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Multi-component multi-phase lattice Boltzmann modeling of droplet coalescence in flow channel of fuel cell

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HIGHLIGHTS

- A multi-component multi-phase lattice Boltzmann model is presented.
- Drawbacks in original pseudopotential multiphase model are solved.
- A new method for multiphase open boundary is proposed.
- Droplet coalescence is beneficial for droplet motion.
- Shear force exerted on droplet is determined by droplet height and gas velocity.

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ABSTRACT

A multi-component multi-phase lattice Boltzmann model is presented to study the dynamic behavior of droplet coalescence in the flow channel of proton exchange membrane fuel cell. The original pseudopotential multiphase model is developed to realize high density and kinematic viscosity ratios, low spurious velocity, good thermodynamic consistency and independent adjustment of surface tension. Multi-component Laplace law and capillary wave tests are conducted to validate the capability of model in capturing static and dynamic characteristics. A new method for multiphase open boundary is proposed, enabling the droplet to pass the outlet naturally. The droplet coalescence is studied elaborately with the consideration of different droplet size arrangement, distance between two droplets, wall contact angle and gas flow velocity. The droplet shapes are shown with detailed description during the coalescence processes, and the evolutions of droplet height and position throughout the whole processes are measured. Results show that droplet coalescence is beneficial for droplet motion, because the shear force exerted on the droplet, which is determined by the droplet height and gas flow velocity, is strengthened during the coalescence.

1. Introduction

Proton exchange membrane fuel cell (PEMFC) has become one of the most promising power sources for vehicles, due to its high power density and rapid response to various loads [1,2]. Among the various drawbacks restricting the popularization of PEMFC, complicated water management, especially the water flooding in cathode porous electrode and flow channel, is still of primary importance for further improvement of performance and durability [3,4].

In regarding to the experimental works in flow channel, Yu et al. [5] studied the flow regimes in the cathode channel with double parallel conductance probes inspecting system. Ous and Arcoumanis [6] designed a transparent fuel cell to observe the water accumulation during its operation with a charge coupled device (CCD) camera. Hussaini et al. [7] investigated the cathode channel flooding under various working conditions and introduced a new parameter called wetted area ratio. Based on the above visulaization experiments, it is found that the flow patterns in flow channel are related to the droplet coalescence phenomenon, as film flow is often observed when water accumulates as tiny droplets on gas diffusion layer (GDL) surface, while it may evolve into droplet flow or slug flow when larger droplet forms during the coalescence process. In addition, droplet deformation and oscillation during coalescence process are also more violent than the single droplet flow [8,9], which is more likely to cause channel blockage. Therefore, it is of great importance to study droplet coalescence in PEMFC flow channel.

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Nomenclature

a	parameter in EOS
b	parameter in EOS
c	lattice constant
C_ρ	density conversion coefficient, 105.9 kg m^{-3}
C_l	length conversion coefficient, 1 μm
C_t	time conversion coefficient, 1.089 × 10^{-5} ms
C_s	lattice sound speed
D	distance between two droplets
e	discrete velocity
f	distribution function
F	interaction force
G	interaction strength
h	wave amplitude
I	unit tensor
k	wave number
p	pressure
m	distribution function at moment space
M	transformation matrix
Q	variables to tune surface tension
R	universal gas constant; radius, μm
Re	Reynolds number
S	forcing term
t	time, ms
T	temperature, K; oscillating period
v	velocity, m s^{-1}
w	weight coefficient
x	lattice site; direction
y	direction

Greek letters

α	velocity direction; parameter in EOS; moment space
β	velocity space
ζ	bulk viscosity
κ	scalar
λ	surface tension, N m^{-1}
θ	contact angle, °
P	density, kg m^{-3}
σ	component; thermodynamic consistency parameter
τ	relaxation time
υ	kinematic viscosity
ψ	pseudopotential
ω	weight coefficient; acentric factor
γ	surface tension adjustment parameter
Λ	diagonal relaxation matrix

Subscripts and superscripts

1	water component
2	air component
Ads	adhesion force
C	critical point
Eq	equilibrium
EOS	equation of state
Int	interaction
l	length
t	time
w	wall

Considerable efforts have also been devoted to the numerical simulation, because experiment is expensive and deficient to capture more details of dynamic mechanism. Various computational fluid dynamics (CFD) methods, such as the volume-of-fluid (VOF) and level-set-method, have been widely employed in the past decade to investigate the droplet flow in channel, considering the effect of typical factors like wall contact angle, gas inlet velocity and structural designs [10–12]. Specifically to the droplet coalescence, Nikolopoulos et al. simulated the central collision of two droplets by VOF method and adaptive local grid is employed for refining the resolution around the multi-phase interface [13]. Lee et al. investigated the droplet coalescence process using sharp-interface level-set-method [14]. However, the artificially constructed interface makes these methods high resources consumption to capture the shape characteristics during droplet coalescence process and variation of dynamic contact angle [15]. Thus, the macroscopic interface capturing method is imperfect and preferable method is still pursued.

Mesoscopic methods are expected to reveal the underlying mechanism at small-scale view, and with acceptable computational cost compared to molecular dynamics (MD) model. Over the past decades, lattice Boltzmann (LB) method, which is based on the mesoscopic kinetic theory, has evolved into a powerful technique in various research areas, especially for multiphase flow. The main advantages, such as linear convective operator, extraordinary capability of dealing with complex boundary and its perfect scheme for parallel computing, distinguish the LB method from other numerical methodologies [16]. Simple implementation makes the Shan-Chen psedopotential method outstand in comparison with other multiphase LB model [17]. The key of psedopotential method lies in that the phases seperate naturally via the effect of lattice interaction force, which is realized by introducing density-based pseudopotential.

Based on single-component psedopotential model, Han et al. [18,19] applied the original Shan-Chen model to simulate the droplet transport in flow channel and the effects of some crucial properties like the gas inlet velocity, wall contact angle and structure of the turning part are discussed. Gong et al. [20] presented a 3D Shan-Chen model which is capable of achieving high density ratio and investigated the droplet coalescence processes on surface driven by various forms of wettability gradient. Clime et al. [21] investigated the droplet motion and coalescence at different contact angles and geometries of fuel cell.

However, the pseudopotential models presented in the above works are limited to single-component condition and cannot simulate the realistic droplet coalescence process in flow channel for some deficiencies including the large spurious velocity, thermodynamic inconsistency, low density and kinematice viscosity ratios and coupling between surface tension and some other critical properties [17]. In the capillary dominated area such as the GDL and catalyst layer (CL), the effects of these drawbacks may be neglectable. While in flow channel where capillary number is much larger, the effect of density and viscosity ratio must be considered [22]. Recently, Xu et al. [23] successfully simulated large density and kinematic viscosity ratio multiphase flow with tunable surface tension via single-component pseudopotential model, which is a huge progress. However, multi-component condition is not considered in this work, thus the droplet motion is driven by a defined body force instead of the shear force caused by air flow, which still cannot reflect the realistic droplet dynamic behavior in flow channel.

To the best of the authors' knowledge, realistic droplet coalescence in the flow channel of PEMFC has not been realized using LB method. In the present work, a developed multi-component multi-phase LB model with multiple-relaxation-time (MRT) collision operator is presented, realizing good thermodynamic consistency [24], tunable surface tension [25], low spurious current [26], high density [27] and kinematic viscosity ratios. Unlike the previous work, the droplet is driven by the air component flow instead of the extra body force or wall wettability gradient. And a new method for multiphase boundary is proposed