Contents

Biographies ix
Series Preface xi
Preface xiii
Symbols and Abbreviations xvii

1 The Nature of Fluid Flow 1
   1.1 Introduction 1
   1.2 Basics of fluid motion 1
      1.2.1 Continuum/bulk properties 3
      1.2.2 Continuum approximations 8
      1.2.3 Continuum scale simulation 11
   1.3 Molecular mechanics 16
      1.3.1 Molecular properties 16
      1.3.2 Molecular simulations 18
   1.4 Types of simulation 20
      1.4.1 Monte Carlo simulation 22
      1.4.2 Molecular dynamics 25
      1.4.3 Introduction to the physics of MD simulations 25
      1.4.4 Hard sphere model 32
      1.4.5 Soft sphere model 35
   1.5 Effects at molecular scale 36
      1.5.1 Phase change in confined systems 36
      1.5.2 Adsorption/desorption in pores 39
   1.6 Summary 43
CONTENTS

2 Fluid Physics at Meso Scales
  2.1 Introduction 45
  2.2 Top-down approach for meso scale computation 46
      2.2.1 Continuum limit 46
      2.2.2 Top-down meso scale methods 50
  2.3 Bottom up approach for meso scale computation 55
      2.3.1 Molecular dynamics model 55
      2.3.2 Boundary conditions 57
      2.3.3 Bottom-up meso scale methods 60
  2.4 Summary 65

3 Meso Scale Model Based on First Principles
  3.1 Introduction 67
  3.2 Fluid physics model 68
      3.2.1 Book keeping 68
      3.2.2 Force interactions 70
      3.2.3 Time integration scheme 70
      3.2.4 Boundary conditions 75
      3.2.5 Modified boundary potential 80
  3.3 Extracting local bulk properties 81
      3.3.1 Approximation method 82
      3.3.2 Bin averaging 82
      3.3.3 Smooth particle hydrodynamics (SPH) 83
      3.3.4 Moving least squares 86
      3.3.5 Weight functions 92
      3.3.6 Grid structure implementation 94
      3.3.7 Sampling 95
  3.4 Verification of proposed meso scale model 96
  3.5 Summary 102

4 Enhancements to the Meso Scale Model
  4.1 Introduction 103
  4.2 Driving forces 104
  4.3 Thermostats 106
      4.3.1 Gaussian thermostat 106
      4.3.2 Nosé–Hoover 108
  4.4 Case studies 110
      4.4.1 Sampling 110
      4.4.2 Gradient study 119
  4.5 Summary 125
CONTENTS

5 Modelling Fluid Regimes at Nano/Meso Scales 127
5.1 Introduction 127
5.2 Flow regimes 128
  5.2.1 Laminar flow 130
  5.2.2 Turbulent flow 132
5.3 Fluid flow characterization from molecular simulation 133
  5.3.1 Characteristics of low-speed molecular flow 134
  5.3.2 Characteristics of high-speed molecular flow 136
  5.3.3 Comparisons and data analysis 137
5.4 Summary 142

6 Performance of Proposed Meso Scale Model 143
6.1 Introduction 143
6.2 Issues in using large numbers of molecules 143
  6.2.1 Processing large numbers of molecules 144
  6.2.2 Boundary conditions 150
  6.2.3 Bulk property extraction 150
6.3 Meso scale simulations 151
  6.3.1 Performance of meso scale simulations 155
6.4 Summary 158

7 Experimental Aspects of Fluid Properties at the Nano/Meso Scale 159
7.1 Introduction 159
7.2 Colloidal interactions in nano-fluids 160
  7.2.1 Particle-particle interactions 161
7.3 Osmotic phenomena and osmotic pressure 163
  7.3.1 Measurement of osmotic pressure 164
  7.3.2 Numerical calculation of the osmotic pressure for nano-fluids 170
7.4 Gradient diffusion coefficient 172
  7.4.1 Experimental measurement of the gradient diffusion coefficient 173
  7.4.2 Experimental data analysis 174
  7.4.3 Gradient diffusion coefficient calculation 176
7.5 Viscosity 180
  7.5.1 Viscosity experiments 181
  7.5.2 Viscosity calculation 184
7.6 Membrane separations 184
7.7 Membrane ultrafiltration models 185
  7.7.1 Frontal ultrafiltration model 185
  7.7.2 Cross-flow ultrafiltration model 186
  7.7.3 Comparison of experimental and theoretical data 189
CONTENTS

7.8 Tensile and other rheological properties of liquids on the meso scale 190
  7.8.1 Metastability and cavitation phenomena 190
  7.8.2 Experimental techniques 194
  7.9 Summary 202

8 Future Advancement 203
  8.1 Future advancement 203

References 205

Index 215