NATIONAL UNIVERSITY OF ENGINEERING
COLLEGE OF CHEMICAL AND TEXTILE ENGINEERING
CHEMICAL ENGINEERING PROGRAM

PI523 – CALCULATIONS IN CHEMICAL ENGINEERING I

I. GENERAL INFORMATION

CODE	**:**	PI523 Calculations in Chemical Engineering I
SEMESTER	**:**	5
CREDITS	**:**	4
HOURS PER WEEK	**:**	5 (Theory, Practice)
PREREQUISITES	**:**	MA143 Mathematics IV
CONDITION	**:**	Compulsory

II. COURSE DESCRIPTION

The course prepares students in the analysis and application of numerical methods for solving different types of equations and mathematical problems appearing in chemical engineering. Students apply numeric methods for solving linear and nonlinear equation systems, function approximation and interpolation, solution of differential equations. The methods and algorithms are describe in computer code or pseudo-code and implemented using software applications

III. COURSE OUTCOMES

At the end of the course, students:

1. Analyze numerical methods for determining their convergence properties.
2. Understand, analyze and apply numeric methods for solving linear and nonlinear equation systems, function approximation and interpolation, solution of differential equations.
3. Represent numerical methods through computer code or pseudo-code.
4. Interpret obtained results and verify their precision and validity.

IV. LEARNING UNITS

1. SOLUTION OF NONLINEAR EQUATIONS
Fixed point method / Newton-Raphson method / Bisection method / False position method / Secant method.

2. LINEAR EQUATION SYSTEMS
Jacobi method / Gauss- Seidel method

3. NONLINEAR EQUATION SYSTEMS
Multivariable Newton-Raphson method

4. FUNCTION APPROXIMATION AND INTERPOLATION
Simple polynomial approximation and interpolation / Lagrange polynomials.

5. NUMERIC DIFFERENTIATION AND INTEGRATION
Numeric differentiation / Newton-Cotes method / Gauss quadrature / Multiple integrals.

6. ORDINARY DIFFERENTIAL EQUATIONS
Initial value problem / Euler method / Runge-Kutta Method / High order ordinary differential equations / Systems of ordinary differential equations.

7. PARTIAL DIFFERENTIAL EQUATIONS

Derivative approximation by finite differences / Solution of one-dimensional heat equation.

V. LABORATORY AND PRACTICAL EXPERIENCES

Practice 1. Solution of nonlinear equations
Practice 2. Linear and nonlinear equation systems
Practice 3 Function approximation and interpolation
Practice 4. Numeric differentiation and integration
Practice 5. Ordinary and partial differential equations

VI. METHODOLOGY

The course takes place in theory, practice and computer laboratory sessions. In theory sessions, faculty presents the methods and techniques. In practice sessions, students solve diverse problems related to the numeric methods presented in theory sessions. In computer laboratory sessions, students implement the numeric methods using specialized software applications. Student's active participation is promoted throughout the course for solving real-world chemical engineering problems.

VII. GRADING FORMULA

The Final Grade PF is calculated as follow:

PF = (EP + EF + PL) / 3

EP: Mid-term Exam. EF: Final Exam.
PL: Average of Laboratory and Practice Works.

VIII. BIBLIOGRAPHY

1. **NIEVES A.**
   Numeric Methods Applied to Engineering
   Patria Editorial, Mexico, 2012
2. **CONSTANTINIDES Mostoufi**
   Numerical Methods for Chemical Engineers with MATLAB Applications
   Physical Chemistry
   Prentice Hall, 2010