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Review Article

Lattice Boltzmann simulation of proton exchange membrane fuel cells – A review on opportunities and challenges

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ABSTRACT

Proton exchange membrane (PEM) fuel cells are presently at the center of attention due to their major role in the fuel cell vehicles (FCVs). To simulate multi-species multi-phase flow through complicated non-homogenous and anisotropic porous media of PEM fuel cells electrodes, one of the best choices is lattice Boltzmann method (LBM) which offers several advantages. Numerous LB simulations of PEM fuel cells have been conducted in recent years. In the current study, these simulations are classified based on the simulation target into three classes and through a strict review pros and cons of simulations of each class are explained. The main research gaps are: (a) LB calculation of micro-porous layer (MPL) and catalyst layer (CL) transport properties, (b) investigation of water droplet dynamic behavior through gas channel with high density ratio LB techniques, and (c) LB simulation of multi-component multi-phase reactive flow through an operating electrode via an active approach. Since different features of LB models which are applicable for the simulation of PEM fuel cells are elucidated in the current review article, it will be supportive for researchers interested in LB investigation of PEM fuel cells.

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Nomenclature

Bo	Bond number
Ca	Capillary number
$\vec{c}$	Particle velocity[1], lu ts^{-1}
c_s	Speed of sound in lattice, lu ts^{-1}
$\vec{F}_{coh}$	Fluid–fluid interaction force[2], lm lu ts^{-2}
$\vec{F}_{adh}$	Fluid–solid interaction force, lm lu ts^{-2}
f	Density distribution function
G^{jk}_{coh}	Cohesion factor between components k and j
G^{k}_{adh}	Adhesion factor of component k to the wall
Kn	Knudsen number
$\vec{r}$	Particle position vector, lu
t	Time, ts
$\vec{u}$	Velocity vector, lu ts^{-1}
We	Webber number
w	Weighting factor
x, y, z	Cartesian coordinates

Greek symbols

ϕ	Scalar quantity
ν	Kinematic viscosity, lu^2 ts^{-1}
ρ	Density, lm lu^{-3} or kg m^{-3}
τ	Relaxation time, ts
ψ	Inter-particle potential function and also bulk free-energy density

Subscripts and superscripts

eq	Equilibrium
i	Direction *i* of lattice
k	Species (component) *k*
LB	Lattice Boltzmann

Abbreviations

BGK	Bhatnagar–Gross–Krook
CL	Catalyst layer
CFVLBM	Coupling FVM and LBM modeling scheme
DDF	Density distribution function
FVM	Finite volume method
GC	Gas Channel
GDL	Gas diffusion layer
KC	Kozeny–Carman
LB	Lattice Boltzmann
LBM	Lattice Boltzmann method
MPL	Micro-porous layer
MRT	Multi-relaxation time
NPMC	Non-precious metal catalyst
PEM	Proton exchange membrane
SC	Shan and Chen
SRT	Single-relaxation time

Introduction

While energy demands are increasing and fossil fuel resources are depleting, fuel cell systems can serve as safe, clean, efficient and reliable power generating device in a wide range of portable, stationary and transport applications, ranging from very small devices such as mobile phones and laptops, right through passenger cars, forklifts, buses and ships, to combined heat and power (CHP) systems and huge distributed electrical power generators [1]. Besides, they can easily be coupled with energy storage systems to provide a robust and effectively controllable power systems such as recently developed fuel cell/battery hybrid systems [2–4].

In order to have a more practical sense, status of fuel cell vehicles (FCVs) will be succinctly explained. The Toyota Mirai and the Hyundai ix35 were two FCVs which have been introduced since 2015 for commercial sale and lease in limited quantities. From June 2011, demonstration of FCVs showed the capabilities of being driven more than 4,800,000 km (3,000,000 mi), with about 27,000 times refueling [5]. In their production process, a driving range exceeding 400 km (250 mi) between each refueling was considered which would take less than 5 min [6].

The fuel cell technology program of U.S. Department of Energy claims that, commencing 2011, fuel cells achieved 53–59% and 42–53% efficiency at one-quarter power and full power respectively and also more than 120,000 km (75,000 mi) durability with less than 10% degradation [6].

General Motors and its partners in a well-to-wheels simulation analysis evaluated that a FCV driven by a compressed

[1] lu and ts are the units of length and time in LBM, respectively.
[2] lm is the unit of mass in LBM.