On continuum models for heat transfer in micro/nano-scale porous structures relevant for fuel cells

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ABSTRACT

Micro or even nano-scale solid particles are applied in porous structures in different energy systems, such as fuel cells, for the objectives to enhance the catalytic reaction activities and improve the fuel utilization efficiency or/and reduce the pollutants. In addition to the charge transport and reactions, heat transfer processes in fuel cell porous electrodes are strongly affected by the small scale and complex porous structures. In this paper, the thermal energy equations commonly used for continuum models at pore-level and porous-average level are outlined and highlighted, with the purpose to provide a general overview of the validity and the limitation of these approaches. Various models in the open literature are reviewed and discussed focusing on the important properties in the continuum methods, e.g., the effective thermal conductivity and interfacial/volumetric heat transfer coefficient between the fluid and solid surfaces. It is revealed that both the rarefaction and tortuous effects may be significant, but these have not been extensively studied yet in the micro/nano-scale heat transfer models relevant for the fuel cells. Comments and suggestions are presented for better understanding and implementation of the continuum heat transfer models for fuel cell electrodes.

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1. Introduction

Finite resources of conventional fossil fuels and associated gas emissions are two immense problems facing human beings. During recent years, a new trend is to apply micro or even nano-size particles in multi-functional porous materials within energy systems, for the objectives to improve the fuel utilization efficiency or/and reduce the pollutants exhausted from, e.g., in fuel cells, batteries, reformers and electrolysers [1]. Various heat transfer processes appear in heterogeneously distributed pores and solid matrices. These are strongly coupled with catalytic reactions and

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Nomenclature

A_{sf}	interfacial area		Nu	Nusselt number
Bi	Biot number		p	fluid pressure
c	specific heat		PEMFCs	proton exchange membrane fuel cells
CFD	computational fluid dynamics		Pr	Prandtl number
CG	coarse-graining		PTFE	polytetrafluoroethylene
CLs	catalyst layers		q	heat flux
CT	computer tomography		Re	Reynolds number
d	characteristic length		RVE	representative volume element
d_g	effective diameter of a fluid molecule		SOFCs	solid oxide fuel cells
D_k	Knudsen diffusion coefficient		SPH	smoothed particle hydrodynamics
d_{nom}	nominal pore diameter		T	temperature
DPD	dissipative particle dynamics		TPBs	triple phase boundaries
EMT	effective medium theory		u	velocity
FDM	finite difference method		$\mathbf{v}$	fluid velocity vector
FEM	finite element method			
FVM	finite volume method		*Greek symbols*	
GDL	gas diffusion layer		β	coefficient
h_f	interfacial heat transfer coefficient		ε	porosity
h_v	volumetric heat transfer coefficient		θ	dimensionless temperature
k	conductivity		λ	mean free path
k_B	Boltzmann constant (1.3807×10^{-23} J/K)		μ	dynamic viscosity
Kn	Knudsen number		ρ	density
k_r	conductivity ratio between the solid and the fluid phase (k_s/k_f)		τ	tortuosity
l	edge length		*Subscripts*	
LBM	lattice Boltzmann modeling		cont	continuous
LTE	local thermal equilibrium		disp	dispersed
LTNE	local thermal non-equilibrium		eff	effecitive
MD	molecular dynamics		f	fluid
ME	Maxwell–Eucken model		s	solid
Nr	necking ratio			

charge (proton/ions and electrons) transfer, e.g., in proton exchange membrane fuel cells (PEMFCs) and solid oxide fuel cells (SOFCs) [2–7].

In addition to the complex porous structures, rarefaction of the fluid flow and mass transfer at small scales has a significant effect on heat transfer. The Knudsen number, Kn, based on the ratio of average distance between gas collisions (or the mean free path) and the pore/particle size falls into the slip flow (temperature jump) or transition regions. The interactions between the fluid and solid walls within the small scale and porous structures become strong and should be taken into account. Recently there are several microscopic models available trying to capture the real material structures and transport processes in the porous electrodes and catalyst layers (CLs) from atomistic to nano-scales, involving molecular dynamics (MD) and pseudo-particle methods. MD approach takes into account the movements and collisions of all individual molecules at sub-nanoscales, and provides realistic equations of transport processes with/without reactions, to study the mechanisms of fluid and charge transport and surface reactions. However, it is computationally too expensive (or impossible) to cover all the interactions for such a big number of molecules representing the actual electrodes and CLs [8,9]. On the other hand, the so-called pseudo-particle models (PPMs), e.g., lattice-based lattice Boltzmann modeling (LBM), and off-lattice ones including the coarse-graining (CG) MD, dissipative particle dynamics (DPD), smoothed particle hydrodynamics (SPH), have been developed for self-organization of membrane electrolytes at different hydration levels and CL material morphology [10–16]. In these models, a particle represents a small cluster of atoms or molecules, and the particle–particle interactions are much softer than those in

MD models. Therefore it is feasible to take much larger particle sizes and time steps to study the material structures and hydrodynamics occurring in larger length- and time scales than in the less coarse models (e.g., MD). However, none of them were able to take all the important aspects into account, such as the CL microscopic materials and structures (heat transfer at the interfaces between the solid surface and the fluid), catalytic reactions (heat generation/consumption) [8], particularly multi-phase flow (heat transfer between liquid water and vapor due to state change) [17].

On the other hand, the macroscopic transport model (such as computational fluid dynamics, CFD) have been extensively developed, based on the volume averaging method and treating the porous structure as a black box or as a macrohomogeneous porous region (uniformly distributed spheres or agglomerates) [18–20]. With a specified set of suitable boundary conditions, the governing differential equations can be properly discretized on a computational grid using standard CFD techniques, such as finite difference method (FDM), finite volume method (FVM) or finite element method (FEM) [21,22]. These approaches lead to a much simpler mathematical modeling method and correspondingly less numerical effort is required. However, these methodologies are developed on the basis of the so-called continuum theory, and the significant challenge is how to capture the effects of both rarefaction (small particle/pore size) and structural morphology of the porous electrodes/catalyst layers, and how to take into account effects of the interactions at the interfaces between the fluid and solid particle surfaces.

Regarding the continuum method for mass transfer analysis, several approaches are available for determining the gas-phase species diffusion flux in the connected pores, e.g., Fick's law, the