

Contents

Preface	xi
Acknowledgements	xiii
1 Introduction	1
1.1 What is CFD?	1
1.2 How does a CFD code work?	2
1.3 Problem solving with CFD	4
1.4 Scope of this book	6
2 Conservation laws of fluid motion and boundary conditions	9
2.1 Governing equations of fluid flow and heat transfer	9
2.1.1 Mass conservation in three dimensions	10
2.1.2 Rates of change following a fluid particle and for a fluid element	12
2.1.3 Momentum equation in three dimensions	14
2.1.4 Energy equation in three dimensions	16
2.2 Equations of state	20
2.3 Navier–Stokes equations for a Newtonian fluid	21
2.4 Conservative form of the governing equations of fluid flow	24
2.5 Differential and integral forms of the general transport equations	24
2.6 Classification of physical behaviours	26
2.7 The role of characteristics in hyperbolic equations	29
2.8 Classification method for simple PDEs	32
2.9 Classification of fluid flow equations	33
2.10 Auxiliary conditions for viscous fluid flow equations	35
2.11 Problems in transonic and supersonic compressible flows	36
2.12 Summary	38
3 Turbulence and its modelling	40
3.1 What is turbulence?	40
3.2 Transition from laminar to turbulent flow	44
3.3 Descriptors of turbulent flow	49

3.4	Characteristics of simple turbulent flows	52
3.4.1	Free turbulent flows	53
3.4.2	Flat plate boundary layer and pipe flow	57
3.4.3	Summary	61
3.5	The effect of turbulent fluctuations on properties of the mean flow	61
3.6	Turbulent flow calculations	65
3.7	Reynolds-averaged Navier–Stokes equations and classical turbulence models	66
3.7.1	Mixing length model	69
3.7.2	The k – ε model	72
3.7.3	Reynolds stress equation models	80
3.7.4	Advanced turbulence models	85
3.7.5	Closing remarks – RANS turbulence models	97
3.8	Large eddy simulation	98
3.8.1	Spacial filtering of unsteady Navier–Stokes equations	98
3.8.2	Smagorinsky–Lilly SGS model	102
3.8.3	Higher-order SGS models	104
3.8.4	Advanced SGS models	105
3.8.5	Initial and boundary conditions for LES	106
3.8.6	LES applications in flows with complex geometry	108
3.8.7	General comments on performance of LES	109
3.9	Direct numerical simulation	110
3.9.1	Numerical issues in DNS	111
3.9.2	Some achievements of DNS	113
3.10	Summary	113

4 The finite volume method for diffusion problems 115

4.1	Introduction	115
4.2	Finite volume method for one-dimensional steady state diffusion	115
4.3	Worked examples: one-dimensional steady state diffusion	118
4.4	Finite volume method for two-dimensional diffusion problems	129
4.5	Finite volume method for three-dimensional diffusion problems	131
4.6	Summary	132

5 The finite volume method for convection–diffusion problems 134

5.1	Introduction	134
5.2	Steady one-dimensional convection and diffusion	135
5.3	The central differencing scheme	136
5.4	Properties of discretisation schemes	141
5.4.1	Conservativeness	141
5.4.2	Boundedness	143
5.4.3	Transportiveness	143
5.5	Assessment of the central differencing scheme for convection–diffusion problems	145
5.6	The upwind differencing scheme	146
5.6.1	Assessment of the upwind differencing scheme	149
5.7	The hybrid differencing scheme	151
5.7.1	Assessment of the hybrid differencing scheme	154

5.7.2	Hybrid differencing scheme for multi-dimensional convection–diffusion	154
5.8	The power-law scheme	155
5.9	Higher-order differencing schemes for convection–diffusion problems	156
5.9.1	Quadratic upwind differencing scheme: the QUICK scheme	156
5.9.2	Assessment of the QUICK scheme	162
5.9.3	Stability problems of the QUICK scheme and remedies	163
5.9.4	General comments on the QUICK differencing scheme	164
5.10	TVD schemes	164
5.10.1	Generalisation of upwind-biased discretisation schemes	165
5.10.2	Total variation and TVD schemes	167
5.10.3	Criteria for TVD schemes	168
5.10.4	Flux limiter functions	170
5.10.5	Implementation of TVD schemes	171
5.10.6	Evaluation of TVD schemes	175
5.11	Summary	176

6 Solution algorithms for pressure–velocity coupling in steady flows

179

6.1	Introduction	179
6.2	The staggered grid	180
6.3	The momentum equations	183
6.4	The SIMPLE algorithm	186
6.5	Assembly of a complete method	190
6.6	The SIMPLER algorithm	191
6.7	The SIMPLEC algorithm	193
6.8	The PISO algorithm	193
6.9	General comments on SIMPLE, SIMPLER, SIMPLEC and PISO	196
6.10	Worked examples of the SIMPLE algorithm	197
6.11	Summary	211

7 Solution of discretised equations

212

7.1	Introduction	212
7.2	The TDMA	213
7.3	Application of the TDMA to two-dimensional problems	215
7.4	Application of the TDMA to three-dimensional problems	215
7.5	Examples	216
7.5.1	Closing remarks	222
7.6	Point-iterative methods	223
7.6.1	Jacobi iteration method	224
7.6.2	Gauss–Seidel iteration method	225
7.6.3	Relaxation methods	226
7.7	Multigrid techniques	229
7.7.1	An outline of a multigrid procedure	231
7.7.2	An illustrative example	232
7.7.3	Multigrid cycles	239
7.7.4	Grid generation for the multigrid method	241
7.8	Summary	242

8	The finite volume method for unsteady flows	243
8.1	Introduction	243
8.2	One-dimensional unsteady heat conduction	243
8.2.1	Explicit scheme	246
8.2.2	Crank–Nicolson scheme	247
8.2.3	The fully implicit scheme	248
8.3	Illustrative examples	249
8.4	Implicit method for two- and three-dimensional problems	256
8.5	Discretisation of transient convection–diffusion equation	257
8.6	Worked example of transient convection–diffusion using QUICK differencing	258
8.7	Solution procedures for unsteady flow calculations	262
8.7.1	Transient SIMPLE	262
8.7.2	The transient PISO algorithm	263
8.8	Steady state calculations using the pseudo-transient approach	265
8.9	A brief note on other transient schemes	265
8.10	Summary	266
9	Implementation of boundary conditions	267
9.1	Introduction	267
9.2	Inlet boundary conditions	268
9.3	Outlet boundary conditions	271
9.4	Wall boundary conditions	273
9.5	The constant pressure boundary condition	279
9.6	Symmetry boundary condition	280
9.7	Periodic or cyclic boundary condition	281
9.8	Potential pitfalls and final remarks	281
10	Errors and uncertainty in CFD modelling	285
10.1	Errors and uncertainty in CFD	285
10.2	Numerical errors	286
10.3	Input uncertainty	289
10.4	Physical model uncertainty	291
10.5	Verification and validation	293
10.6	Guidelines for best practice in CFD	298
10.7	Reporting/documentation of CFD simulation inputs and results	300
10.8	Summary	302
11	Methods for dealing with complex geometries	304
11.1	Introduction	304
11.2	Body-fitted co-ordinate grids for complex geometries	305
11.3	Catesian vs. curvilinear grids – an example	306
11.4	Curvilinear grids – difficulties	308

11.5	Block-structured grids	310
11.6	Unstructured grids	311
11.7	Discretisation in unstructured grids	312
11.8	Discretisation of the diffusion term	316
11.9	Discretisation of the convective term	320
11.10	Treatment of source terms	324
11.11	Assembly of discretised equations	325
11.12	Example calculations with unstructured grids	329
11.13	Pressure–velocity coupling in unstructured meshes	336
11.14	Staggered vs. co-located grid arrangements	337
11.15	Extension of the face velocity interpolation method to unstructured meshes	340
11.16	Summary	342

12 CFD modelling of combustion 343

12.1	Introduction	343
12.2	Application of the first law of thermodynamics to a combustion system	344
12.3	Enthalpy of formation	345
12.4	Some important relationships and properties of gaseous mixtures	346
12.5	Stoichiometry	348
12.6	Equivalence ratio	348
12.7	Adiabatic flame temperature	349
12.8	Equilibrium and dissociation	351
12.9	Mechanisms of combustion and chemical kinetics	355
12.10	Overall reactions and intermediate reactions	355
12.11	Reaction rate	356
12.12	Detailed mechanisms	361
12.13	Reduced mechanisms	361
12.14	Governing equations for combusting flows	363
12.15	The simple chemical reacting system (SCRS)	367
12.16	Modelling of a laminar diffusion flame – an example	370
12.17	CFD calculation of turbulent non-premixed combustion	376
12.18	SCRS model for turbulent combustion	380
12.19	Probability density function approach	380
12.20	Beta pdf	382
12.21	The chemical equilibrium model	384
12.22	Eddy break-up model of combustion	385
12.23	Eddy dissipation concept	388
12.24	Laminar flamelet model	388
12.25	Generation of laminar flamelet libraries	390
12.26	Statistics of the non-equilibrium parameter	399
12.27	Pollutant formation in combustion	400
12.28	Modelling of thermal NO formation in combustion	401
12.29	Flamelet-based NO modelling	402
12.30	An example to illustrate laminar flamelet modelling and NO modelling of a turbulent flame	403
12.31	Other models for non-premixed combustion	415
12.32	Modelling of premixed combustion	415
12.33	Summary	416

13	Numerical calculation of radiative heat transfer	417
13.1	Introduction	417
13.2	Governing equations of radiative heat transfer	424
13.3	Solution methods	426
13.4	Four popular radiation calculation techniques suitable for CFD	427
	13.4.1 The Monte Carlo method	427
	13.4.2 The discrete transfer method	429
	13.4.3 Ray tracing	433
	13.4.4 The discrete ordinates method	433
	13.4.5 The finite volume method	437
13.5	Illustrative examples	437
13.6	Calculation of radiative properties in gaseous mixtures	442
13.7	Summary	443
	Appendix A Accuracy of a flow simulation	445
	Appendix B Non-uniform grids	448
	Appendix C Calculation of source terms	450
	Appendix D Limiter functions used in Chapter 5	452
	Appendix E Derivation of one-dimensional governing equations for steady, incompressible flow through a planar nozzle	456
	Appendix F Alternative derivation for the term $(\mathbf{n} \cdot \text{grad } \phi A_i)$ in Chapter 11	459
	Appendix G Some examples	462
	Bibliography	472
	Index	495