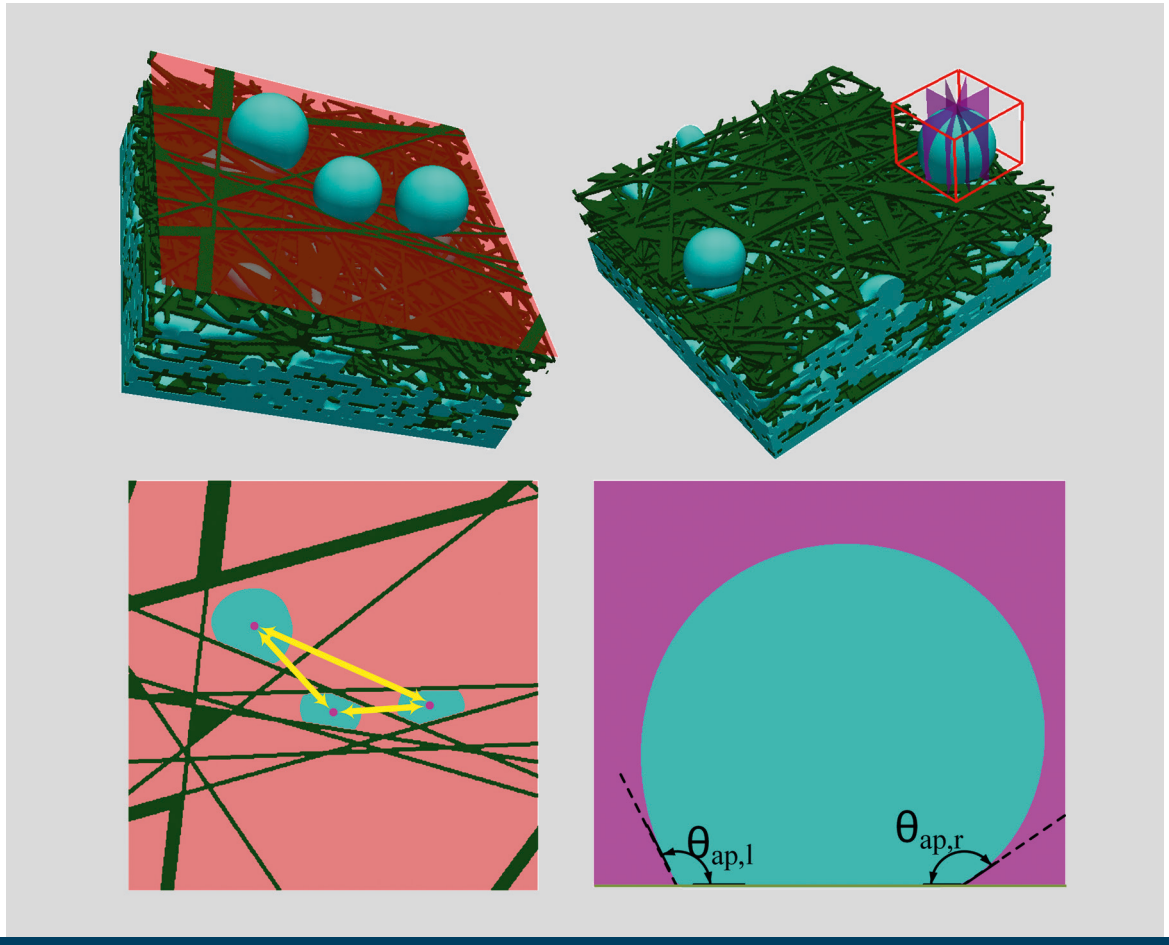

Lattice Boltzmann Simulation in Components of Polymer Electrolyte Fuel Cell

Junliang Yu

Energie & Umwelt / Energy & Environment
Band / Volume 438
ISBN 978-3-95806-360-0

Mitglied der Helmholtz-Gemeinschaft

JÜLICH
Forschungszentrum

Forschungszentrum Jülich GmbH
Institut für Energie- und Klimaforschung
Elektrochemische Verfahrenstechnik (IEK-3)

Lattice Boltzmann Simulation in Components of Polymer Electrolyte Fuel Cell

Junliang Yu

Schriften des Forschungszentrums Jülich
Reihe Energie & Umwelt / Energy & Environment Band / Volume 438

ISSN 1866-1793 ISBN 978-3-95806-360-0

Contents

1 Introduction and literature review **1**
- 1.1 Motivation and goal . . . 3
- 1.2 Two-phase flow in GDL of PEFC . . . 4
  - 1.2.1 Two-phase flow mechanisms . . . 5
  - 1.2.2 Two-phase flow simulations and experiments . . . 8

2 Methods **11**
- 2.1 ShanChen MCMP model . . . 12
  - 2.1.1 ShanChen MCMP model with SRT approach . . . 13
  - 2.1.2 ShanChen MCMP model with MRT approach . . . 15
- 2.2 Force schemes in ShanChen MCMP model . . . 16
- 2.3 Open boundary condition . . . 18
- 2.4 Unit conversion . . . 19
- 2.5 Apparent contact angle on rough surface . . . 21

3 Simulation framework **25**
- 3.1 Simulation process . . . 25
- 3.2 Geometry introduction . . . 27

4 Model validation **31**
- 4.1 External force driving Poiseuille flow test . . . 31
- 4.2 Flat interface test . . . 37
  - 4.2.1 Steady flat interface test . . . 37
  - 4.2.2 External force driving layered Poiseuille flow . . . 43
- 4.3 Droplet test . . . 47
  - 4.3.1 Single ideal droplet test . . . 47
  - 4.3.2 Cubic initialization test . . . 52
  - 4.3.3 Coalescence test . . . 54
- 4.4 Contact angle test . . . 57
- 4.5 Open boundary condition test . . . 63
- 4.6 Summary . . . 67

5 Simulation of liquid water through GDL **69**
- 5.1 Simulation setups and conditions . . . 69
- 5.2 Buffer space thickness effect . . . 71
- 5.3 Domain size effect . . . 75
- 5.4 Capillary number effect . . . 78
- 5.5 Geometry effect . . . 82
- 5.6 Wettability effect . . . 91
- 5.7 Summary . . . 93

6 Statistic analysis of liquid water through GDL **95**
6.1 Apparent contact angle . . . 95
6.2 Breakthrough point distance . . . 100

7 PTFE effects on water through GDL **107**
7.1 Simulation setups and conditions . . . 107
7.2 In-plane PTFE distribution . . . 110
7.3 Whole-GDL PTFE distribution . . . 115
7.4 Two-sections-through-plane PTFE distribution . . . 117
7.5 Sandwich-through-plane PTFE distribution . . . 121
7.6 Quasi-linear-through-plane PTFE distribution . . . 128

8 Discussion **131**

9 Conclusion **135**

References **137**

A Appendix **151**
A.1 Transformation matrix in MRT . . . 151
A.2 Example of unit conversion . . . 152
A.3 SPPF method in MATLAB . . . 152

B Abbreviate **155**
B.1 Acronyms . . . 155
B.2 Latin symbols . . . 159

List of Figures **165**

List of Tables **171**

C Acknowledgments **173**

Energie & Umwelt / Energy & Environment
Band / Volume 438
ISBN 978-3-95806-360-0

Mitglied der Helmholtz-Gemeinschaft

JÜLICH
Forschungszentrum