Contents

Part I Introductory Concepts

1 The Role of Combustion Technology in the 21st Century ............. 3
   R.W. Bilger
   1.1 Introduction ......................................................... 3
   1.2 Sustainable Energy ................................................. 6
   1.3 Technology Forecasts .............................................. 7
   1.4 Implications for Combustion Technology ......................... 12
   1.5 Prospects for Advanced Computer Modeling of Combustors ..... 14
   1.6 Concluding Remarks ............................................... 17
   References .............................................................. 17

2 Turbulent Combustion: Concepts, Governing Equations and
   Modeling Strategies .................................................. 19
   Tarek Echekki and Epaminondas Mastorakos
   2.1 Introduction .......................................................... 19
   2.2 Governing Equations ............................................... 22
      2.2.1 Conservation Equations ....................................... 22
      2.2.2 Constitutive Relations, State Equations and Auxiliary
           Relations ........................................................ 24
   2.3 Conventional Mathematical and Computational Frameworks for
       Simulating Turbulent Combustion Flows ......................... 28
      2.3.1 Direct Numerical Simulation (DNS) .......................... 28
      2.3.2 Reynolds-Averaged Navier-Stokes (RANS) .................. 30
      2.3.3 Large-Eddy Simulation (LES) ............................... 32
   2.4 Addressing the Closure Problem .................................. 35
   2.5 Outline of Upcoming Chapters ..................................... 36
   References .............................................................. 37
Part II Recent Advances and Trends in Turbulent Combustion Models

3 The Flamelet Model for Non-Premixed Combustion ..................... 43
Bénédicte Cuenot

3.1 Introduction ............................................. 43
3.2 Fundamental Concepts ..................................... 44
  3.2.1 The Mixture Fraction .................................. 45
  3.2.2 The Flamelet Solution .................................. 46
  3.2.3 The Counterflow Diffusion Flame ....................... 47
  3.2.4 Validity of the Flamelet Approach ..................... 48
3.3 RANS Flamelet Modeling .................................... 49
  3.3.1 Steady Flamelets ...................................... 50
  3.3.2 Transient Flamelets .................................... 53
  3.3.3 Representative Interactive Flamelets (RIF) Model ...... 55
  3.3.4 Eulerian Particle Flamelet Model (EPFM) ................ 56
  3.3.5 Flamelet–Progress Variable (FPV) Models ............... 56
3.4 LES Flamelet Modeling .................................... 58
  3.4.1 Subgrid Scale Modelling ............................... 58
3.5 Conclusion ................................................................ 59
References .................................................................... 59

4 RANS and LES Modelling of Premixed Turbulent Combustion ...... 63
Stewart Cant

4.1 Introduction to Premixed Flames .................................. 63
4.2 Modelling Framework for RANS and LES ...................... 64
  4.2.1 Introduction ............................................. 64
  4.2.2 Regimes of Premixed Turbulent Combustion ............ 65
  4.2.3 Averaging and Filtering .................................. 66
  4.2.4 Modelling Principles ..................................... 68
4.3 Transport Modelling for Premixed Turbulent Flames .......... 70
4.4 Reaction Rate Modelling for Premixed Turbulent Flames .... 71
  4.4.1 Simple Models ........................................... 71
  4.4.2 Flame Surface Density Modelling ....................... 73
  4.4.3 G-equation Modelling .................................... 80
  4.4.4 Scalar Dissipation Rate Modelling ....................... 83
  4.4.5 Other Approaches ....................................... 85
4.5 Future .................................................................. 86
References .................................................................... 87

5 The Conditional Moment Closure Model ............................... 91
A. Kronenburg and E. Mastorakos

5.1 Introduction ................................................... 91
5.2 Methodological Developments in CMC ......................... 93
  5.2.1 The CMC Equations ...................................... 93
  5.2.2 Advances in Second Order Closures .................... 96
10 The Linear-Eddy Model ........................................... 221
Suresh Menon and Alan R. Kerstein
10.1 Motivation ....................................................... 221
10.2 Triplet Map ..................................................... 222
10.3 Map Sizes and Frequency of Occurrence ....................... 223
10.4 Application to Passive Mixing .................................. 225
10.5 Application to Reacting Flows ................................... 226
10.6 Application to Reacting Flows as a Subgrid Model .......... 228
10.6.1 The LEM Subgrid Model ...................................... 231
10.6.2 Large-Scale Advection of the Subgrid Field ................. 232
10.7 LEMLES Applications to Reacting Flows ....................... 237
10.8 Summary and Future Prospects .................................. 243
References .............................................................. 244

11 The One-Dimensional-Turbulence Model ......................... 249
Tarek Echekki, Alan R. Kerstein, and James C. Sutherland
11.1 Motivation ......................................................... 249
11.2 Constant-Property ODT .......................................... 251
11.2.1 Model Formulation .......................................... 251
11.2.2 Numerical Implementation ................................... 255
11.2.3 Generalizations and Couplings .............................. 255
11.2.4 Features of the ODT Representation of Turbulent Flow .. 256
11.3 Applications of ODT in Combustion ............................ 258
11.3.1 Governing Equations ........................................ 258
11.3.2 Stand-Alone ODT Simulations ............................... 261
11.3.3 Hybrid ODTLES ............................................. 265
11.4 Concluding Remarks ............................................. 272
References .............................................................. 274

12 Unsteady Flame Embedding ....................................... 277
Hossam A. El-Asrag and Ahmed F. Ghoniem
12.1 Introduction ...................................................... 278
12.2 Historical Perspective on the Flame Embedding Concept ...... 280
12.3 Elemental Flame Model Formulation ............................ 283
12.4 Numerical Solution for the Elemental Flame Model .......... 286
12.5 UFE LES Sub-grid Combustion Model .......................... 288
12.6 Numerical Results ............................................... 291
12.7 Conclusions .................................................... 296
References .............................................................. 298
Chapter 13: Adaptive Methods for Simulation of Turbulent Combustion
John Bell and Marcus Day

13.1 Introduction
13.2 Mathematical Formulation
13.3 AMR Basic Concepts
  13.3.1 Creating and Managing the Grid Hierarchy
  13.3.2 AMR Discretization
  13.3.3 Hyperbolic Conservation Laws
  13.3.4 Elliptic
  13.3.5 Parabolic Systems
13.4 AMR for Low Mach Number Combustion
13.5 Implementation Issues and Software Design
  13.5.1 Performance of Adaptive Projection
13.6 Application – Lean Premixed Hydrogen Flames
  13.6.1 Background
  13.6.2 Models and Setup
  13.6.3 Simulation Results
13.7 Summary
References

Chapter 14: Wavelet Methods in Computational Combustion
Robert Prosser and R. Stewart Cant

14.1 Introduction
14.2 Wavelet Transforms
  14.2.1 Orthogonal Wavelets
  14.2.2 Biorthogonal Wavelet Transforms
  14.2.3 Second Generation Wavelets
14.3 Wavelets as a Method for DNS
  14.3.1 The Wavelet Representation of the Derivative
  14.3.2 Higher Dimensional Discretizations
14.4 An Application of Wavelets to Reacting Flows
  14.4.1 Governing Equations
14.5 Results
14.6 Conclusions
References

Part IV: Cross-Cutting Science

Chapter 15: Design of Experiments for Gaining Insights and Validating Modeling of Turbulent Combustion
A.R. Masri

15.1 Introduction
15.2 The Turbulent Combustion Domain
15.3 Basic Considerations
  15.3.1 Design Issues
15.3.2 Operational Envelopes ............................... 362
15.3.3 Experimental Considerations ......................... 364
15.3.4 Numerical Considerations ............................ 366
15.4 Case Studies ........................................... 367
15.4.1 The Swirl Stabilised Burner ......................... 367
15.4.2 The Premixed Burner in Vitiated Coflows ............ 370
15.4.3 The Piloted Spray Burner ............................ 372
15.5 Concluding Remarks .................................... 375
References .................................................... 377

16 Uncertainty Quantification in Fluid Flow ....................... 381
Habib N. Najm
16.1 Introduction ........................................... 381
16.1.1 Polynomial Chaos .................................... 384
16.1.2 Challenges in PC UQ Methods ......................... 389
16.2 Polynomial Chaos UQ in Fluid Flow Applications ....... 392
16.2.1 Incompressible Flow ................................ 393
16.2.2 Reacting Flow ....................................... 396
16.2.3 Compressible Flow ................................... 398
16.2.4 Turbulence .......................................... 399
16.3 Closure ............................................... 401
References .................................................... 401

17 Computational Frameworks for Advanced Combustion Simulations . 409
17.1 Introduction ........................................... 409
17.2 Literature Review of Computational Frameworks ........... 410
17.3 The Common Component Architecture ..................... 413
17.3.1 Features of the Common Component Architecture ...... 414
17.4 Computational Facility for Reacting Flow Science ........ 416
17.4.1 Numerical Methods and Capabilities .................. 416
17.4.2 The Need for Componentization ....................... 417
17.5 Computational Investigations Using CCA .................. 420
17.5.1 Fourth-order Combustion Simulations with Adaptive Mesh Refinement ................................ 421
17.5.2 Computational Singular Perturbation and Tabulation ... 425
17.6 Research Topics in Computational Frameworks ............. 431
17.7 Conclusion ............................................ 432
References .................................................... 433

18 The Heterogeneous Multiscale Methods with Application to Combustion .............................. 439
Weinan E, Björn Engquist and Yi Sun
18.1 The Heterogeneous Multiscale Method ...................... 439
18.1.1 The Basic Framework ........................................ 440
18.1.2 The Seamless Algorithm ................................. 443
18.1.3 Stability and Accuracy .................................. 446
18.2 Capturing Macroscale Interface Dynamics .................... 447
  18.2.1 Macroscale Solver: The Interface Tracking Methods .... 447
  18.2.2 Estimating The Macroscale Interface Velocity ...... 448
18.3 HMM Interface Tracking of Combustion Fronts ............. 451
  18.3.1 Majda’s Model ........................................ 451
  18.3.2 Reactive Euler Equations ............................. 454
18.4 Conclusions .................................................. 456
References ......................................................... 457

19 Lattice Boltzmann Methods for Reactive and Other Flows .... 461
Christos E. Frouzakis
19.1 Introduction .................................................. 461
19.2 The Boltzmann Equation ..................................... 463
  19.2.1 Basic Considerations .................................. 463
  19.2.2 Lattice Boltzmann Model .............................. 465
  19.2.3 Variations on the LBM Theme ........................ 470
  19.2.4 Initial and Boundary Conditions ...................... 472
  19.2.5 Computational Cost ................................... 473
19.3 Applications ................................................ 473
  19.3.1 Isothermal Flows ...................................... 473
  19.3.2 Non-Isothermal Flows ................................. 476
  19.3.3 Multicomponent Mixtures ............................. 478
  19.3.4 Reactive Flows ........................................ 479
19.4 Conclusions .................................................. 481
References ......................................................... 482

Index ............................................................. 487