

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

By Richard A Davis



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This latest edition expands *Practical Numerical Methods* with more *VBA* to boost *Excel's* power for modeling and analysis using the same numerical techniques found in more specialized math software. Visit the companion web site:

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to access all of the book's *Excel* and *VBA* files, and learn how to customize your own *Excel* workbooks with:

- 1. A refined macro-enabled *Excel* workbook with a suite of over 170 *VBA* userdefined functions, macros and user-forms for learning *VBA* and implementing advanced numerical techniques in *Excel*.
- 2. More than 200 example and animation workbook files from the book that demonstrate the power of numerical methods. Customize the example files and macros to tackle your own problems using *VBA* in Excel.
- 3. Hundreds of practice problems for self-guided study to sharpen your *Excel* and *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 & ordinary & partial differential equations:

- 1. Numerical Methods & Mathematical Modeling: expert problem solving
- 2. Excel: Documentation, Graphing, Worksheet Functions, Input Validation and Formatting, What-if Analysis
- VBA: Editor and objects, Function and Sub Procedures, Data Types, Structured Programming, Arithmetic and Worksheet Functions, Flow Control, Arrays, Communication, Message and Input Boxes, User Forms, Reading/Writing Files, Debugging, Unit Conversions

- Linear Equations: Matrix Algebra, Gaussian Elimination and Crout Reduction with Pivoting, Thomas, Cholesky, Power, Jacobi, and Interpolation Methods for Eigenvalues and Eigenvectors, Jacobi and Gauss-Seidel Iteration, Relaxation
- 5. Taylor Series Analysis: Finite Difference Derivative Approximation, Richardson's Extrapolation, Ridder's algorithm, Sensitivity
- Nonlinear Equations Root Finding: Methods of Bisection, Regula Falsi, Newton, Secant, Pade, Wegstein, Quasi-Newton, Aitkin/Steffensen, Homotopy, Bairstow (for polynomial roots), Goal Seek and Solver
- 7. Optimization: Solver, Luus-Jaakola, Quadratic, Golden Section, Powell, Downhill Simplex, Firefly, Constraints, Scaling and Sensitivity
- 8. Uncertainty and Risk Analysis: Bootstrap, Confidence Intervals, Law of Propagation, Monte Carlo Simulations with Latin Hypercube Sampling
- Least-squares Regression: Linear, Nonlinear, LINEST, Gauss-Newton, Levenberg-Marquardt, Validation and Assessment, Uncertainty Analysis, Weighted Regression
- Interpolation: Linear, Newton Divided Difference and Lagrange Polynomials, Rational, Bulirsh-Stoer, Pade, Stineman, Cubic, B, Akima and Constrained Hermite Splines, Bivariate Interpolation
- Integration: Graphical, Trapezoidal, Midpoint and transformation for Improper Integrals, Romberg, Adaptive Simpson and Gauss-Kronrod, Multiple Integrals by Simpson, Kronrod and Monte Carlo
- 12. Initial-value Problems: Single Step Euler and Backward Euler, Implicit Trapezoidal for Stiffness, Variable Step Runge-Kutta Cash-Karp, Dormand-Prince, Multi-step Adams-Bashforth-Moulton, Differential-Algebraic Systems
- Boundary-value Problems and Partial Differential Equations: Shooting, Finite Difference, Orthogonal Collocation, Quasilinearization, Method of Lines, Crank-Nicholson
- 14. Review: Reference Tables of Excel and VBA Functions, User-defined Functions, Macros, User Forms
- 15. Primer on chemical reaction engineering

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Editorial Review

About the Author

Richard Davis is a *Jean G. Blehart Distinguished Professor* of Chemical Engineering at the University of Minnesota Duluth. He earned Ph.D. and B.S. Chemical Engineering degrees from UCSB and BYU, respectively.

Professor Davis has over two decades experience teaching a variety of courses including computational methods, unit operations of momentum, heat and mass transfer, chemical reactor design, engineering economics, bioprocessing and green engineering.

His current teaching and research interests include process modeling and simulation applied to mineral processing, energy conversion, air pollution control, chemical process safety, and environmental management.

Professor Davis serves as the Executive Secretary for the National Chemical Engineering Honor Society Omega Chi Epsilon, and is active in AIChE and ASEE. He is the academic adviser to the local engineering student chapters of Tau Beta Pi, Omega Chi Epsilon, and the Society for Mining, Metallurgy, and Exploration.

He is the recipient of the University's Outstanding Adviser and Exceptional Teaching awards.

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