

Contents

<i>Preface</i>	<i>page</i> xiii	
<i>Acknowledgements</i>	xvi	
<i>Notation</i>	xvii	
1	Introductory Concepts	1
1.1	Overview of the Population Balance Methodology	1
1.1.1	Introduction	1
1.1.2	Applications of the Population Balance	2
1.1.3	Scope and Methodology of Population Balance	8
1.2	Distributions and Their Properties	9
1.2.1	Discrete and Continuous Distributions	9
1.2.2	Number Density and Probability Density Function	11
1.2.3	Properties of Distributions	12
1.3	Choice of Distributed Variables	14
1.4	Kinetic and Transport Processes	15
1.5	Population Balance and Fluid Dynamics	16
1.6	Two Examples of Population Balance in Flows	18
1.6.1	Precipitation of Crystals	18
1.6.2	Formation of Soot and Carbonaceous Nanoparticles	18
1.7	A Brief Historical Survey	19
1.8	Summary	22
2	Formulation of the Population Balance	24
2.1	Overview of Population Balance Formulations	24
2.2	Discrete Population Balance Equation (PBE)	25
2.2.1	Smoluchowski Equation	25
2.2.2	Formulation of the Complete Discrete PBE	27
2.2.3	Applications of Discrete PBE	29
		vii

2.2.4	Limitations of Discrete PBE	29
2.3	Continuous PBE	30
2.3.1	Derivation Based on Discrete PBE	30
2.3.2	Derivation from Continuum Principles	33
2.3.3	Applications of Continuous PBE	37
2.4	PBE with Multiple Distributed Properties	38
2.4.1	Multidimensional PBE	39
2.4.2	Coupled PBEs	42
2.5	Monodisperse PBE	47
2.6	Coupling of the PBE with Ideal Reactor Models	48
2.7	Spatially Dependent PBE and Coupling with Fluid Dynamics	52
2.7.1	Preliminary Considerations	52
2.7.2	PBE for Non-Inertial Particles	54
2.7.3	PBE for Inertial Particles with Low Stokes Number	55
2.7.4	PBE for Inertial Particles with Arbitrary Stokes Number	56
2.8	Summary	57
3	Kinetic and Transport Processes	59
3.1	Scope and Classification of Models	59
3.2	Aggregation	61
3.2.1	Preliminary Concepts	61
3.2.2	Collision Mechanisms and Kernels	64
3.2.3	Aggregate Morphology	73
3.3	Fragmentation	76
3.3.1	Overview	76
3.3.2	Models for the Fragment Size Number Density	78
3.3.3	Models for the Fragmentation Rate	82
3.4	Particle Formation Processes	83
3.4.1	Overview	83
3.4.2	Crystal Nucleation and Growth	84
3.4.3	Aerosols, Soot and Carbonaceous Nanoparticles	87
3.5	Determination of Kinetic Parameters: The Inverse Population Balance	90
3.5.1	Overview	90
3.5.2	Crystal Nucleation and Growth	91
3.5.3	Growth, Aggregation and Fragmentation	93
3.6	Transport Processes	97
3.6.1	Overview	97
3.6.2	Drag Force	99
3.6.3	Body Forces	102

	<i>Contents</i>	
		ix
3.6.4	Brownian Motion	102
3.6.5	Incorporation of Transport Models in the PBE	105
3.7	Concluding Remarks	109
4	Solution of the PBE	110
4.1	Introduction and Overview	110
4.1.1	General Features of the PBE	110
4.1.2	Overview of Solution Methods	111
4.2	Aggregation and Fragmentation	116
4.2.1	General Features	116
4.2.2	Analytical Solutions	119
4.2.3	Similarity Solutions	123
4.2.4	Moment Methods: Fundamentals and Closed Forms	125
4.2.5	Moment Methods: Closure Models	129
4.2.6	Discretisation Methods: Pointwise Approximation	134
4.2.7	Discretisation Methods: One-Dimensional Quadrature	138
4.2.8	Discretisation Methods: Two-Dimensional Quadrature	142
4.2.9	Monte Carlo Methods	150
4.2.10	Multidimensional PBEs	153
4.2.11	Coupled PBEs	154
4.3	Population Balance with a Growth Term	155
4.3.1	General Features	155
4.3.2	Analytical Solutions	157
4.3.3	Moment Methods	161
4.3.4	Discretisation Methods: Fixed Grid	163
4.3.5	Discretisation Methods: Characteristics-Based	169
4.3.6	Discretisation Methods: Adaptive Grids	171
4.3.7	Monte Carlo Method	172
4.3.8	Multidimensional and Coupled PBEs	173
4.4	Coupling of PBE with CFD: Non-Inertial and Low-Inertia Particles	174
4.4.1	Overview	174
4.4.2	Moment Methods	176
4.4.3	Discretisation Methods	178
4.4.4	Introduction of the PBE Source Term in CFD	182
4.4.5	Convection and Diffusion of Particles	184
4.4.6	Lagrangian Monte Carlo Methods	185
4.4.7	Data-Driven Methods	186
4.5	Coupling of PBE with CFD: Inertial Particles	188
4.5.1	PBE with Discretised Velocity Coordinates	188

4.5.2	Moment Methods and Multi-Fluid Models	189
4.5.3	Lagrangian Methods	190
4.6	Summary and Concluding Remarks	190
5	Population Balance in Turbulent Flow	193
5.1	Overview	193
5.2	Fundamentals of Turbulent Flow Modelling and Simulation	195
5.2.1	Turbulent Flow, Averages and PDFs	195
5.2.2	Reynolds-Averaged Navier–Stokes (RANS) Models	196
5.2.3	Scales of Turbulent Motion	199
5.2.4	Direct Numerical Simulation (DNS)	200
5.2.5	Large Eddy Simulation (LES)	201
5.2.6	Reacting Flows	204
5.2.7	Variable Density Flows	205
5.3	Closure Problem for Population Balance in Turbulent Flow	206
5.3.1	Averaging of the PBE	206
5.3.2	Averaging of the Moment Equations	208
5.3.3	Classification of Unclosed Terms	210
5.3.4	Overview of Closure Methods	211
5.4	Presumed PDF Methods	212
5.5	Transported PDF Methods	215
5.5.1	PDF Equation for Scalar Transport with a Nonlinear Source Term	216
5.5.2	The PBE-PDF Approach	223
5.5.3	Numerical Methods for Solving the PBE-PDF Equation	227
5.5.4	Computational Implementation	231
5.6	Concluding Remarks	233
6	Case Studies of CFD-PBE Application	235
6.1	Silica Nanoparticle Synthesis in a Laminar Flame	236
6.1.1	Introduction	236
6.1.2	Formulation of the Population Balance Model	238
6.1.3	Kinetic Models	242
6.1.4	Fluid Dynamics and Transport Phenomena	244
6.1.5	Numerical Methods	245
6.1.6	Simulation of Silica Synthesis in a Laminar Flame: The Camenzind et al. Case	245
6.1.7	Concluding Remarks	251
6.2	Soot Formation in Laminar and Turbulent Flames	252
6.2.1	Introduction	252

<i>Contents</i>	xi
6.2.2 Formulation of the Population Balance Model	254
6.2.3 Kinetic Models	259
6.2.4 Fluid Dynamics and Transport Phenomena	263
6.2.5 Turbulence, Turbulence–Chemistry and Turbulence–PBE Interactions	264
6.2.6 Numerical Methods	265
6.2.7 Simulation of Soot Formation in a Laminar Flow: The Santoro Flame	265
6.2.8 Simulation of Soot Formation in a Turbulent Flow: The Sandia Flame	274
6.2.9 Concluding Remarks	285
6.3 Precipitation in a Turbulent T-Mixer Flow	287
6.3.1 Introduction	287
6.3.2 Formulation of the Population Balance Model	290
6.3.3 Kinetic Models	291
6.3.4 Fluid Dynamics and Transport Phenomena	294
6.3.5 Numerical Methods	294
6.3.6 Simulation of Precipitation of BaSO ₄ in a Turbulent T-Mixer Flow: The Schwarzer et al. Case	297
6.3.7 Scaled-Down T-Mixer: Effect of Sub-Kolmogorov Scales on Precipitation	311
6.3.8 Concluding Remarks	318
<i>Appendix A Coupling of PBE with Fluid Flow, Heat and Mass Transfer</i>	320
A.1 Mass Transport	320
A.1.1 Continuity Equation	321
A.1.2 Multicomponent Mixtures	321
A.1.3 The Diffusion Flux	323
A.1.4 The Reaction Source Term	324
A.1.5 The Population Balance Kinetics Source Term	325
A.2 Momentum Transport	325
A.3 Energy Transport	326
A.3.1 The First Law of Thermodynamics	327
A.3.2 The Transport Equation for Chemical and Thermal Energy	328
A.3.3 Heat Conduction	329
A.3.4 Radiative Heat Transfer	329
A.3.5 Multicomponent and Reacting Flows	329

xii	<i>Contents</i>	
	<i>Appendix B Implementation of the Conservative Finite Volume Discretisation Method</i>	331
	B.1 Construction of Aggregation and Fragmentation Map	331
	B.1.1 Aggregation Map	331
	B.1.2 Fragmentation Map	336
	B.2 Time Advancement	337
	<i>Appendix C Derivation of the PDF Transport Equation</i>	339
	C.1 Random Variables and Stochastic Processes	339
	C.2 Fine-Grained Density and Essential Identities	340
	C.3 Derivation of the PDF Transport Equation for a Single Scalar	341
	C.4 The Diffusion Term and Scalar Dissipation	344
	<i>Appendix D Derivation of the Stochastic Field Equation</i>	345
	D.1 Essential Results from Stochastic Calculus	345
	D.2 Derivation of the Stochastic Field Equation for a Single Scalar	347
	<i>References</i>	350
	<i>Index</i>	379