

Table of Contents

1	Introduction, Fundamental Definitions and Phenomena	1
1.1	Introduction	1
1.2	Some Fundamental Definitions	1
1.3	Basic Flame Types	4
1.4	Exercises	8
2	Experimental Investigation of Flames	9
2.1	Velocity Measurements	10
2.2	Density Measurement	11
2.3	Concentration Measurements	13
2.4	Temperature Measurements	18
2.5	Pressure Measurements	20
2.6	Measurement of Particle Sizes	21
2.7	Simultaneous Diagnostics	22
2.8	Exercises	27
3	Mathematical Description of Premixed Laminar Flat Flames	29
3.1	Conservation Equations for Laminar Flat Premixed Flames	29
3.2	Heat and Mass Transport	33
3.3	The Description of a Laminar Premixed Flat Flame Front	33
3.4	Exercises	38
4	Thermodynamics of Combustion Processes	39
4.1	The First Law of Thermodynamics	39
4.2	Standard Enthalpies of Formation	41
4.3	Heat Capacities	43
4.4	The Second Law of Thermodynamics	44
4.5	The Third Law of Thermodynamics	45
4.6	Equilibrium Criteria and Thermodynamic Variables	46
4.7	Equilibrium in Gas Mixtures; Chemical Potential	47
4.8	Determination of Equilibrium Compositions in Gases	49
4.9	Determination of Adiabatic Flame Temperatures	51
4.10	Tabulation of Thermodynamic Data	52
4.11	Exercises	55

5	Transport Phenomena	57
5.1	A Simple Physical Model of Transport Processes	57
5.2	Heat Conduction in Gases	60
5.3	Viscosity of Gases	62
5.4	Diffusion in Gases	64
5.5	Thermal Diffusion, Dufour Effect, and Pressure Diffusion	66
5.6	Comparison with Experiments	67
5.7	Exercises	71
6	Chemical Kinetics	73
6.1	Rate Laws and Reaction Orders	73
6.2	Relation of Forward and Reverse Reactions	75
6.3	Elementary Reactions, Reaction Molecularity	75
6.4	Experimental Investigation of Elementary Reactions	77
6.5	Temperature Dependence of Rate Coefficients	79
6.6	Pressure Dependence of Rate Coefficients	81
6.7	Surface Reactions	84
6.8	Exercises	88
7.	Reaction Mechanisms	91
7.1	Characteristics of Reaction Mechanisms	91
7.1.1	Quasi-Steady States	92
7.1.2	Partial Equilibrium	94
7.2	Analysis of Reaction Mechanisms	97
7.2.1	Sensitivity Analysis	97
7.2.2	Reaction Flow Analysis	101
7.2.3	Eigenvalue Analyses of Chemical Reaction Systems	103
7.3	Stiffness of Ordinary Differential Equation Systems	107
7.4	Simplification of Reaction Mechanisms	107
7.5	Radical Chain Reactions	115
7.6	Exercises	117
8	Laminar Premixed Flames	119
8.1	Zeldovich's Analysis of Flame Propagation	119
8.2	Flame Structures	121
8.3	Flame Velocities	124
8.4	Sensitivity Analysis	127
8.5	Exercises	128
9	Laminar Nonpremixed Flames	129
9.1	Counterflow Nonpremixed Flames	129
9.2	Laminar Jet Nonpremixed Flames	133
9.3	Nonpremixed Flames With Fast Chemistry	135
9.4	Exercises	138

10	Ignition Processes	141
10.1	Semenov's Analysis of Thermal Explosions	142
10.2	Frank-Kamenetskii's Analysis of Thermal Explosions	143
10.3	Autoignition: Ignition Limits	145
10.4	Autoignition: Ignition-Delay Time	148
10.5	Induced Ignition, Minimum Ignition Energies	149
10.6	Spark Ignition	153
10.7	Detonations	157
10.8	Exercises	163
11	Low-Temperature Oxidation, Engine Knock	165
11.1	Fundamental Phenomena in Otto Engines	165
11.2	Oxidation at Intermediate Temperatures	168
11.3	Low-Temperature Oxidation	169
11.4	Ignition Processes in Reciprocating Engines	173
11.4.1	Knock Damages in Otto Engines	173
11.4.2	Ignition in Diesel Engines	174
11.4.3	The HCCI Concept	175
11.4.4	The DICI Concept	177
11.5	Exercises	178
12	The Navier-Stokes-Equations for Three-Dimensional Reacting Flow	179
12.1	The Conservation Equations	179
12.1.1	Overall Mass Conservation	180
12.1.2	Species Mass Conservation	181
12.1.3	Momentum Conservation	181
12.1.4	Energy Conservation	182
12.2	The Empirical Laws	183
12.2.1	Newton's Law	183
12.2.2	Fourier's Law	184
12.2.3	Fick's Law and Thermal Diffusion	184
12.2.4	Calculation of the Transport Coefficients from Molecular Parameters	185
12.3	Exercises	185
13	Turbulent Reacting Flows	187
13.1	Some Fundamental Phenomena	187
13.2	Direct Numerical Simulation	189
13.3	Concepts for Turbulence Modeling: Time- and Favre-Averaging	192
13.4	Reynolds-Averaged Navier-Stokes (RANS) Equations	194
13.5	Turbulence Models	196
13.6	Mean Reaction Rates	200
13.7	Concepts for Turbulence Modeling: Probability Density Functions	202
13.8	Eddy-Break-Up Models	206
13.9	Turbulent Scales	207
13.10	Large-Eddy Simulation (LES)	209
13.11	Exercises	211

14	Turbulent Nonpremixed Flames	213
14.1	Nonpremixed Flames with Equilibrium Chemistry	214
14.2	Finite-Rate Chemistry in Nonpremixed Flames	217
14.3	Flame Extinction	221
14.4	PDF-Simulations of Turbulent Non-Premixed Flames Using a Monte-Carlo Method	224
14.5	Exercises	226
15	Turbulent Premixed Flames	227
15.1	Classification of Turbulent Premixed Flames	227
15.2	Flamelet Models	230
15.2.1	Flamelet Modelling Using a Reaction Progress Variable	231
15.2.2	Flamelet Modelling Using a Level-Set Method	232
15.3	Turbulent Flame Velocity	233
15.4	Flame Extinction	235
15.5	Other Models of Turbulent Premixed Combustion	237
15.6	Exercises	238
16	Combustion of Liquid and Solid Fuels	239
16.1	Droplet Combustion	239
16.1.1	Combustion of Single Droplets	240
16.1.2	Combustion of Droplet Groups	244
16.2	Spray Combustion	246
16.2.1	Formation of Sprays	246
16.2.2	Spray Combustion Modes	247
16.2.3	Statistical Description of Sprays	249
16.2.4	Modeling of Turbulent Spray Combustion	252
16.2.5	Flamelet-Type Models for Spray Combustion	253
16.3	Coal Combustion	255
16.3.1	Pyrolysis of Coal	255
16.3.2	Burning of Volatile Compounds	256
16.3.3	Burning of the Coke	256
16.3.4	Coal Gasification	257
16.4	Exercises	258
17	Formation of Nitric Oxides	259
17.1	Thermal NO (Zeldovich NO)	259
17.2	Prompt NO (Fenimore NO)	262
17.3	NO Generated via Nitrous Oxide	265
17.4	Conversion of Fuel Nitrogen into NO	265
17.5	NO Reduction by Combustion Modifications	267
17.6	Catalytic Combustion	271
17.7	NO Reduction by Post-Combustion Processes	272
17.8	Exercises	275

18	Formation of Hydrocarbons and Soot	277
18.1	Unburnt Hydrocarbons	277
18.1.1	Flame Extinction Due to Strain	278
18.1.2	Flame Extinction at Walls and in Gaps	278
18.2	Formation of Polycyclic Aromatic Hydrocarbons (PAH)	280
18.3	The Phenomenology of Soot Formation	283
18.4	Modelling and Simulation of Soot Formation	287
18.5	Exercises	296
19	Effects of Combustion Processes on the Atmosphere	297
19.1	The Structure of the Atmosphere	297
19.1.1	Pressure in the Atmosphere	297
19.1.2	Temperature and Classification of Compartments in the Atmosphere	299
19.1.3	Composition of the Atmosphere	300
19.2.	The Atmosphere as a Photochemical System	300
19.2.1	Lambert-Beer Law	300
19.2.2	Stern-Vollmer Equation	301
19.2.3	Formation of Photochemical Layers	302
19.3	Incoming Sun Radiation, Photochemical Primary Processes	303
19.4.	Physical Processes in the Atmosphere	305
19.4.1	Conservation of the Mass of Species	305
19.4.2	Conservation of Energy	306
19.4.3	Solution of the Conservation Equations	307
19.5	Chemistry of the Unpolluted Atmosphere	307
19.5.1	Pure Oxygen Atmosphere	307
19.5.2	Oxygen-Nitrogen-Hydrogen-Carbon Atmosphere	308
19.6	Chemistry of the Polluted Atmosphere	310
19.6.1	Photochemical Smog	310
19.6.2	Supersonic Transports	314
19.6.3	Green-House Effect	315
19.6.4	Acid rain	316
19.7	The Role of Combustion Sources in Atmospheric Pollution	317
20	Appendix 1: Mathematics	319
20.1	Some Definitions and Laws for Vectors and Tensors	319
20.2.1	Formulation of the Problem	320
20.2.2	General Remarks on Solution Algorithms for ODE Systems	321
20.2.3	Euler Method	322
20.2.4	Extrapolation Method	324
20.3	Numerical Solution of Partial Differential Equation Systems	325
20.3.1	Spatial Discretization	326
20.3.2	Initial Values, Boundary Conditions, Stationary Solution	328
20.3.3	Explicit Solution Methods	329
20.3.4	Implicit Solution Methods	330
20.3.5	Semi-implicit Solution of Partial Differential Equations	330
20.3.6	Implicit Solution of Partial Differential Equations	331

XII	Table of Contents	
21	Appendix 2: Reaction Mechanisms	333
21.1	Mechanism of the Oxidation of H ₂ , CO, C ₁ and C ₂ Hydrocarbons	333
21.2	Reaction Mechanism of the Generation and Consumption of NO _x	340
22	References	345
23	Index	367