

Contents

Preface — V

Introduction — VII

Part I: Applied matrix algebra

1	Matrices and linear algebraic equations — 3
1.1	Simultaneous linear equations — 3
1.2	Review of basic matrix operations — 4
1.2.1	Matrix addition and subtraction — 5
1.2.2	Matrix multiplication — 5
1.2.3	Special matrices — 6
1.3	Elementary row operations and row echelon form of a matrix — 7
1.3.1	Representation of elementary row operations — 8
1.4	Rank of a matrix and condition for existence of solutions — 10
1.4.1	The homogeneous system $\mathbf{A}\mathbf{u} = \mathbf{0}$ — 10
1.4.2	The inhomogeneous system $\mathbf{A}\mathbf{u} = \mathbf{b}$ — 12
1.5	Gaussian elimination and LU decomposition — 15
1.5.1	Lower and upper triangular systems — 15
1.5.2	Gaussian elimination — 16
1.5.3	LU decomposition/factorization — 18
1.6	Inverse of a square matrix — 19
1.6.1	Properties of inverse — 19
1.6.2	Calculation of inverse — 20
1.7	Vector-matrix formulation of some chemical engineering problems — 21
1.7.1	Batch reactor: evolution equations with multiple reactions — 22
1.7.2	Continuous-flow stirred tank reactor (CSTR): transient and steady-state models with multiple reactions — 24
1.7.3	Two interacting tank system: transient model for mixing with in- and outflows — 25
1.7.4	Models for transient diffusion, convection and diffusion-convection (compartment models) — 27
1.8	Application of elementary matrix concepts — 30
1.9	Application of computer algebra and symbolic manipulation — 33
1.9.1	Example 1: mass transfer disguised matrix for a five species system — 35
1.9.2	Example 2: mass transfer disguised matrix for a ten species system — 36

2 Determinants — 44

- 2.1 Definition of determinant — 44
- 2.2 Properties of the determinant — 46
- 2.3 Computation of determinant by pivotal condensation — 48
- 2.4 Minors, cofactors and Laplace's expansion — 49
- 2.4.1 Classical adjoint and inverse matrices — 51
- 2.5 Determinant of the product of two matrices — 52
- 2.6 Rank of a matrix defined in terms of determinants — 53
- 2.7 Solution of $\mathbf{A}\mathbf{u} = \mathbf{0}$ and $\mathbf{A}\mathbf{u} = \mathbf{b}$ by Cramer's rule — 54
- 2.8 Differentiation of a determinant — 56
- 2.9 Applications of determinants — 57

3 Vectors and vector expansions — 65

- 3.1 Linear dependence, basis and dimension — 66
- 3.2 Dot or scalar product of vectors — 67
- 3.3 Linear algebraic equations — 70
- 3.4 Applications of vectors and vector expansions — 72
- 3.4.1 Stoichiometry — 72
- 3.4.2 Dimensional analysis — 74
- 3.5 Application of computer algebra and symbolic manipulation — 76
- 3.5.1 Determination of independent reactions — 76

4 Solution of linear equations by eigenvector expansions — 82

- 4.1 The matrix eigenvalue problem — 82
- 4.2 Left eigenvectors and the adjoint eigenvalue problem (eigenrows) — 85
- 4.3 Properties of eigenvectors/eigenrows — 87
- 4.4 Orthogonal and biorthogonal expansions — 96
- 4.4.1 Vector expansions — 96
- 4.4.2 Orthogonal expansions — 96
- 4.4.3 Biorthogonal expansions — 98
- 4.5 Solution of linear equations using eigenvector expansions — 99
- 4.5.1 Solution of linear algebraic equations $\mathbf{A}\mathbf{u} = \mathbf{b}$ — 99
- 4.5.2 (*Fredholm alternative*): solution of linear algebraic equations $\mathbf{A}\mathbf{u} = \mathbf{b}$ when \mathbf{A} is singular — 100
- 4.5.3 Linear coupled first-order differential equations with constant coefficients — 102
- 4.5.4 Linear coupled inhomogeneous equations — 104
- 4.5.5 A second-order vector initial value problem — 105
- 4.5.6 Multicomponent diffusion and reaction in a catalyst pore — 107
- 4.6 Diagonalization of matrices and similarity transforms — 109
- 4.6.1 Examples of similarity transforms — 110
- 4.6.2 Canonical form — 112

4.6.3	Similarity transform when $\mathbf{A}^T = \mathbf{A}$ — 114
5	Solution of linear equations containing a square matrix — 122
5.1	Cayley–Hamilton theorem — 122
5.2	Functions of matrices — 125
5.3	Formal solutions of linear differential equations containing a square matrix — 129
5.4	Sylvester’s theorem — 131
5.5	Spectral theorem — 135
5.6	Projections operators and vector projections — 142
5.6.1	Standard basis and projection in \mathbb{R}^2 — 142
5.6.2	Nonorthogonal projections — 143
5.6.3	Geometric interpretation with real and negative eigenvalues — 145
5.6.4	Geometrical interpretation with complex eigenvalues with negative real part — 148
5.6.5	Geometrical interpretation with one zero eigenvalue — 149
5.6.6	Physical and geometrical interpretation of transient behavior of interacting tank systems for various initial conditions — 150
6	Generalized eigenvectors and canonical forms — 160
6.1	Repeated eigenvalues and generalized eigenvectors — 160
6.1.1	Linearly independent solutions of $\frac{du}{dt} = \mathbf{A}u$ with repeated eigenvalues — 161
6.1.2	Examples of repeated EVs and GEVs — 162
6.2	Jordan canonical forms — 164
6.3	Multiple eigenvalues and generalized eigenvectors — 166
6.4	Determination of $f(\mathbf{A})$ when \mathbf{A} has multiple eigenvalues — 173
6.5	Application of Jordan canonical form to differential equations — 175
7	Quadratic forms, positive definite matrices and other applications — 179
7.1	Quadratic forms — 179
7.2	Positive definite matrices — 183
7.3	Rayleigh quotient — 184
7.4	Maxima/minima for a function of several variables — 185
7.5	Linear difference equations — 190
7.6	Generalized inverse and least square solutions — 196

Part II: Abstract vector space concepts

8	Vector space over a field — 207
8.1	Definition of a field — 207

- 8.2 Definition of an abstract vector or linear space: — 208
- 8.2.1 Subspaces — 209
- 8.2.2 Bases and dimension — 210
- 8.2.3 Coordinates — 211

9 Linear transformations — 214

- 9.1 Definition of a linear transformation — 214
- 9.2 Matrix representation of a linear transformation — 216
- 9.2.1 Change of basis — 221
- 9.2.2 Kernel and range of a linear transformation — 222
- 9.2.3 Relation to linear equations — 223
- 9.2.4 Isomorphism — 224
- 9.2.5 Inverse of a linear transformation — 225

10 Normed and inner product vector spaces — 229

- 10.1 Definition of normed linear spaces — 229
- 10.2 Inner product vector spaces — 231
- 10.2.1 Gram–Schmidt orthogonalization procedure — 236
- 10.3 Linear functionals and adjoints — 238

11 Applications of finite-dimensional linear algebra — 253

- 11.1 Weighted dot/inner product in \mathbb{R}^n — 253
- 11.2 Application of weighted inner product to interacting tank systems — 258
- 11.3 Application of weighted inner product to monomolecular kinetics — 262

Part III: Linear ordinary differential equations-initial value problems, complex variables and laplace transform

12 The linear initial value problem — 277

- 12.1 The vector initial value problem — 277
- 12.2 The n -th order initial value problem — 280
- 12.2.1 The n -th order inhomogeneous equation — 284
- 12.3 Linear IVPs with constant coefficients — 286

13 Linear systems with periodic coefficients — 292

- 13.1 Scalar equation with a periodic coefficient — 292
- 13.2 Vector equation with periodic coefficient matrix — 295

14 Analytic solutions, adjoints and integrating factors — 302

14.1	Analytic solutions —	302
14.2	Adjoins and integrating factors —	307
14.2.1	First-order equation —	307
14.2.2	Second-order equation —	308
14.3	Relationship between solutions of $Lu = 0$ and $L^*v = 0$ —	310
14.4	Vector initial value problem —	310
15	Introduction to the theory of functions of a complex variable —	318
15.1	Complex valued functions —	318
15.1.1	Algebraic operations with complex numbers —	318
15.1.2	Polar form of complex numbers —	318
15.1.3	Roots of complex numbers —	320
15.1.4	Complex-valued functions —	320
15.2	Limits, continuity and differentiation —	321
15.2.1	Limits —	321
15.2.2	Continuity —	321
15.2.3	Derivative —	321
15.2.4	The Cauchy–Riemann equations —	322
15.2.5	Some elementary functions of a complex variable —	323
15.2.6	Zeros and singular points of complex-valued functions —	325
15.3	Complex integration, Cauchy’s theorem and integral formulas —	326
15.3.1	Simply and multiply connected domains —	327
15.3.2	Contour integrals and traversal of a closed path —	327
15.3.3	Cauchy’s theorem —	328
15.3.4	Cauchy’s integral formulas —	330
15.4	Infinite series: Taylor’s and Laurent’s series —	332
15.4.1	Taylor’s series —	333
15.4.2	Practical methods of obtaining power series —	334
15.4.3	Laurent series —	334
15.5	The residue theorem and integration by the method of residues —	335
15.5.1	Other methods for evaluating residues —	338
15.5.2	Residue theorem —	340
16	Series solutions and special functions —	344
16.1	Series solution of a first-order ODE —	344
16.2	Ordinary and regular singular points —	345
16.3	Series solutions of second-order ODEs —	350
16.4	Special functions defined by second-order ODEs —	353
16.4.1	Airy equation —	353
16.4.2	Bessel equation —	354
16.4.3	Modified Bessel equation —	354
16.4.4	Spherical Bessel equation —	356

16.4.5	Legendre equation —	357
16.4.6	Associated Legendre equation —	358
16.4.7	Hermite's equation —	359
16.4.8	Laguerre's equation —	360
16.4.9	Chebyshev's equation —	360
17	Laplace transforms —	361
17.1	Definition of Laplace transform —	361
17.2	Properties of Laplace transform —	363
17.2.1	Examples of Laplace transform —	366
17.3	Inversion of Laplace transform —	369
17.3.1	Bromwich's complex inversion formula —	371
17.4	Solution of linear differential equations by Laplace transform —	374
17.4.1	Initial value problems with constant coefficients —	374
17.4.2	Elementary derivation of Heaviside's formula —	377
17.4.3	Two-point boundary value problems —	381
17.4.4	Linear ODEs with variable coefficients: —	382
17.4.5	Simultaneous ODEs with constant coefficients —	383
17.5	Solution of linear differential/partial differential equations by Laplace transform —	384
17.5.1	Heat transfer in a finite slab —	385
17.5.2	TAP reactor model —	386
17.5.3	Dispersion of tracers in unidirectional flow —	389
17.5.4	Unsteady-state operation of a packed-bed —	398
17.6	Control system with delayed feedback —	404
17.6.1	PI control with delayed feedback —	404

Part IV: Linear ordinary differential equations-boundary value problems

18	Two-point boundary value problems —	423
18.1	The adjoint differential operator —	423
18.1.1	The Lagrange identity for an n -th order linear differential operator —	426
18.2	Two-point boundary value problems —	428
18.3	The adjoint boundary value problem —	434
18.3.1	Adjoint BCs and conditions for self-adjointness of the BVP —	438
19	The nonhomogeneous BVP and Green's function —	445
19.1	Introduction to Green's function —	445
19.2	Green's function for second-order self-adjoint TPBVP —	447

- 19.3 Properties of the Green's function for the second-order self-adjoint BVP — **454**
- 19.4 Green's function for the n -th order TPBVP — **458**
- 19.4.1 Physical interpretation of the Green's function — **466**
- 19.5 Solution of TPBVP with inhomogeneous boundary conditions — **471**

- 20 Eigenvalue problems for differential operators — 478**
- 20.1 Definition of eigenvalue problems — **478**
- 20.2 Determination of the eigenvalues — **480**
- 20.2.1 Relationship between the n -th order eigenvalue problem and the vector eigenvalue problem — **481**
- 20.3 Properties of the characteristic equation — **483**

- 21 Sturm–Liouville theory and eigenfunction expansions — 496**
- 21.1 Sturm–Liouville theory — **496**
- 21.2 Eigenfunction expansions — **503**
- 21.3 Convergence in function spaces and introduction to Banach and Hilbert spaces — **505**
- 21.3.1 Cauchy sequence — **505**
- 21.3.2 Riemann and Lebesgue integration — **506**
- 21.3.3 Banach and Hilbert spaces — **506**
- 21.3.4 Convergence theorems for eigenfunction expansions — **507**
- 21.3.5 Fourier series (eigenfunction expansions) and Parseval's theorem — **508**
- 21.3.6 Example of Fourier series (eigenfunction expansions) — **509**
- 21.3.7 Fourier series (eigenfunction expansion) of the Green's function — **514**

- 22 Introduction to the solution of linear integral equations — 520**
- 22.1 Introduction — **520**
- 22.2 Transformation of an IVP into an IE of Volterra type — **521**
- 22.3 Transformation of TPBVP into an IE of Fredholm type — **523**
- 22.4 Solution of Fredholm integral equations with separable kernels — **524**
- 22.4.1 Homogeneous equation — **524**
- 22.4.2 Inhomogeneous equation — **526**
- 22.5 Solution procedure for Volterra integral equations of the second kind — **530**
- 22.5.1 Method of successive approximation — **530**
- 22.5.2 Adomian decomposition method — **533**
- 22.6 Solution procedure for Volterra integral equations of the first kind — **534**
- 22.6.1 Differentiation approach — **534**
- 22.6.2 Integration approach — **535**

22.7	Volterra integral equations with convolution kernel —	536
22.8	Fredholm integral equations of the second kind —	538
22.8.1	Solution by successive substitution —	538
22.8.2	Solution by Adomian decomposition method —	539
22.9	Fredholm integral equations with symmetric kernels —	540
22.10	Adjoint operator and Fredholm alternative —	542
22.11	Solution of FIE of the second kind with symmetric kernels —	543

Part V: Fourier transforms and solution of boundary and initial-boundary value problems

23	Finite Fourier transforms —	551
23.1	Definition and general properties —	551
23.1.1	Example 1 (solution of Poisson's equation) —	552
23.1.2	Example 2 (solution of heat/diffusion equation) —	553
23.1.3	Example 3 (solution of the wave equation) —	553
23.2	Application of FFT for BVPs in 1D —	554
23.2.1	Example 1 (Poisson's equation in 1-D) —	554
23.2.2	Example 2: higher-order boundary value problems (coupled equations) in 1D —	559
23.3	FFT for parabolic, hyperbolic and elliptic PDEs (two independent variables) —	560
23.3.1	Example 3: heat/diffusion equation in a finite domain —	560
23.3.2	Example 4: Green's function for the heat/diffusion equation in a finite domain —	565
23.3.3	Example 5: heat/diffusion equation in the finite domain with time dependent boundary condition —	566
23.3.4	Example 6: heat/diffusion equation in a finite domain with general initial and boundary conditions —	569
23.3.5	Example 7 (wave equation) —	569
23.3.6	Example 8 (Poisson's equation in 2-D) —	571
23.4	Additional applications of FFT in rectangular coordinates —	576
23.4.1	Example 9 (diffusion and reaction in a catalyst cube) —	576
23.4.2	Example 10 (axial dispersion model) —	579
23.4.3	Example 11 (Fourier's ring problem) —	588
23.4.4	Example 12: (coupled equations) reaction–diffusion equations —	590
24	Fourier transforms on infinite intervals —	598
24.1	Fourier transform on $(-\infty, \infty)$ —	598
24.1.1	Fourier integral formula —	600
24.2	Finite Fourier transform and the Fourier transform —	602

24.2.1	Physical interpretation — 604
24.2.2	Properties of the Fourier transform — 605
24.2.3	Moments theorem for Fourier transform — 607
24.2.4	Fourier transform in spatial and cyclic frequencies — 609
24.2.5	Fourier transform and Plancherel's theorem — 611
24.3	Solution of BVPs and IBVPs in infinite intervals using the FT — 612
24.3.1	Heat equation in an infinite rod — 612
24.3.2	Solution of the heat equation in semi-infinite domain — 618
24.3.3	Transforms on the half-line — 623
24.3.4	Solution of heat/diffusion equation with radiation BC — 625
24.3.5	Fourier transforms on an infinite domain: solution of the wave equation — 628
24.3.6	Laplace's equation in infinite and semi-infinite domains — 631
24.3.7	Multiple Fourier transforms — 635
24.4	Relationship between Fourier and Laplace transforms — 637
25	Fourier transforms in cylindrical and spherical geometries — 642
25.1	BVP and IBVP in cylindrical and spherical geometries — 642
25.1.1	Cylindrical geometries — 643
25.1.2	Spherical geometries — 644
25.1.3	3D eigenvalue problems in cylindrical geometries — 646
25.1.4	3D eigenvalue problems in spherical geometries — 648
25.2	FFT method for 1D problems in spherical and cylindrical geometries — 651
25.2.1	Steady-state diffusion and reaction in a cylindrical catalyst — 651
25.2.2	Transient heat/mass transfer in an 1D infinite cylinder — 654
25.2.3	Steady-state 1D diffusion and reaction in a spherical catalyst particle — 658
25.2.4	Transient 1D heat conduction in a spherical geometry — 660
25.3	2D and 3D problems in cylindrical geometry — 662
25.3.1	Solution of Laplace's equation inside a unit circle — 662
25.3.2	Vibration of a circular membrane — 664
25.3.3	Three-dimensional problems in cylindrical geometry — 669
25.4	2D and 3D problems in spherical geometry — 671
25.4.1	Poisson's equation in a sphere — 671

Part VI: Formulation and solution of some classical chemical engineering problems

26	The classical Graetz–Nusselt problem — 683
26.1	Model formulations and formal solution — 683

26.1.1	Analysis of constant wall temperature boundary condition —	684
26.2	Parallel plate with fully-developed velocity profile —	688
26.3	Circular channel with fully-developed velocity profile —	690
27	Friction factors for steady-state laminar flow in ducts —	695
27.1	Model formulations and formal solution —	695
27.2	Specific example: parallel plates —	697
27.2.1	Direct solution —	697
27.2.2	FFT approach —	698
27.3	Specific case: elliptical ducts —	699
28	Multicomponent diffusion and reaction —	704
28.1	Generalized effectiveness factor problem —	704
28.1.1	Effectiveness factor —	706
28.1.2	Sherwood number (for internal mass-transfer coefficient) —	707
28.1.3	Exact expressions for Sh_i for some common geometries —	708
28.2	Multicomponent diffusion and reaction in the washcoat layer of a monolith reactor —	709
28.3	Isothermal monolith reactor model for multiple reactions —	712
28.3.1	Example: reversible sequential reactions —	713
29	Packed-bed chromatography —	721
29.1	Model formulation —	721
29.1.1	Adsorption isotherm —	722
29.1.2	Nondimensional form —	724
29.1.3	Limiting case: $p \rightarrow 0$ —	725
29.2	Similarity with heat transfer in packed-beds —	727
29.3	Impact of interphase mass transfer —	727
29.3.1	Pseudo-homogeneous model —	729
29.4	Solution of the hyperbolic model by Laplace transform —	729
29.5	Chromatography model with dispersion in fluid phase —	731
29.5.1	Limiting cases —	732
29.5.2	Lumped model for $p \rightarrow 0$ —	732
29.5.3	Lumped model for $p > 0$ —	733
29.5.4	Chromatography model with dispersion in fluid phase for unit impulse input —	735
29.5.5	Finite stage chromatography model —	736
29.6	Impact of intraparticle gradients —	737
30	Stability of transport and reaction processes —	740
30.1	Lapwood convection in a porous rectangular box —	740
30.1.1	Model formulation —	740

30.1.2	Conduction state and its stability —	742
30.1.3	Neutral curve and critical Ra_d —	745
30.2	Chemical reactor stability and dynamics —	748
30.2.1	Model of a cooled CSTR —	749
30.2.2	Dimensionless form of model for a single reaction —	750
30.2.3	Stability analysis —	751

Bibliography — 759

Index — 761