

Index

A

- Adiabatic
 - system, 21, 32, 45
 - tank, 21, 32
- Algebraic equations (AEs), 2, 3
 - linear, 89, 90, 92, 94, 95, 99, 100, 107, 151, 152
 - non-linear, 102–105, 109
- Algorithm, 103, 130–144
- Analytical solution, 18, 115, 120, 121, 163
- Area
 - cross-section area, 11, 58, 60, 63, 65, 66, 72, 73, 75, 78, 81, 143, 157
 - for heat transfer, 24, 37, 47
- Argument, 134, 135, 141
- Array, 137, 138
- Arrhenius law, 30, 32, 34

B

- Backward difference, 101, 157, 158, 162, 163
- Batch
 - stirred tank reactor, 32
- Benzene, 54–57, 126
- Bitubular heat transfer, 54, 126
- Boundary condition, 54, 65, 66, 70, 73, 76, 77, 79, 81–87, 113, 122, 123, 127, 143, 145, 157, 158, 161–165

C

- Centered difference formula, 101, 147, 149
- Chemical engineering, vii–ix, 1, 5, 13, 42, 74, 89, 160, 164

- Chemical reactions, 5, 6, 13, 14, 17, 21, 28–33, 35, 36, 39, 73, 78

Codes

- computational, viii, 129, 130

Computational

- languages, 5
- program, 129, 130

- Concentration profile, 16, 142

- Concentric tubes, 54

Conduction

- heat, 58, 63, 71, 81, 84, 151, 164

- Conservation laws, 1, 6, 7, 9, 10, 14–16, 18–20, 25, 34, 36, 39, 50–52, 56, 63, 65, 66, 69, 71, 74, 78–80, 83, 91

Continuous

- stirred tank reactors, 31, 37, 39, 41, 43, 47, 97, 109, 136–144
- stirred tanks, 31, 37, 143

- Control volume, 7–9, 14, 18, 27, 32, 34, 36, 39, 49–53, 55, 56, 63, 65, 66, 69, 71–76, 78–82, 86

Convection

- heat, 76

- Convective heat transfer, 21, 24, 25, 27, 66

- Convergence, 100, 103, 149

- Customize ribbon, 130, 132

Cylindrical

- metal bar, 62, 65, 143, 145, 154, 160
- tank, 5
- tube, 49, 122

D

- Dependent variable, 7, 14, 50, 78, 80, 113, 116, 124, 127, 134, 137, 138, 146

- Derivative
 first, 120, 124, 127, 128, 146–148, 163
 second, 148
 partial, 73, 102, 145, 146, 148
- Deterministic model, 1, 3
- Developer tab, 130
- Differentiation, 100–102
- Diffusion coefficient of mass, 60, 70, 75
- Diffusive
 transport of heat, 58
 transport of mass, 59, 75
 transport of momentum, 61
- Diffusivity, 60, 69, 75, 86, 164
- Dimension (Dim), 9, 10, 14, 15, 18, 19, 29–31, 33, 49, 51, 53, 55, 74, 77, 84, 138, 141
- Dimensional analysis, 9
- Discretization, 146, 149, 154, 157, 161, 162
- Distributed-parameter models, 1, 2
- E**
- Endothermic
 chemical reactions, 17
 system, 17, 28, 36
 tank, 17
- Energy balance, 6, 17, 18, 20–22, 24, 27, 30, 32, 34, 36, 37, 39–42, 50, 53, 55, 56, 64, 65, 67, 72–77, 79, 82, 86, 94–97, 136, 137
- Enthalpy of reaction, 156
- Error, 114, 118, 147, 149
- Ethylene, 59, 60
- Euler method, 116, 117, 120–124, 127–135, 138, 139, 141, 142, 155, 156
- Excel
 macro-enabled workbook, 135
 spreadsheet, ix, 92, 121–130, 133, 141, 153
- Exothermic
 chemical reactions, 6, 17, 28, 32, 35, 36
 system, 6, 17, 28, 32, 35–37, 40, 74, 85, 109
 tank, 32
- Explicit methods, 113
- F**
- Fick, Fick's law, 62, 69
- Fill handle, 124, 125, 127, 149, 155
- Finite difference method, x, 145, 146, 148–165
- Flux boundary conditions, 150, 160–165
- Forward difference, forward difference approximation, 101, 147, 163, 164
- Fourier, 66
- Fourier, Fourier's law of heat conduction, 62, 63
- Function
 derivative, 134, 135, 137
 space, 92, 93, 105, 123, 125, 155
- G**
- Global heat transfer coefficient, 23, 24, 37, 45, 46
- Grid, 146, 151, 153
- H**
- Heat transfer
 coefficient, 23, 47, 58, 95, 143
 by convection, 62, 63, 65, 66, 81, 86, 161
 by diffusion, 58–77
- I**
- Implicit methods, 113
- Increment, 7, 55, 115, 116, 141, 142, 163
- Independent variable, 7, 9, 14, 50, 54, 73, 78, 80, 84, 96, 113, 114, 127, 135, 146, 148–150, 154, 164
- Infinitesimal variation of the dependent variable, 7, 9, 14, 50, 78, 80
- Initial condition, 7, 10, 11, 15, 17, 20, 21, 26, 28, 34, 36, 37, 44, 46, 47, 54, 73, 79, 83, 86, 96, 131, 135, 137, 142, 158
- Initial guess, 96, 100–103, 105, 107
- Insert function area, 102, 103
- Insulated
 perfectly stirred tank, 18
 stirred tank, 17, 18
- Iterations, number of iterations, 100
- J**
- Jacket
 linear algebraic equations, 109
- Jacobian
 matrix, 100–102, 104
- K**
- Kinetics
 rate constant, 29
- L**
- Lumped-parameter models, 1, 2, 13
- Lumped-parameters problem, ix, 13, 14, 32, 49
- M**
- Macro
 macro-enabled workbook, 135
- Mass
 balances, 10, 13–17, 32–34, 37, 39, 40, 70, 75, 76, 82, 86, 91, 97, 107, 110, 137, 143

- flow by diffusion, 69
 - transfer, 59, 76
- Material (mass) balance, 10, 13–17, 32–35, 37, 39, 40, 70, 75, 76, 82, 86, 91, 97, 107, 110, 137, 143
- Mathematical model, vii, 2, 3, 13, 15, 24, 28, 31, 32, 49, 62, 71, 74, 83, 142, 143
- Mathematical software, 32
- Matrix
 - identity and inverse, 90
 - inversion and multiplication, ix, 92
 - Jacobian, 99–102, 104
- Modeling, vii, ix, x, 1–3, 5, 6, 8, 10, 11, 32, 34, 52, 62, 65, 83, 84, 131, 145, 151, 157

- N**
- Newton-Raphson (NR) method, ix, 96, 97, 102, 107, 109
- Nonlinear
 - algebraic equations, 40, 89, 96, 97, 99, 103, 104, 106
 - nonlinear equations, ix, 89, 104
- Numerical
 - derivative, 101, 102
 - differentiation, 101, 104
 - integration, 113
 - method, vii–ix, 2, 3, 5, 10, 89, 113–121, 124, 131, 141, 143, 145, 154, 155, 157

- O**
- One-sided difference, 147
- Optimization, 105
- Ordinary differential equations (ODE), ix, x, 2, 10, 13, 15, 16, 20, 26, 34, 36, 44–47, 49, 56, 76, 84, 85, 113–145, 154, 155, 161, 162

- P**
- Partial differential equations (PDE), ix, x, 2, 3, 49, 52, 54, 64, 79, 82, 84, 107, 145
- Perfect agitation, 2
- Perfectly mixed, 18, 19, 27, 32
- Perfectly stirred tank, 1, 13, 14, 16–18, 44, 45, 91
- Phenomenological modeling, 1

- R**
- Reaction
 - of first order, 29, 33, 108
 - of second order, 29, 30, 39
- Reactor, vii, 1, 28–47, 74–77, 80, 82, 83, 85–87, 100, 107–109, 136, 137, 142, 143, 156–158, 160
- Roots, 96–98, 103, 105, 107
- Runge–Kutta methods, x, 115, 116, 120, 141, 158

- S**
- Second derivative, 148
- Second partial derivative, 147, 148
- Semi-batch, 31
- Set objective, 105
- Simulation, vii–ix, 1–3, 5, 6, 10, 15, 19, 89, 130, 132
- Solver, ix, 104–110
- Spatial coordinates, 2
- Specific heat, 18, 19, 21, 23, 24, 35, 37, 46, 51, 72, 75, 86, 94, 123, 126
- Spreadsheet, 93, 105, 123, 133, 138, 149, 155, 156, 162, 163
- Square metal plate, 151
- Stability, 149
- Steady state, ix, 2, 11, 13, 16, 18, 20, 24, 26, 27, 37, 39–42, 45, 47, 49, 50, 52, 54, 58, 60–66, 70, 71, 74, 77, 78, 80, 83, 84, 86, 87, 89, 91, 94–97, 100, 103, 107–110, 113, 122, 141–144, 151, 159, 163–165
- Step, vii, ix, 5, 6, 8, 19, 24, 30, 105, 121–127, 133, 134, 141, 142
- Stirred tank, Stirred Tank Reactor (STR), 15, 24, 26, 30

- T**
- Tangent, 7, 96, 117
- Taylor series, Taylor series expansion, 8, 98, 114, 115, 117–120, 146, 147
- Temperature profile, 20, 21, 26, 51, 52, 54, 56, 58, 66, 77, 78, 84, 86, 125, 143, 144
- Thermal conductivity, 22, 23, 59, 63–65, 72, 75, 77–79, 86, 87, 143, 161, 164
- Toluene, 54–57, 127
- Transient regime, transient state, ix, 2, 13, 16, 41–44, 79, 83, 113, 136, 137, 156
- Tubular reactor, 1, 31, 74, 80, 83, 85, 87, 142, 156

- V**
- Vector, 93, 99, 102, 103, 153
- Visual basic for applications (VBA), viii, ix, 121, 129–144, 158, 159
- Volume balance, 10, 13, 16, 17, 21

- W**
- Workbook, 135