algorithm development using SCILAB and python for solution of system of linear equations (Iterative Methods) |
| 6 | Data visualization in SCILAB and python |
| 7 | Data Analysis and manipulation in SCILAB and python |
| 8 | Algorithm development using SCILAB and python for Numerical Differentiation & Integration |
| 9 | Algorithm development using SCILAB and python for Initial value problem & boundary value problems of ordinary differential equations |
| 10 | Algorithm development using SCILAB and python for partial differential equations |

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| **4. Books Recommended:** | |
| 1. | “Introduction to Computer Science”, Fourth Impression, Pearson Education, ITL Education Solutions Limited, 2009. |
| 2. | Gottfried B.S., “Programming with C Schaum’s outline Series”, Outline Series, 2nd Edition, Tata McGraw-Hill, 2006. |
| 3. | Pradip Dey, “Programming in C”, 2nd Edition, Oxford University Press, 2012. |
| 4 | Paul Barry, Head First Python: A Learner's Guide to the Fundamentals of Python Programming, A Brain-Friendly Guide, Third Edition, O’Reilly Media, Inc., 2023 |
| 5. | Gilat, A.. MATLAB: An introduction with Applications. 4th Edition, John Wiley & Sons, 2017 |
| 6. | Kapuno, J. R. R. A. (2010). *Programming for chemical engineers using C, C++, and MATLAB*. Laxmi Publications, Ltd.. |