An Introduction to Computational Fluid Dynamics

THE FINITE VOLUME METHOD

Second Edition

H K Versteeg and W Malalasekera

PEARSON
Prentice Hall

Harlow, England • London • New York • Boston • San Francisco • Toronto
Sydney • Tokyo • Singapore • Hong Kong • Seoul • Taipei • New Delhi
Cape Town • Madrid • Mexico City • Amsterdam • Munich • Paris • Milan

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 Smagorinksy–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 (n . grad ϕA_i) in Chapter 11 459
Appendix G Some examples 462
Bibliography 472
Index 495