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Agglomerate modeling of cathode catalyst layer of a PEM fuel cell by the lattice Boltzmann method

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ABSTRACT

Lattice Boltzmann method is a relatively new micro-scale modeling technique for complex fluid systems that offers several advantages over more conventional numerical methods and hence has attracted interest of researchers. However, lattice Boltzmann modeling of PEM fuel cell electrodes has faced with some challenges in tackling electrochemical reaction in the catalyst layer. In the present study, a two-dimensional single-phase lattice Boltzmann agglomerate model of the cathode catalyst layer of a PEM fuel cell is developed for the first time. After validation of different aspects of the model, the reactive air flow in a cathode electrode is simulated through a multi-scale lattice Boltzmann approach. Species distributions in the pore region, electrical potential distribution in the electrolyte film, and current density distribution at the interface of membrane and catalyst layer are presented and analyzed; both uniform and non-uniform agglomerate arrangements are simulated. The novel model can be adopted to simulate reactive flow in a cathode catalyst layer with a more complicated arrangement of agglomerates representing a realistic microstructure.

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Introduction

New safe, reliable, cheap, and efficient energy sources and energy conversion devices are needed to respond to concerns over increased pollution and dwindling fossil fuel resources [1]. Among energy conversion devices compatible with such renewable energy sources, proton exchange membrane (PEM) fuel cells are currently in an advanced stage of development with a wide variety of promising applications. They can be a power source for mobile phones and computers, right through

boats and domestic systems, cars, buses and industrial combined heat and power systems [2].

Nevertheless, to decrease the cost and increase the durability of PEM fuel cells some challenges still exist which restrain their wide commercialization. This makes fundamental research for PEM fuel cell development inevitable. Modeling of reactant gas transport accompanied by electrochemical reactions in electrodes is critically demanded, particularly in the cathode where the oxygen reduction reaction is sluggish and inefficient [3]. Several numerical models of the cathode electrode with different features have been proposed in the literature [4]. In most of these models, the porous

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Nomenclature			
a_{agg}^{eff}	effective surface ratio of agglomerate	α	transfer coefficient
\vec{c}	particle velocity, $lu\ ts^{-12}$	ϵ_{agg}	Nafion fraction in agglomerate
c_s	speed of sound in lattice, $lu\ ts^{-1}$	η	local activation over-potential
D	diffusivity, $m^2\ s^{-1}$	λ	water content
D^{LB}	lattice Boltzmann diffusivity	λ_n	eigen-parameter in Eq. (40)
Da	Damköhler number	μ	dynamic viscosity, $kg\ m^{-1}\ s^{-1}$
E_{agg}	agglomerate effectiveness factor	ν	kinematic viscosity, $lu^2\ ts^{-1}$
E_{oc}	open-circuit potential, V	ρ	density, $lm\ lu^{-3}$ or $kg\ m^{-3}$
EW	equivalent molar mass of Nafion, $kg\ kmol^{-1}$	ρ^*	dimensionless density
e_{Pt}	effective surface ratio of Pt particles	σ	local proton conductivity of electrolyte, $S\ m^{-1}$
F	Faraday's constant, $A\ s\ mol^{-1}$	τ	relaxation time, ts
\vec{F}_{adh}^k	fluid–solid interaction force acting on a particle of type k, $lm\ lu\ ts^{-23}$	ϕ	local electrical potential, V
\vec{F}_{coh}^k	fluid–fluid interaction force acting on a particle of type k, $lm\ lu\ ts^{-2}$	Φ_1	Thiele's modulus
Fo	Fourier number	<i>Subscripts and superscripts</i>	
f	gas phase density distribution function	A	type A species
g	electrolyte phase density distribution function	agg	agglomerate
H	Henry's constant, $Pa\ m^3\ mol^{-1}$	as	agglomerate surface
j	current density, $A\ m^{-2}$	C	type C species
k	rate constant, $m\ s^{-1}$	c	cathode
k^{LB}	lattice Boltzmann rate constant	DN	dry Nafion
l	characteristic length scale, m	elect	electrolyte phase
MW	molar mass, $kg\ kmol^{-1}$	eq	equilibrium
P	pressure, Pa	er	electrochemical reaction
R_u	universal gas constant, $J\ mol^{-1}\ K^{-1}$	gas	gas phase
\vec{r}	particle position vector, lu	i	direction i of lattice
r	radius, m	if	interface
r''	rate of reaction per unit surface, $mol\ m^{-2}\ s^{-1}$	k	kth species
S_a	surface area per unit mass of a Pt particle, $m^2\ kg^{-1}$	LB	lattice Boltzmann
T	temperature, K	n	nitrogen
t	time, ts	N	Nafion
\vec{u}	velocity vector, $lu\ ts^{-1}$	o	oxygen
\vec{u}'	composite velocity vector in Eq. (4), $lu\ ts^{-1}$	Pt	platinum
V_{cell}	operating cell potential, V	p,q	position (p,q) of lattice
w	weighting factor	ref	reference
		sat	saturation
		sr	surface reaction
		w	water
<i>Greek symbols</i>			

medium of the cathode electrode is considered homogeneous and isotropic while it is highly non-homogeneous and anisotropic in reality [5]. In this regard, pore-scale numerical methods, which can capture real microstructure of the cathode electrode porous medium, are at the center of attention.

In recent years, the lattice Boltzmann method is applied as a powerful tool for pore-scale modeling of transport phenomena in complicated heterogeneous and anisotropic porous media such as gas diffusion layer (GDL) of PEM fuel cells. In fact, lattice Boltzmann method is superior to other conventional numerical methods through many aspects such as dealing with complex boundaries of a domain with complicated morphology, parallelization of the algorithm and modeling multi-phase fluid flow with a dynamic interface in a porous medium [6].

However, a significant challenge for lattice Boltzmann modeling of the cathode electrode is the simulation of electrochemical reaction in the catalyst layer (CL) [7]. To the best of the authors' knowledge, electrochemical reaction is taken into account in only a few of recent lattice Boltzmann investigations. In three of them [8–10], the catalyst layer is considered as a thin interface, so it is treated just as a boundary condition. In another case [11], the catalyst layer has an idealized microstructure with a solid phase with a reactive surface. Since electrolyte phase is not considered in this investigation, effective processes such as dissolution of oxygen at the pore-electrolyte interface, diffusion of oxygen in the electrolyte film toward reactive sites and back diffusion of produced water at the reactive sites out of electrolyte film are not considered. These processes have been taken into account in the agglomerate models of the catalyst layer implemented by conventional computational fluid dynamic methods [12–22]. Agglomerate models, which are more

² lu and ts are the unit of length and time in lattice Boltzmann method, respectively.

³ lm is the unit of mass in lattice Boltzmann method.

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