

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	12
2.4	Temperature Measurements	18
2.5	Pressure Measurements	20
2.6	Measurement of Particle Sizes	20
2.7	Simultaneous Diagnostics	21
2.8	Exercises	22
3	Mathematical Description of Premixed Laminar Flat Flames	23
3.1	Conservation Equations for Laminar Flat Premixed Flames	23
3.2	Heat and Mass Transport	27
3.3	The Description of a Laminar Premixed Flat Flame Front	27
3.4	Exercises	32
4	Thermodynamics of Combustion Processes	33
4.1	The First Law of Thermodynamics	33
4.2	Standard Enthalpies of Formation	35
4.3	Heat Capacities	37
4.4	The Second Law of Thermodynamics	38
4.5	The Third Law of Thermodynamics	39
4.6	Equilibrium Criteria and Thermodynamic Variables	40
4.7	Equilibrium in Gas Mixtures; Chemical Potential	41
4.8	Determination of Equilibrium Compositions in Gases	43
4.9	Determination of Adiabatic Flame Temperatures	45
4.10	Tabulation of Thermodynamic Data	46
4.11	Exercises	48

5	Transport Phenomena	49
5.1	A Simple Physical Model of the Transport Processes	49
5.2	Heat Conduction in Gases	52
5.3	Viscosity of Gases	54
5.4	Diffusion in Gases	56
5.5	Thermal Diffusion, Dufour Effect, and Pressure Diffusion	58
5.6	Comparison with Experiments	59
5.7	Exercises	63
6	Chemical Kinetics	65
6.1	Rate Laws and Reaction Orders	65
6.2	Relation of Forward and Reverse Reactions	67
6.3	Elementary Reactions, Reaction Molecularity	67
6.4	Experimental Investigation of Elementary Reactions	74
6.5	Temperature Dependence of Rate Coefficients	75
6.6	Pressure Dependence of Rate Coefficients	76
6.7	Surface Reactions	80
6.8	Exercises	84
7.	Reaction Mechanisms	85
7.1	Characteristics of Reaction Mechanisms	85
7.1.1	Quasi-Steady States	86
7.1.2	Partial Equilibrium	88
7.2	Analysis of Reaction Mechanisms	91
7.2.1	Sensitivity Analysis	91
7.2.2	Reaction Flow Analysis	95
7.2.3	Eigenvalue Analyses of Chemical Reaction Systems	97
7.3	Stiffness of Ordinary Differential Equation Systems	101
7.4	Simplification of Reaction Mechanisms	101
7.5	Radical Chain Reactions	107
7.6	Exercises	109
8	Laminar Premixed Flames	111
8.1	Zeldovich's Analysis of Flame Propagation	111
8.2	Numerical Solution of the Conservation Equations	113
8.2.1	Spatial Discretization	113
8.2.2	Initial Values, Boundary Conditions, Stationary Solution	115
8.2.3	Explicit Solution Methods	116
8.2.4	Implicit Solution Methods	117
8.2.5	Semi-implicit Solution of Partial Differential Equations	118
8.2.6	Implicit Solution of Partial Differential Equations	118
8.3	Flame Structures	119
8.4	Flame Velocities	122
8.5	Sensitivity Analysis	124
8.6	Exercises	125

9	Laminar Nonpremixed Flames	127
9.1	Counterflow Nonpremixed Flames	127
9.2	Laminar Jet Nonpremixed Flames	131
9.3	Nonpremixed Flames With Fast Chemistry	133
9.4	Exercises	136
10	Ignition Processes	137
10.1	Semenov's Analysis of Thermal Explosions	138
10.2	Frank-Kamenetskii's Analysis of Thermal Explosions	139
10.3	Autoignition: Ignition Limits	141
10.4	Autoignition: Ignition-Delay Time	144
10.5	Induced Ignition, Minimum Ignition Energies	145
10.6	Spark Ignition	149
10.7	Detonations	150
10.8	Exercises	152
11	The Navier-Stokes-Equations for Three-Dimensional Reacting Flows	153
11.1	The Conservation Equations	153
11.1.1	Overall Mass Conservation	154
11.1.2	Species Mass Conservation	155
11.1.3	Momentum Conservation	155
11.1.4	Energy Conservation	156
11.2	The Empirical Laws	157
11.2.1	Newton's Law	157
11.2.2	Fourier's Law	158
11.2.3	Fick's Law and Thermal Diffusion	158
11.2.4	Calculation of the Transport Coefficients from Molecular Parameters	159
11.3	Appendix: Some Definitions and Laws from Vector- and Tensor-Analysis	159
11.4	Exercises	161
12	Turbulent Reacting Flows	163
12.1	Some Fundamental Phenomena	163
12.2	Direct Numerical Simulation	165
12.3	Concepts for Turbulence Modeling: Probability Density Functions (PDFs)	167
12.4	Concepts for Turbulence Modeling: Time- and Favre-Averaging	168
12.5	Averaged Conservation Equations	170
12.6	Turbulence Models	172
12.7	Mean Reaction Rates	176
12.8	Eddy-Break-Up-Models	182
12.9	Large-Eddy Simulation (LES)	182
12.10	Turbulent Scales	182
12.11	Exercises	184

13	Turbulent Nonpremixed Flames	187
13.1	Nonpremixed Flames with Equilibrium Chemistry	188
13.2	Finite-Rate Chemistry in Nonpremixed Flames	191
13.3	Flame Extinction	195
13.4	PDF-Simulations of Turbulent Non-Premixed Flames	198
13.5	Exercises	200
14	Turbulent Premixed Flames	201
14.1	Classification of Turbulent Premixed Flames	201
14.2	Flamelet Models	204
14.3	Turbulent Flame Velocity	206
14.4	Flame Extinction	208
14.5	Other Models of Turbulent Premixed Combustion	210
14.6	Exercises	211
15	Combustion of Liquid and Solid Fuels	213
15.1	Droplet and Spray Combustion	213
15.1.1	Combustion of Single Droplets	214
15.1.2	Combustion of Sprays	218
15.2	Coal Combustion	224
16	Low-Temperature Oxidation, Engine Knock	227
16.1	Fundamental Phenomena	227
16.2	High-Temperature Oxidation	230
16.3	Low-Temperature Oxidation	231
16.4	Knock Damages	235
16.5	Exercises	236
17	Formation of Nitric Oxides	237
17.1	Thermal NO (Zeldovich-NO)	237
17.2	Prompt NO (Fenimore-NO)	240
17.3	NO Generated via Nitrous Oxide	243
17.4	Conversion of Fuel Nitrogen into NO	243
17.5	NO Reduction by Combustion Modifications	249
17.6	Catalytic Combustion	251
17.7	NO-Reduction by Post-Combustion Processes	253
18	Formation of Hydrocarbons and Soot	257
18.1	Unburnt Hydrocarbons	257
18.1.1	Flame Extinction Due to Strain	258
18.1.2	Flame Extinction at Walls and in Gaps	258
18.2	Formation of Polycyclic Aromatic Hydrocarbons (PAH)	260
18.3	The Phenomenology of Soot Formation	262
18.4	Modelling and Simulation of Soot Formation	266
19	References	273
20	Index	289