

Practical Numerical Methods for Chemical Engineers: Using Excel with VBA, 3rd Edition

Richard A Davis

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This NEW 3rd edition expands *Practical Numerical Methods* with more VBA and Excel programming to boost Excel's power for numerical modeling and analysis. Excel is the *de facto* computational tool used by engineers & scientists worldwide. Learn how to customize your Excel workbooks with VBA using the same powerful numerical techniques found in specialized math software.

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- 1. The refined Excel *PNM3Suite* workbook with 120 VBA user-defined functions, macros & user forms for learning VBA & implementing advanced numerical techniques in Excel.
- 2. Excel workbooks used to create the book's more than 200 practical examples demonstrating the power of the numerical methods in the book. Customize the examples & macros to tackle your own numerical problems using VBA in Excel.
- 3. Hundreds of practice problems for self-guided study to sharpen your Excel & VBA skills.

The first chapter sets the stage for problem solving with numerical methods. The next two chapters cover frequently overlooked features of Excel and VBA for implementing numerical methods in Excel, as well as documenting results. The remaining chapters present powerful numerical techniques using Excel and VBA to find roots to algebraic equations, approximate derivatives, optimize, model data by least-squares regression and interpolation, analyze risk and uncertainty, solve integrals and ordinary & partial differential equations:

- 1. Numerical Methods & Mathematical Modeling: expert problem solving
- 2. Excel: Documentation, Graphing, Worksheet Functions, Input Validation & Formatting, What-if Analysis
- 3. VBA: Editor and objects, Function & Sub Procedures, Data Types, Structured Programming, Arithmetic and Worksheet Functions, Flow Control, Arrays, Communication, Message & Input Boxes, User Forms, Reading/Writing Files, Debugging, Unit Conversions
- 4. Linear Equations: Matrix Algebra, Gaussian Elimination and Crout Reduction with Pivoting, Thomas, Cholesky, Power, Jacobi, & Interpolation Methods for Eigenvalues & Eigenvectors, Jacobi & Gauss-Seidel Iteration, Relaxation
- 5. Taylor Series Analysis: Finite Difference Derivative Approximation, Richardson's Extrapolation, Ridder's algorithm, Sensitivity
- 6. Nonlinear Equations Root Finding: Methods of Bisection, Regula Falsi, Newton, Secant, Pade, Wegstein, Quasi-Newton, Aitkin/Steffensen, Homotopy, Bairstow (for polynomial roots), Goal Seek & Solver
- 7. Optimization: Solver, Luus-Jaakola, Quadratic Interpolation, Golden Section, Powell, Firefly, Constraints, Scaling & Sensitivity

- 8. Uncertainty & Risk Analysis: Law of Propagation, Monte Carlo Simulations with Latin Hypercube Sampling
- 9. Least-squares Regression: Linear, Nonlinear, LINEST, Gauss-Newton, Levenberg-Marquardt, Validation and Assessment, Uncertainty Analysis, Weighted Regression
- 10. Interpolation: Linear, Newton Divided Difference and Lagrange Polynomials, Rational, Bulirsh-Stoer Pade, Stineman, Cubic & Constrained Splines, Linear & Spline Bivariate Interpolation
- 11. Integration: Graphical, Trapezoidal, Midpoint & transformation for Improper Integrals, Romberg, Adaptive Simpson & Gauss-Kronrod, Multiple Integrals by Simpson, Kronrod & Monte Carlo
- 12. Initial-value Problems: Single Step Euler & Backward Euler, Implicit Trapezoidal for Stiffness, Variable Step Runge-Kutta Cash-Karp, Dormand-Prince, Multi-step Adams-Bashforth-Moulton, Differential-Algebraic Systems
- 13. Boundary-value Problems & Partial Differential Equations: Shooting, Finite Difference, Orthogonal Collocation, Quasilinearization, Method of Lines, Crank-Nicholson
- 14. Review: Reference Tables of Excel & VBA Functions, User-defined Functions, Macros, User Forms
- 15. Primer on chemical reaction engineering

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