

# MADHAV INSTITUTE OF TECHNOLOGY & SCIENCE, GWALIOR-05

(A Govt. Aided UGC Autonomous Institute Affiliated to RGPV, Bhopal)

## Department of Chemical Engineering

# Computational Methods in Chemical Engineering Lab

1. Data representation and treatment by graphical methods, pressure volume, temperature and concentration relationship for gases and their mixtures
2. Redlich-Kwong equation of state and other Viral equations to estimate thermodynamic properties like compressibility factor, molar volume and P-V-T relationship
3. Estimation of properties from empirical correlations
4. Estimation of critical properties from group contribution method
5. Measurement errors their propagation and minimization of random errors, selection of confidence limits
6. Numerical solutions of quadratic and linear algebraic equations using various methods on the solvers in MATLAB
7. Numerical solutions of batch reactor problems using Euler Algorithm
8. Polynomial root finding using “Newton Raphson method and Secant method”
9. Numerical integration by Trapezoidal rule, Simpsons 1/3<sup>rd</sup> and 3/8<sup>rd</sup> rule
10. Approximate solutions of ordinary differential equations by Runge-Kutta algorithm and its application in chemical engineering
11. Numerical solution of transient flow temperature profile of fluid using different computational methods on MATLAB solver
12. Mass balance problem using continuity equation applied to a dynamic system. Formation of differential equations (component balance) and their solutions

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## **Process Modeling & Simulation Lab**

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- 1.** Process dynamics experiments like flow of incompressible fluids at a variable flow rate.
  - 2.** Dynamics of a tank draining through an orifice in the bottom. Differential equation formulation and verification with the experimental data
  - 3.** Mass balance in a tank filling at certain rate and emptying at another rate. Rectangular and wedge-shaped tank and incompressible fluid
  - 4.** Modeling a batch reactor-verification of 1st and 2nd order rate kinetics.
  - 5.** Counter current double pipe heat exchanger modeling-data analysis by iterative methods.
  - 6.** Simulation of a distillation column-binary systems, equimolar overflow, constant relative, volatility.
  - 7.** Input-Output response study in non-ideal flow reactors.
  - 8.** Simulation of a perfectly mixed reactor with heat transfer. Derivation of a mathematical model and solving for steady state heat transfer
  - 9.** Simulation of False Position method.
  - 10.** Simulation of Newton-Raphson method.
  - 11.** Simulation of Muller method.
  - 12.** Simulation of Euler's & R-K methods.
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## **Process Computation Lab**

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1. To apply mass balance for a process situation using excel
  2. To apply energy balance for a process situation using excel
  3. To plot and learn duhrings plot
  4. To plot various time changing plots for parameters involved in a process
  5. To analysis parameter relations in a process situation using in-out relations
  6. To develop flow-sheet in excel
  7. To develop balance sheet for a process situation
  8. To develop understanding of calling of workbooks for use at one time
  9. To learn about data validation and consolidation in excel
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