Journal of Power Sources 187 (2009) 431–443

Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

Two-phase flow and maldistribution in gas channels of a polymer electrolyte fuel cell

Suman Basu*, Jun Li, Chao-Yang Wang

Department of Mechanical and Nuclear Engineering, and Electrochemical Engine Center (ECEC), The Pennsylvania State University, University Park, PA 16802, United States

ARTICLE INFO

Article history:
Received 7 October 2008
Received in revised form 7 November 2008
Accepted 7 November 2008
Available online 21 November 2008

Keywords:
PEFC
Two-phase flow
Gas channel
Flow maldistribution
Pressure drop

ABSTRACT

Liquid water transport in a polymer electrolyte fuel cell (PEFC) is a major issue for automotive applications. Mist flow with tiny droplets suspended in gas has been commonly assumed for channel flow while two-phase flow has been modeled in other cell components. However, experimental studies have found that two-phase flow in the channels has a profound effect on PEFC performance, stability and durability. Therefore, a complete two-phase flow model is developed in this work for PEFC including two-phase flow in both anode and cathode channels. The model is validated against experimental data of the wetted area ratio and pressure drop in the cathode side. Due to the intrusion of soft gas diffusion layer (GDL) material in the channels, flow resistance is higher in some channels than in others. The resulting flow maldistribution among PEFC channels is of great concern because non-uniform distributions of fuel and oxidizer result in non-uniform reaction rates and thus adversely affect PEFC performance and durability. The two-phase flow maldistribution among the parallel channels in an operating PEFC is explored in detail.

1. Introduction

The portability, compactness, zero emission and high power output at low temperature has made the polymer electrolyte fuel cell (PEFC) one of the most potent replacements for the internal combustion engines [1]. This new focus has led to an urgent need for identification, understanding, prediction, control, and optimization of various transport and electrochemical processes that occur on disparate length scales in fuel cells [2]. Recent studies have shown that among all transport phenomena, the two-phase transport of water in the PEFC to maintain water balance is the most critical to cell performance.

A typical PEFC and its components are schematically displayed in Fig. 1a. A PEFC model should consider transport phenomena with electrochemical kinetics and charge transport of both electrons and protons in disparate length and time scales [2]. The need for detailed model validation has been increasingly acknowledged by the PEFC research community because the global current–voltage curve is largely inadequate to differentiate various transport and electrochemical processes.

Much effort has been directed toward PEFC modeling [2–5]. Although water is essential for membrane proton conductivity, excess water can initiate channel flooding, blocking the pores of GDL and catalyst layer and hampering the reactant transport [6,7]. Channel flooding refers to a situation where a substantial fraction of liquid water accumulates in gas channels. Given the low startup temperatures (room temperature) for automobile applications, two-phase flow is unavoidable for automobile fuel cells. Therefore, its understanding and prediction is critical for good PEFC design. Two-phase transport in a PEFC consists of three subprocesses: (1) liquid water accumulation and transport in catalyst layers, (2) two-phase transport in GDL and MPLs, along with the interfacial coverage at the GDL surface, and (3) two-phase flow in gas channels. All two-phase flow modeling efforts in PEFC in the literature were on the first two sub-processes [8–13]. Ample experimental evidence, however, indicates that the channel flooding plays a pivotal role in water management, particularly at low current densities where gas velocity is insufficiently low to drain liquid water out of the channels. The low load regime is particularly important for PEFC engines due to its potential of high energy conversion efficiency and it is most frequently used.

The flooding problem is compounded by GDL intrusion into the channels. PEFC is operated under high compression to minimize the contact resistance between the land and GDL. The high compression pressure pushes the softer GDL material into the channel, blocking the channels partially as shown in Fig. 1b. Compression pressure is highest at the edge (near the location of tightening bolts) and therefore GDL intrusion is most severe at the edge channels. Flow through the intruded channel is reduced under the same pressure drop, thereby making it more difficult to flush liquid water out of

* Corresponding author. Tel.: +1 814 865 9768.
E-mail address: sxb967@psu.edu (S. Basu).

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doi:10.1016/j.jpowsour.2008.11.039

Nomenclature

A	area
C_i	local concentration of species i, mol m^{-3}
D_i	diffusion coefficient of species i, m^2 s^{-1}
d	diameter
I	current density, A cm^{-2}
K	permeability of the porous media
k	relative permeability of the phase
M	molecular weight
mf_l^k	mass fraction of species k in liquid phase
n	normal direction
P	pressure, Pa
S	source term in the governing equations
s	liquid water saturation/volume fraction
T	absolute temperature, K
u	velocity
x	x coordinate, μm
y	y coordinate, μm
z	z coordinate, μm

Greek letters

α	net water transport coefficient
ρ	density
ε	porosity
γ	correction factor
κ	electrolyte conductivity, S m^{-1}
λ	relative mobility
σ	surface tension coefficient (N m^{-1})
ξ	Stoichiometry at gas channel inlet (anode or cathode)
ν	kinematic viscosity

Subscripts and superscripts

g	gas phase
l	liquid species
eff	effective
sat	saturation
r	relative
c	convective correction
mem	membrane
in	inlet
ph	phase
avg	average
H_2O	water
O_2	oxygen

the channel. This exacerbates channel flooding and accelerates the mass transport loss as well as leads to operational instability. The worst scenario is total blockage of a channel by liquid water. The maldistribution of flow in parallel channels has profound performance and durability implications, and a serious loss of efficiency is possible as the whole channel is lost due to blockage. Hence, for a PEFC to maintain stable performance, flooding of the channels must be avoided.

Channel flooding in PEFCs has received increased attention in the fuel cell community [14–26]. A friction factor similar to that in the case of laminar flow through a circular channel was proposed for the PEFC channels [14]. Preferential entry of inlet flow in parallel channels was attributed partly to the formation of recirculation vortex at the inlet [15]. Single-phase flow in the channel has been used widely in the gas channel for design purposes [16,17,18] but experimental observations indicate presence of liquid water in the PEFC gas channels [19,20]. Attempts have been made to use analytically calculated dry length of a gas channel as a design tool for PEFC channel flow field design [21]. Others used the void-in-fluid (VOF) method [22–26] to compute two-phase flow in the gas channels. Unfortunately, these models are computationally expensive and have not been integrated with the other components of a PEFC.

Few experimental investigations on flow distribution in the PEFC channels exist in literature [14,19,20,27]. While mist flow model and film flow model have been used for the extreme cases of high gas velocity (liquid volume fraction <0.1%) and low gas velocity/highly hydrophilic channel wall (liquid volume fraction >10%), respectively, a general model covering a common range of liquid fraction and capable of capturing flow maldistribution was absent. Such a general model will enable the prediction of channel flooding, two-phase flow maldistribution in multiple, parallel channels, and the flow-field effect on liquid water removal in operating PEFCs.

In the present work, we first couple a recently developed two-phase channel flow model with other two-phase models for the catalyst layer and GDL previously developed in our laboratory to form a complete two-phase model for an entire PEFC. The channel two-phase model [28,29] is based on the framework of multi-phase mixture model (M^2 model) and capable of predicting the liquid water volume fraction and pressure along the flow direction. Then, the complete model is validated against experimental data of wetted area ratio and pressure drop over a range of operating conditions. Finally, this complete two-phase model is employed to study the effects of GDL intrusion and manifold design on reducing flow maldistribution.

2. Mathematical model

A PEFC consists of seven sub-regions – anode gas channel, anode GDL, anode catalyst layer, ionomeric membrane, cathode catalyst layer, cathode GDL and cathode gas channel. In addition, the electron transport through bipolar plates may be important in some cases [30]. The membrane is a solid-state electrolyte with water and proton co-transport taking place through its ionomer phase. Full descriptions of electrochemical and transport phenomena in a PEFC already exist in the literature [2] and are not repeated here.

Two-phase flow and transport in a PEFC are governed by the laws of momentum, mass, energy, species and charge conservation. Under non-isothermal, two-phase conditions the conservation equations of mass, momentum, energy, species and charge equations in the PEFC can be written as [30–32]

$$\text{Mass}: \quad \nabla\cdot(\rho\vec{u}) = 0 \tag{1}$$

$$\text{Momentum}: \quad \frac{1}{\varepsilon^2}\nabla\cdot(\rho\vec{u}\vec{u}) = -\nabla P - \nabla\cdot(\rho\tau) + S_u \tag{2}$$

$$\text{Energy}: \quad \nabla\cdot(\gamma_T\rho C_p\vec{u}T) = \nabla\cdot(k_{eff}\nabla T) + S_T \tag{3}$$

$$\text{Species}: \quad \nabla\cdot(\gamma_c\vec{u}C^k) = \nabla\cdot(D_g^{k,eff}\nabla C_g^k) - \nabla\cdot\left[\left(\frac{mf_l^k}{M^k} - \frac{C_g^k}{\rho_g}\right)\vec{j}_l\right] + S_k \tag{4}$$

$$\text{Charge (electrons)}: \quad \nabla\cdot(\sigma^{eff}\nabla\Phi_s) + S_{\Phi_s} = 0 \tag{5}$$

$$\text{Charge (protons)}: \quad \nabla\cdot(k^{eff}\nabla\Phi_e) + S_{\Phi_e} = 0 \tag{6}$$

The source terms are tabulated in Table 1. Details about these equations and the source terms are available in the literature [31,32]. The present modeling approach is to view all components in a PEFC as porous media. Specially, we model flow channels of typical dimension between 0.2 and 1 mm as a structured porous media or a bundle of straight capillary tubes. Hence, we apply the two-phase flow theory based on extended Darcy's law to describe two-phase