

Contents

<i>Preface</i>	<i>page</i> xiii
<i>Acknowledgments</i>	xiv
1 Introduction	1
1.1 Brief history of meteorological sciences	1
1.2 Brief history of air-pollution science	5
1.3 The merging of air-pollution and meteorological sciences	6
1.4 Weather, climate, and air pollution	6
1.5 Scales of motion	8
1.6 Atmospheric processes	8
2 Atmospheric structure, composition, and thermodynamics	12
2.1 Pressure, density, and composition	12
2.2 Temperature structure	18
2.3 Equation of state	28
2.4 Changes of pressure with altitude	34
2.5 Water in the atmosphere	37
2.6 First law of thermodynamics	47
2.7 Summary	57
2.8 Problems	58
2.9 Computer programming practice	60
3 The continuity and thermodynamic energy equations	61
3.1 Definitions	61
3.2 Continuity equations	65
3.3 Expanded continuity equations	68
3.4 Thermodynamic energy equation	78
3.5 Summary	80
3.6 Problems	80
3.7 Computer programming practice	81
4 The momentum equation in Cartesian and spherical coordinates	82
4.1 Horizontal coordinate systems	82
4.2 Newton's second law of motion	87
4.3 Applications of the momentum equation	111
4.4 Summary	135

Contents

4.5	Problems	136
4.6	Computer programming practice	137
5	Vertical-coordinate conversions	138
5.1	Hydrostatic and nonhydrostatic models	138
5.2	Altitude coordinate	143
5.3	Pressure coordinate	143
5.4	Sigma-pressure coordinate	151
5.5	Sigma-altitude coordinate	160
5.6	Summary	167
5.7	Problems	167
5.8	Computer programming practice	168
6	Numerical solutions to partial differential equations	169
6.1	Ordinary and partial differential equations	169
6.2	Operator splitting	170
6.3	Advection–diffusion equations	171
6.4	Finite-difference approximations	172
6.5	Series expansion methods	192
6.6	Finite-volume methods	199
6.7	Advection schemes used in air-quality models	199
6.8	Summary	202
6.9	Problems	202
6.10	Computer programming practice	203
7	Finite-differencing the equations of atmospheric dynamics	204
7.1	Vertical model grid	204
7.2	The continuity equation for air	208
7.3	The species continuity equation	211
7.4	The thermodynamic energy equation	213
7.5	The horizontal momentum equations	214
7.6	The hydrostatic equation	221
7.7	Order of calculations	222
7.8	Time-stepping schemes	222
7.9	Summary	224
7.10	Problems	224
7.11	Computer programming practice	225
7.12	Modeling project	225
8	Boundary-layer and surface processes	228
8.1	Turbulent fluxes of momentum, energy, and moisture	228
8.2	Friction wind speed	230
8.3	Surface roughness lengths	231
8.4	Parameterizations of kinematic turbulent fluxes	235
8.5	Eddy diffusion above the surface layer	250
8.6	Ground surface temperature and soil moisture	254

Contents

8.7	Summary	271
8.8	Problems	271
8.9	Computer programming practice	272
9	Radiative energy transfer	273
9.1	Energy transfer processes	273
9.2	Electromagnetic spectrum	275
9.3	Light processes	283
9.4	Absorption and scattering by gases and particles	290
9.5	Visibility	313
9.6	Optical depth	316
9.7	Solar zenith angle	317
9.8	The radiative transfer equation	320
9.9	Summary	334
9.10	Problems	334
9.11	Computer programming practice	335
10	Gas-phase species, chemical reactions, and reaction rates	336
10.1	Atmospheric gases and their molecular structures	336
10.2	Chemical reactions and photoprocesses	342
10.3	Reaction rates	344
10.4	Reaction rate coefficients	346
10.5	Sets of reactions	351
10.6	Stiff systems	353
10.7	Summary	355
10.8	Problems	355
10.9	Computer programming practice	356
11	Urban, free-tropospheric, and stratospheric chemistry	357
11.1	Free-tropospheric photochemistry	357
11.2	Urban photochemistry	375
11.3	Stratospheric photochemistry	393
11.4	Summary	415
11.5	Problems	416
11.6	Computer programming practice	417
12	Methods of solving chemical ordinary differential equations	418
12.1	Characteristics of chemical ODEs	418
12.2	Analytical solutions to ODEs	421
12.3	Taylor series solution to ODEs	421
12.4	Forward Euler solution to ODEs	422
12.5	Backward Euler solution to ODEs	424
12.6	Simple exponential and quasi-steady-state solutions to ODEs	426
12.7	Multistep implicit–explicit (MIE) solution to ODEs	427
12.8	Gear’s solution to ODEs	432
12.9	Family solution to ODEs	439

Contents

12.10 Summary	442
12.11 Problems	442
12.12 Computer programming practice	443
12.13 Modeling project	444
13 Particle components, size distributions, and size structures	446
13.1 Introduction to particles	446
13.2 Aerosol, fog, and cloud composition	447
13.3 Discrete size distributions	449
13.4 Continuous size distributions	454
13.5 Evolution of size distributions over time	462
13.6 Summary	467
13.7 Problems	468
13.8 Computer programming practice	468
14 Aerosol emission and nucleation	470
14.1 Aerosol emission	470
14.2 Nucleation	484
14.3 Summary	492
14.4 Problems	493
14.5 Computer programming practice	493
15 Coagulation	494
15.1 Implicit coagulation	494
15.2 Semiimplicit Coagulation	496
15.3 Comparison with analytical solutions	498
15.4 Coagulation among multiple particle distributions	500
15.5 Particle flow regimes	505
15.6 Coagulation kernel	508
15.7 Summary	522
15.8 Problems	523
15.9 Computer programming practice	523
16 Condensation, evaporation, deposition, and sublimation	525
16.1 Fluxes to and from a single drop	525
16.2 Corrections to growth parameters	528
16.3 Fluxes to a particle with multiple components	540
16.4 Fluxes to a population of particles	540
16.5 Solutions to growth equations	542
16.6 Solving homogeneous nucleation with condensation	545
16.7 Effects of condensation on coagulation	547
16.8 Ice crystal growth	548
16.9 Summary	550
16.10 Problems	550
16.11 Computer programming practice	551

Contents

17	Chemical equilibrium and dissolution processes	553
	17.1 Definitions	553
	17.2 Equilibrium reactions	554
	17.3 Equilibrium relation and coefficients	558
	17.4 Forms of equilibrium-coefficient equations	562
	17.5 Mean binary solute activity coefficients	565
	17.6 Temperature dependence of binary solute activity coefficients	567
	17.7 Mean mixed solute activity coefficients	568
	17.8 The water equation	570
	17.9 Solid formation and deliquescence relative humidity	574
	17.10 Example equilibrium problem	575
	17.11 Mass-flux iteration method	577
	17.12 Analytical equilibrium iteration method	579
	17.13 Equilibrium solver results	582
	17.14 Nonequilibrium between gases and particles	583
	17.15 Summary	594
	17.16 Problems	596
	17.17 Computer programming practice	596
18	Cloud thermodynamics and dynamics	598
	18.1 Fog and cloud types and formation mechanisms	598
	18.2 Moist adiabatic and pseudoadiabatic processes	602
	18.3 Cloud development by free convection	606
	18.4 Entrainment	608
	18.5 Vertical momentum equation in a cloud	610
	18.6 Convective available potential energy	612
	18.7 Cumulus parameterizations	612
	18.8 Cloud microphysics	614
	18.9 Summary	642
	18.10 Problems	643
	18.11 Computer programming practice	643
19	Irreversible aqueous chemistry	645
	19.1 Significance of aqueous chemical reactions	645
	19.2 Mechanisms of converting S(IV) to S(VI)	646
	19.3 Diffusion within a drop	652
	19.4 Solving growth and aqueous chemical ODEs	654
	19.5 Summary	659
	19.6 Problems	659
	19.7 Computer programming practice	660
20	Sedimentation, dry deposition, and air–sea exchange	661
	20.1 Sedimentation	661
	20.2 Dry deposition	665

Contents

20.3	Dry deposition and sedimentation calculations	670
20.4	Air–sea flux of carbon dioxide and other gases	672
20.5	Summary	679
20.6	Problems	679
20.7	Computer programming practice	679
21	Model design, application, and testing	681
21.1	Steps in model formulation	681
21.2	Example model simulations	700
21.3	Summary	707
21.4	Problems	707
21.5	Computer programming practice	707
Appendix A	Conversions and constants	709
A.1	Distance conversions	709
A.2	Volume conversions	709
A.3	Mass conversions	709
A.4	Temperature conversions	710
A.5	Force conversions	710
A.6	Pressure conversions	710
A.7	Energy conversions	710
A.8	Power conversions	710
A.9	Speed conversions	710
A.10	Constants	711
Appendix B	Tables	714
B.1	Standard atmospheric variables versus altitude	714
B.2	Solar irradiance at the top of the atmosphere	715
B.3	Chemical symbols and structures of gases	716
B.4	Gas-phase reactions	728
B.5	Chemicals involved in equilibrium and aqueous reactions	738
B.6	Thermodynamic data	740
B.7	Equilibrium reactions and rate coefficients	741
B.8	Irreversible aqueous reactions	743
B.9	Solute activity coefficient data	746
B.10	Water activity data	748
B.11	Surface resistance data	749
B.12	More surface resistance data	751
<i>References</i>		752
<i>Index</i>		784