

INDIAN INSTITUTE OF TECHNOLOGY TIRUPATI

भारतीय प्रौद्योगिकी संस्थान तिरुपति

1.	Title of the course	Computational Techniques for Chemical Engineers
2.	Course number	CH304M
3.	Structure of credits	3-0-3-5
4.	Offered to	UG
5.	New course/modification to	Modification To CH3107/12
6.	To be offered by	Department of Chemical Engineering
7.	To take effect from	July 2022
8.	Prerequisite	Nil

- 9. **Course Objective(s):** To demonstrate solution strategies for algebraic and differential equations (linear and nonlinear). To solve chemical engineering problems for the discussed numerical techniques using suitable software.
- 10. **Course Content:** Significance of numerical methods; Approximations, round-off and truncation errors, uncertainty in experimental data, error propagation, rate of convergence; Solution of linear algebraic equations, eigenvalues and eigenvectors; Solution of nonlinear algebraic equations; Solution to material balance on process units; Regression, curve fitting, cubic splines; Analysis of reaction kinetic data; Numerical differentiation and integrations; Solution to ordinary differential equations: initial value and boundary value problems; Solution to heat conduction equation, falling sphere in a fluid; Solution to partial differential equations; Solution to diffusion equation.

Laboratory: Application of the above techniques to chemical engineering problems using suitable software.

11. Textbook(s):

- 1. Chapra S C and Canale R P, *Numerical Methods for Engineers*, 7th Edition, Tata McGraw Hill (2015).
- 2. Gupta S K, Numerical Methods for Engineers, 2nd Edition, New Age International (2010).

12. Reference(s):

- 1. Beers K J, *Numerical Methods for Chemical Engineering: Applications in MATLAB*, 1st Edition, Cambridge University Press (2006).
- 2. Chidambaram M, *Mathematical Modelling and Simulation in Chemical Engineering*, Cambridge University Press (2018).
- 3. Finlayson B A, Introduction to Chemical Engineering Computing, 2nd Edition, Wiley India (2012).
- 4. Ghosh P, *Numerical, Symbolic and Statistical Computing for Chemical Engineers using Matlab*, PHI Learning (2018).