

---

# Contents

---

## Part I Single Phase Flow

---

<b>1 Single Phase Flow .....</b>	<b>3</b>
1.1 Basic Principles of Fluid Mechanics .....	3
1.2 Equations of Change for Multi-Component Mixtures .....	8
1.2.1 Conservation of mass .....	15
1.2.2 Transport of species mass .....	19
1.2.3 Conservation of momentum .....	24
1.2.4 Conservation of total energy .....	35
1.2.5 Some useful simplifications of the governing equations .....	68
1.2.6 Gross Scale Average Forms of the Governing Equations .....	86
1.2.7 Dispersion Models .....	97
1.3 Application of the Governing Equations to Turbulent Flow .....	99
1.3.1 Origin and Characteristics of Turbulence .....	101
1.3.2 Statistical Turbulence Theory .....	104
1.3.3 Reynolds Equations and Statistics .....	117
1.3.4 Semi-Empirical Flow Analysis .....	121
1.3.5 Reynolds Averaged Models .....	129
1.3.6 Large Eddy Simulation (LES) .....	161
<b>References .....</b>	<b>177</b>
<b>2 Elementary Kinetic Theory of Gases .....</b>	<b>187</b>
2.1 Introduction .....	187
2.2 Elementary Concepts in Classical Mechanics .....	193
2.2.1 Newtonian Mechanics .....	194
2.2.2 Lagrangian Mechanics .....	197
2.2.3 Hamiltonian Mechanics .....	201
2.3 Basic Concepts of Kinetic Theory .....	207

2.3.1	Molecular Models . . . . .	208
2.3.2	Phase Space, Distribution Function, Means and Moments . . . . .	210
2.3.3	Flux Vectors . . . . .	212
2.3.4	Ideal Gas Law . . . . .	217
2.4	The Boltzmann Equation . . . . .	218
2.4.1	The Boltzmann Equation in the Limit of no Collisions . . . . .	219
2.4.2	Binary Collisions . . . . .	223
2.4.3	Generalized Collision Term Formulation . . . . .	243
2.5	The Equation of Change in Terms of Mean Molecular Properties . . . . .	246
2.6	The Governing Equations of Fluid Dynamics . . . . .	249
2.7	The Boltzmann H-Theorem . . . . .	252
2.7.1	The H-Theorem Formulation . . . . .	252
2.7.2	The Maxwellian Velocity Distribution . . . . .	254
2.7.3	The H-Theorem and Entropy . . . . .	255
2.8	Solving the Boltzmann Equation . . . . .	256
2.8.1	Equilibrium Flow - The Euler Equations . . . . .	256
2.8.2	Gradient Perturbations - Navier Stokes Equations	258
2.9	Multicomponent Mixtures . . . . .	262
2.10	Mean Free Path Concept . . . . .	309
2.11	Extending the Kinetic Theory to Denser Gases . . . . .	319
2.12	Governing Equations for Polydispersed Multiphase Systems	324
<b>References</b>	.....	<b>327</b>

**Part II Multiphase Flow**

<b>3</b>	<b>Multiphase Flow . . . . .</b>	<b>335</b>
3.1	Introduction . . . . .	335
3.2	Modeling Concepts for Multiphase Flow . . . . .	339
3.2.1	Averaged Models . . . . .	340
3.2.2	High Resolution Methods . . . . .	344
3.3	Basic Principles and Derivation of Multi-Fluid Models . . .	365
3.3.1	Local Instantaneous Transport Equations . . . . .	370
3.3.2	The Purpose of Averaging Procedures . . . . .	393
3.4	Averaging Procedures . . . . .	394
3.4.1	The Volume Averaging Procedure . . . . .	397
3.4.2	The Time Averaging Procedure . . . . .	419
3.4.3	The Ensemble Averaging Procedure . . . . .	429
3.4.4	The Time After Volume Averaging Procedure . . . . .	441
3.4.5	The Mixture Models . . . . .	463

3.4.6	The Gross Scale Averaged Two-Phase Transport Equations . . . . .	473
3.4.7	Heterogeneous Dispersion Models . . . . .	484
3.5	Mathematical Model Formulation Aspects . . . . .	485
<b>References</b> . . . . .		<b>489</b>
<b>4 Flows of Granular Materials</b> . . . . .		<b>503</b>
4.1	The Two-Fluid Granular Flow Model . . . . .	508
4.1.1	Collisional Rate of Change . . . . .	509
4.1.2	Dynamics of Inelastic Binary Collisions . . . . .	514
4.1.3	Maxwell Transport Equation and Balance Laws . . . . .	516
4.1.4	Transport Equation in Terms of Peculiar Velocity	520
4.1.5	Initial- and Boundary Conditions for the Granular Phase Equations . . . . .	530
4.2	Remarks on the Kinetic Theory of Granular Flows . . . . .	531
4.2.1	Granular Flow Closure Limitations . . . . .	534
<b>References</b> . . . . .		<b>537</b>
<b>5 Constitutive Equations</b> . . . . .		<b>543</b>
5.1	Modeling of Multiphase Covariance Terms . . . . .	545
5.1.1	Turbulence Modeling Analogues . . . . .	545
5.2	Interfacial Momentum Closure . . . . .	553
5.2.1	Drag force on a single rigid sphere in laminar flow	559
5.2.2	Lift forces on a single rigid sphere in laminar flow	564
5.2.3	Lift and drag on rigid spheres in turbulent flows .	569
5.2.4	Drag force on bubbles . . . . .	572
5.2.5	Lift force on bubbles . . . . .	577
5.2.6	The Added mass or virtual mass force on a single rigid sphere in potential flow . . . . .	581
5.2.7	Interfacial Momentum Transfer Due to Phase Change . . . . .	587
5.3	Interfacial Heat and Mass Transfer Closures . . . . .	588
5.3.1	Approximate Interfacial Jump Conditions . . . . .	588
5.3.2	Fundamental Heat and Mass Transport Processes	597
5.3.3	Mass Transport Described by Fick's law . . . . .	599
5.3.4	Heat Transfer Described by Fourier's Law . . . . .	604
5.3.5	Heat and Mass Transfer Coefficient Concepts . . . . .	605
5.3.6	Heat Transfer by Radiation . . . . .	635
<b>References</b> . . . . .		<b>647</b>
<b>APPLICATIONS</b> . . . . .		<b>657</b>

## XLVIII Contents

<b>6 Chemical Reaction Engineering .....</b>	<b>659</b>
6.1 Idealized Reactor Models .....	660
6.1.1 Plug Flow Reactor Models .....	660
6.1.2 Batch and Continuous Stirred Tank Reactors .....	663
6.2 Simplified Reactor Models .....	665
6.3 Chemical Reaction Equilibrium Calculations .....	666
6.3.1 Stoichiometric Formulation .....	670
6.3.2 Non-stoichiometric formulation .....	674
<b>References .....</b>	<b>677</b>
<b>7 Agitation and Fluid Mixing Technology .....</b>	<b>679</b>
7.1 Tank Geometry and Impeller Design .....	679
7.2 Fluid Shear Rates, Impeller Pumping Capacity and Power Consumption .....	684
7.2.1 Fluid shear rates .....	685
7.2.2 Impeller Pumping Capacity .....	686
7.2.3 Impeller Power Consumption .....	687
7.2.4 Fundamental Analysis of Impeller Power Consumption .....	688
7.3 Turbulent Mixing .....	699
7.3.1 Studies on Turbulent Mixing .....	700
7.3.2 Flow Fields in Agitated Tanks .....	703
7.3.3 Circulation and mixing times in turbulent agitated tanks .....	705
7.3.4 Turbulent Reactive Flow in Stirred Tank .....	707
7.4 Heat Transfer in Stirred Tank Reactors .....	714
7.5 Scale-up of Single Phase Non-Reactive Turbulent Stirred Tanks .....	716
7.6 Mixing of Multi-Phase Systems .....	717
7.7 Governing Equations in Relative and Absolute Frames .....	723
7.7.1 Governing Eulerian Flow Equations in the Laboratory Frame .....	723
7.7.2 Coriolis and Centrifugal Forces .....	724
7.7.3 Governing Eulerian Equations in a Rotating Frame	727
7.8 Impeller Modeling Strategies .....	730
7.8.1 The Impeller Boundary Conditions (IBC) Method	730
7.8.2 The Snapshot (SS) Method .....	731
7.8.3 The inner-outer (IO) method and the multiple reference frame approach (MRF) .....	732
7.8.4 The Moving Deforming Mesh (MDM) Technique ..	735
7.8.5 The Sliding Grid (SG) or Sliding Mesh (SM) Method .....	736
7.8.6 Model Validation .....	737

7.9	Assessment of Multiple Rotating Reference Frame Model Simulations .....	740
<b>References</b> .....		<b>751</b>
<b>8</b>	<b>Bubble Column Reactors</b> .....	<b>757</b>
8.1	Hydrodynamics of Simple Bubble Columns .....	757
8.1.1	Experimental Characterization of Cylindrical Bubble Column Flow .....	760
8.2	Types of Bubble Columns .....	764
8.3	Applications of Bubble Columns in Chemical Processes ...	766
8.4	Modeling of Bubble Column Reactors .....	767
8.4.1	Fluid Dynamic Modeling .....	770
8.4.2	Numerical Schemes and Algorithms .....	791
8.4.3	Chemical Reaction Engineering .....	793
8.4.4	Multifluid Modeling Framework .....	794
<b>References</b> .....		<b>797</b>
<b>9</b>	<b>The Population Balance Equation</b> .....	<b>807</b>
9.1	Three Alternative Population Balance Frameworks .....	812
9.1.1	The Continuum Mechanical Approach .....	812
9.1.2	The Microscopic Continuum Mechanical Population Balance Formulation .....	835
9.1.3	The Statistical Mechanical Microscopic Population Balance Formulation .....	853
<b>References</b> .....		<b>859</b>
<b>10</b>	<b>Fluidized Bed Reactors</b> .....	<b>867</b>
10.1	Solids Classification .....	868
10.2	Fluidization Regimes for Gas-Solid Suspension Flow .....	868
10.3	Reactor Design and Flow Characterization .....	872
10.3.1	Dense-Phase Fluidized Beds .....	873
10.3.2	Lean-Phase Fluidized Beds .....	875
10.3.3	Various Types of Fluidized Beds .....	880
10.3.4	Experimental Investigations .....	880
10.4	Fluidized Bed Combustors .....	883
10.5	Milestones in Fluidized Bed Reactor Technology .....	888
10.6	Advantages and disadvantages .....	892
10.7	Chemical Reactor Modeling .....	893
10.7.1	Conventional Models for Bubbling Bed Reactors .	894
10.7.2	Turbulent Fluidized Beds .....	911
10.7.3	Circulating Fluidized Beds .....	911
10.7.4	Simulating Bubbling Bed Combustors Using Two-Fluid Models .....	915

10.7.5	Bubbling Bed Reactor Simulations Using Two-Fluid Models .....	928
<b>References</b> .....		945
<b>11 Packed Bed Reactors</b> .....		953
11.1	Processes Operated in Packed Bed Reactors (PBRs) .....	953
11.2	Packed Bed Reactor Design .....	954
11.3	Modeling and Simulation of Packed Bed Reactors .....	956
11.3.1	Fixed Bed Dispersion Models .....	957
11.3.2	Reactor Process Simulations .....	964
<b>References</b> .....		983
<b>12 Numerical Solution Methods</b> .....		985
12.1	Limitations of Numerical Methods .....	986
12.2	Building Blocks of a Numerical Solution Method .....	987
12.3	Properties of Discretization Schemes .....	989
12.4	Initial and Boundary Condition Requirements .....	991
12.5	Discretization Approaches .....	993
12.5.1	The Finite Difference Method .....	993
12.5.2	The Finite Volume Method .....	995
12.5.3	The Method of Weighted Residuals .....	995
12.5.4	The Finite Element Method .....	1002
12.6	Basic Finite Volume Algorithms Used in Computational Fluid Dynamics .....	1008
12.7	Elements of the Finite Volume Method for Flow Simulations .....	1012
12.7.1	Numerical Approximation of Surface and Volume Integrals .....	1014
12.7.2	Solving Unsteady Problems .....	1017
12.7.3	Approximation of the Diffusive Transport Terms .....	1022
12.7.4	Approximation of the Convective Transport Terms .....	1025
12.7.5	Brief Evaluation of Convection/Advection Schemes .....	1038
12.8	Implicit Upwind Discretization of the Scalar Transport Equation .....	1038
12.9	Solution of the Momentum Equation .....	1040
12.9.1	Discretization of the Momentum Equations .....	1040
12.9.2	Numerical Conservation Properties .....	1041
12.9.3	Choice of Variable Arrangement on the Grid .....	1043
12.9.4	Calculation of Pressure .....	1044
12.10	Fractional Step Methods .....	1056
12.11	Finite Volume Methods for Multi-fluid Models .....	1060
12.11.1	Special Challenges in Solving the Two-fluid Model Equations .....	1061

12.11.2	Explicit Fractional Step Algorithm for Solving the Two-Fluid Model Equations Applied to Bubble Column Flow . . . . .	1067
12.11.3	Implicit Fractional Step Method for Solving the Two-Fluid Granular Flow Model Equations Applied to Fluidized Bed Flow . . . . .	1070
12.11.4	Solution of Multi-fluid Models . . . . .	1076
12.12	Numerical Solution of the Population Balance Equation . .	1077
12.13	Solution of Linear Equation Systems . . . . .	1092
12.13.1	Point-Iterative Methods . . . . .	1092
12.13.2	The Tri-Diagonal Matrix Algorithm (TDMA) . . .	1093
12.13.3	Krylov Subspace Methods . . . . .	1095
12.13.4	Preconditioning . . . . .	1098
12.13.5	Multigrid Solvers . . . . .	1102
12.13.6	Parallelization and Performance Optimization . . .	1105
<b>References</b>	. . . . .	1109

### Part III APPENDIX

<b>APPENDIX</b>	. . . . .	1123
<b>A Mathematical Theorems</b>	. . . . .	1125
A.1	Transport Theorem for a Single Phase Region . . . . .	1125
A.1.1	Leibnitz's Rule . . . . .	1125
A.1.2	Leibnitz Theorem . . . . .	1126
A.1.3	Reynolds Theorem . . . . .	1128
A.2	Gauss Theorem . . . . .	1130
A.3	Surface Theorems . . . . .	1131
A.3.1	Leibnitz Transport Theorem for a Surface . . . . .	1131
A.3.2	Gauss Theorem for a Surface . . . . .	1132
<b>References</b>	. . . . .	1137
<b>B Equation of Change for Temperature for a Multicomponent System</b>	. . . . .	1139
B.1	The Problem Definition . . . . .	1139
B.2	Deriving the Equation of Change for Temperature . . .	1139
<b>References</b>	. . . . .	1145
<b>C Trondheim Bubble Column Model</b>	. . . . .	1147
C.1	Model Formulation . . . . .	1147
C.2	Tensor Transformation Laws . . . . .	1157
C.2.1	Curvilinear Coordinate Systems . . . . .	1158

C.2.2	The Tensor Concept .....	1158
C.2.3	Coordinate Transformation Prerequisites.....	1160
C.2.4	Orthogonal Curvilinear Coordinate Systems and Differential Operators .....	1162
C.2.5	Differential Operators in Cylindrical Coordinates	1165
C.2.6	Differential Operators Required for the Two-fluid Model .....	1169
C.3	Two-Fluid Equations in Cylindrical Coordinates .....	1173
C.4	The 2D Axi-Symmetric Bubble Column Model .....	1176
C.4.1	Discretization of the Trondheim Bubble Column Model .....	1180
C.4.2	The Continuity Equation .....	1185
C.4.3	The Generalized equation .....	1187
C.4.4	The liquid phase radial momentum balance .....	1190
C.4.5	The Liquid phase axial momentum balance .....	1202
C.4.6	The gas phase radial momentum balance .....	1211
C.4.7	The gas phase axial momentum balance .....	1221
C.4.8	The Turbulent Kinetic Energy .....	1227
C.4.9	The Turbulent Kinetic Energy Dissipation Rate ..	1230
C.4.10	The Volume fraction .....	1231
C.4.11	The Pressure-Velocity Correction Equations .....	1234
<b>References</b> .....	1237	
<b>Index</b> .....	1239	