

# Contents

Acknowledgements	vii
Preface	ix
1. Introduction	1
1.1 What is Indoor Air Pollution	2
1.2 Ventilation Systems	2
1.3 Exposure Risks	3
1.4 Numerical Modeling of Indoor Air Flow	5
1.5 Comments	7
2. Fluid Flow Fundamentals	9
2.1 Conservation Equations	9
2.2 Ideal Fluids	11
2.2.1 Conformal mapping	16
2.2.2 Schwarz–Christoffel transform	19
2.2.3 Numerical mapping	23
2.2.4 Superposition for stream functions	24
2.3 Turbulence	26
2.4 Species Transport	30
2.5 Comments	32
3. Contaminant Sources	33
3.1 Types of Contaminants	33
3.2 Units	35
3.3 Materials	36
3.4 Typical Operations	38
3.5 The Diffusion Equation	39
3.6 Diffusion in Air	41
3.7 Evaporation of Droplets	43
3.8 Resuspension of Particulate	46
3.9 Coagulation of Particulate	48
3.10 Comments	49
4. Assessment Criteria	51
4.1 Exposure	51
4.2 Economics	54
4.3 Comments	56

5. Simple Modeling Techniques	57
5.1 Analytical Tools	57
5.2 Advection Model	65
5.3 Box Model	67
5.4 Comments	75
6. Dynamics of Particles, Gases and Vapors	77
6.1 Drag, Shape, and Size of Particles	77
6.2 Particle Motion	80
6.2.1 Deposition of particulate with aerodynamic diameters $> 1\mu$ by settling	84
6.2.2 Particle motion in electrostatic field	86
6.2.3 Particle motion induced by temperature gradients	87
6.2.4 Thermophoretic motion for gases and particles with diameter less than the molecular mean free path	87
6.2.5 Thermophoretic transport for particles with diameter greater than the molecular mean free path	87
6.3 Particle Flow in Inlets and Flanges	88
6.4 Comments	91
7. Numerical Modeling – Conventional Techniques	93
7.1 Finite Difference Method	94
7.1.1 Explicit	97
7.1.2 Implicit	97
7.1.3 Upwinding	98
7.2 Finite Volume Method	104
7.2.1 FDM	109
7.2.2 FVM	109
7.3 The Finite Element Method	112
7.3.1 One-dimensional elements	115
7.3.1.1 Linear element	115
7.3.1.2 Quadratic and higher order elements	116
7.3.2 Two-dimensional elements	122
7.3.2.1 Triangular elements	122
7.3.2.2 Quadrilateral elements	124
7.3.2.3 Isoparametric elements	125
7.3.3 Three-dimensional elements	128
7.3.4 Quadrature	130
7.3.5 Time dependence	132
7.3.6 Petrov–Galerkin method	133
7.3.7 Mesh generation	135
7.3.8 Bandwidth	140
7.3.9 Adaptation	141

7.3.9.1 Element subdivision .....	145
7.4 Further CFD Examples .....	150
7.5 Model Verification and Validation .....	153
7.6 Comments .....	156
<b>8. Numerical Modeling – Advanced Techniques</b> .....	<b>159</b>
8.1 Boundary Element Method .....	160
8.2 Lagrangian Particle Technique .....	171
8.3 Particle-in-cell .....	175
8.4 Meshless Method .....	182
8.4.1 Application of meshless methods .....	187
8.4.1.1 Smoothed particle hydrodynamics (SPH) techniques including Kernel Particle Methods (RKPM), and general kernel reproduction methods (GKR) .....	187
8.4.1.2 Meshless Petrov–Galerkin (MLPG) methods including moving least squares (MLS), point interpolation methods (PIM), and hp-clouds .....	188
8.4.1.3 Local radial point interpolation methods (LRPIM) using finite difference representations .....	189
8.4.1.4 Radial basis functions (RBFs) .....	189
8.4.2 Example cases – Heat Transfer .....	196
8.4.2.1 Heat transfer in a 2-D plate .....	196
8.4.2.2 Singular point in a 2-D domain .....	197
8.4.2.3 Heat transfer within an irregular domain .....	199
8.4.2.4 Natural Convection .....	201
8.5 Molecular Modeling .....	208
8.6 Boundary Conditions for Mass Transport Analysis .....	212
8.7 Comments .....	215
<b>9. Turbulence Modeling</b> .....	<b>217</b>
9.1 Brief History of Turbulence Formulation .....	217
9.2 Physical Model .....	221
9.2.1 Turbulent flow .....	222
9.2.2 Two-equation turbulence closure models .....	224
9.2.2.1 Two-equation $k-\epsilon$ .....	225
9.2.2.2 Two-equation $k-w$ .....	226
9.2.3 Large Eddy Simulation (LES) .....	227
9.2.4 Direct Numerical Simulation (DNS) .....	229
9.2.5 Turbulent transport of energy or enthalpy .....	230
9.2.6 Derivation of enthalpy transport .....	231
9.2.7 Turbulent energy transport .....	236
9.2.8 Turbulent transport species .....	237
9.2.9 Coupled fluid-thermal flow .....	237

9.3 Numerical Modeling .....	239
9.3.1 Projection algorithm .....	240
9.3.2 Finite volume approach .....	243
9.3.3 Finite element approach .....	245
9.3.3.1 Weak forms of the governing equations.....	246
9.3.3.2 Matrix equations.....	250
9.3.3.3 Time advancement of the explicit/implicit matrix equations .....	252
9.3.3.4 Mass lumping .....	253
9.3.3.5 General numerical solution.....	254
9.4 Stability and Time Dependent Solution .....	255
9.5 Boundary Conditions.....	256
9.5.1 Boundary conditions for velocity under decomposition.....	257
9.5.1.1 Viscous boundary condition for velocity.....	258
9.5.2 Boundary conditions for pressure and velocity correction....	258
9.5.3 Boundary conditions for turbulent kinetic energy and specific dissipation rate .....	259
9.5.4 Boundary conditions for thermal and species transport .....	262
9.5.5 Thermal and species flux calculation in the presence of Dirichlet boundaries .....	263
9.6 Validation of Turbulence Models .....	264
9.7 Comments .....	274
10. Homeland Security Issues .....	277
10.1 Introduction.....	277
10.2 Potential Hazards .....	278
10.2.1 Prevention and protection.....	283
10.3 A Simple Model .....	286
10.4 Other Indoor Air Quality Models .....	296
10.4.1 CONTAM 2.4 (NIST).....	296
10.4.2 I-BEAM (EPA) .....	298
10.4.3 COMIS-MIAQ (APTG-LBNL) .....	299
10.4.4 FLOVENT (Flomerics, Inc.) .....	300
10.5 Comments .....	301
Appendix A Diffusion Coefficients in Gas .....	303
Appendix B 2-D Office Simulations: COMSOL and ANSWER Software .....	309
Bibliography .....	323
<i>Index</i> .....	341