



Review

On mechanisms and models of multi-component gas diffusion in porous structures of fuel cell electrodes



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ARTICLE INFO

Article history:

Received 6 September 2013
 Received in revised form 16 October 2013
 Accepted 16 October 2013
 Available online 9 November 2013

Keywords:

Mass diffusion
 Porous structures
 Fuel cells
 Modeling
 Tortuosity factor

ABSTRACT

Small scale particles/pores from micrometers and down to nanometers often occur in multi-functional porous electrodes in fuel cells, to enhance the catalytic reaction activities and accordingly the cell performance. Multi-component and -phase mass transport phenomena of reactants and products are strongly coupled with other transport processes as well as various reactions. All these processes form inter-linked circuits for the mass, heat and electricity, which determine electrode design, cell structure/configuration and operation, hence overall performance. Understanding of gas diffusion mechanisms and accurate estimating of the overall diffusion coefficient are essential for the operation and design of fuel cells, especially at high current density conditions. Several intensive research and investigations have appeared in recent years involving both experimental and modeling approaches for porous structure reconstruction and evaluation of effective diffusion coefficients. In this paper, the mass transfer equations commonly used for continuum models at porous-average level are outlined and highlighted, with the purpose to provide a general overview of the validity and the limitation of these approaches. The most often used models in the open literature are reviewed and discussed focusing on the effective gas diffusion coefficients and tortuosity factors. It is revealed that the effects of both small scale (Knudsen number) and tortuous pathways (tortuosity factor) on the effective diffusion coefficients are significant for the specific layers in the electrodes. Summary and suggestions are also provided for better understanding of gas diffusion phenomena and implementation of the effective gas diffusion coefficient models for fuel cell electrodes.

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1. Introduction

Limited resources of conventional fossil fuels, as well as the generated harmful chemical and greenhouse gas emissions bring

immense problems for earth inhabitants. With its high energy efficiency and minimal total emission emitted, fuel cells are considered as a new player in energy technologies, ranging from mobile (transportation), to stationary co-generation, and to portable consumer electronics. Micro- or even nanometer scale particles have been often employed in multi-functional porous materials within fuel cell electrodes, including support substrate layer or gas

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Nomenclature

BFM	binary friction model	Pr	Prandtl number
c	specific heat or gas concentration	PTFE	polytetrafluoroethylene
CFD	computational fluid dynamics	\mathfrak{R}	universal gas constant
CG	coarse-graining	RVE	representative volume element
CL	catalyst layer	S	cross-section area
CT	computer tomography	SEM	scanning electron microscopy
d_p	characteristic pore diameter	SOFCs	solid oxide fuel cells
d_g	effective diameter of a fluid molecule	SPH	smoothed particle hydrodynamics
D_K	Knudsen diffusion coefficient	t	time
DGM	dusty gas model	T	temperature
DPD	dissipative particle dynamics	TPBs	triple phase boundaries
FDM	finite difference method	u	velocity
FEM	finite element method	v	diffusion volume
FIB	focused ion beam	\mathbf{v}	velocity vector
FVM	finite volume method	y	molar fraction
GDL	gas diffusion layer in PEMFCs		
IP	in-plane		
J	mass diffusion flux	<i>Greek symbols</i>	
k_B	Boltzmann constant (1.3807×10^{-23} J/K)	β	coefficient
Kn	Knudsen number	ε	porosity
l	length or thickness	λ	mean free path
LBM	lattice Boltzmann modeling	μ	dynamic viscosity
M	molecular weight	ρ	density
MBFM	modified binary friction model	τ	tortuosity
MD	molecular dynamics	ω	mass fraction
ME	Maxwell–Eucken model		
MPL	micro porous layer in PEMFCs	<i>Sub- and superscripts</i>	
MSD	mean-square displacement	eff	effective
MSM	Maxwell–Stefan model	f	fluid
MSP	Method of Standard Porosimetry	K	Knudsen
N	molar diffusion flux	m	gas species mixture
p	pressure	s	solid
PEMFCs	proton exchange membrane fuel cells		

diffusion layer (GDL), micro porous layer (MPL) and catalyst layer (CL) [1,2]. Various mass transfer processes appear in heterogeneously distributed pores, which are strongly coupled with catalytic reactions and other transport processes including heat and charge (proton/ions and electrons) transfer, e.g., in proton exchange membrane fuel cells (PEMFCs) [3–8] and solid oxide fuel cells (SOFCs) [9].

A fuel cell is an electrochemical device to convert the chemical energy of hydrogen and oxygen efficiently into electricity at the active interface regions between the electrode and electrolyte. A typical electrode consists of various porous layers wherein charges and chemical species are transported and reacting. The catalyst layer in the electrode consists of electrochemical catalyst particles (often platinum in PEMFCs and Ni in SOFCs), supported on larger carbon particles for electron transfer and ionomer for proton transfer in PEMFCs, while YSZ (yttria stabilized zirconia) for oxygen ion transfer and metal materials (Ni or lanthanum strontium manganite, the so-called LSM) for electrons in SOFCs, surrounded by connected voids for the reactants and products. During fuel cell operation, hydrogen and oxygen gases supplied in the channels (or ducts) will be transported through the gas diffusion layer (GDL) or support substrate to the reaction regions. In PEMFCs, a micro porous layer (MPL) is often employed between the GDL and CL for objectives to facilitate water transport and removal, which is a specific issue important for the PEMFC cathode operation and performance [2]. The porous electrodes in fuel cells are usually called the multi-functional components consisting of

various phases for transport of the fluid, heat and charges (ions and electrons), respectively. The composition of the involved solid materials and the size of voids should be well designed and controlled to improve the inter-related mass, heat and electricity transport processes. Any weak spot in an individual process will adversely impact the other transport phenomena, and further the reactions and the overall performance of the cell.

To evaluate the fuel cell performance, three types of energy losses (or polarizations) need consideration, i.e., activation loss, concentration loss and ohmic loss. The ohmic loss is due to charge transfer occurring across all fuel cell components based on the generated current density. The activation loss, on the other hand, appears by offsetting the energy barrier for the electrochemical reactions in the so-called TPB (triple phase boundary between the electron phase, charge phase and void space) sites, in the PEMFC CLs or SOFC active reaction regions close to the electrolyte layer. The concentration loss is deduced due to limited transport rates of the reactants and/or the products to/from the reaction sites. It should be mentioned that the concentration loss is particularly significant when the current density is high, because the required reactant flow rate is big [2]. Due to the solid materials through which there is no mass transport, the rates for the fluid species transfer can be significantly lower than those through air, depending on porosity, pore size distribution and pore connection features [10]. As revealed in [11,12], the measured oxygen with nitrogen binary diffusion coefficient through the PEMFC GDL/MPL assembly is only about 5–15% of the ordinary (molecular) diffusion

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