

Mass/electron co-transport in an air-breathing cathode of a PEM fuel cell

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Abstract

Mass/electron transports in a passive cathode of a proton exchange membrane (PEM) fuel cell have been studied numerically. The porous cathode in contact with a perforated current collector breathes fresh air through an array of orifices. Diffusions of reactant species in the porous cathodes are described by the Stefan–Maxwell equation. Electrochemical reaction on the surfaces of the porous cathode is depicted via the Butler–Volmer equation. Gas flow in the air-breathing porous cathodes is governed by isotropic linear resistance model with constant porosity and permeability. The electron/ion transports in the catalyst/electrolyte are dealt with the charge conservations based on the Ohm's law. A finite-element method is employed to solve the above-coupled equations. The effect of overpotential on the fluid flow, mass transport and electrochemistry is examined. Detailed electrochemical/mass characteristics such as flow velocities, species mass fraction, species flux and current density distributions are presented. They can provide a solid basis for optimizing the geometry of the PEM fuel cell stack running with a passive mode.

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1. Introduction

The increasing number of portable electronic devices on the market today such as laptop computers, cellular phones, PDAs, remote-controlled toys, is creating a demand for improved, more environmentally friendly technologies in energy storage and conversion. Small-scale fuel cells are regarded as a potential candidate in replacing batteries in portable applications [1,2]. However, up to the present time, fuel cells were still too complicated and expensive to meet the need because they required cooling, humidification and pressurization sub-systems in operation. In response, researchers and engineers are trying to develop passive fuel cells for portable power applications. One interesting approach is air-breathing fuel cells, i.e. the oxygen needed by the electrochemical reaction is taken directly from the surrounding air by diffusion and/or natural convection. The fuel cell running in a passive manner has the benefits of minimizing the number of power consumed auxiliary devices that enhances the

system efficiency. However, the power density of cell itself is not as good as that running in an active mode due to poor transport mechanisms [3–13]. It is well known that the current production by electrochemical reaction is directly proportional to the local oxygen concentration in the fuel cell. Inadequate airflow cannot provide enough oxygen for the electrochemical reaction on the active surfaces. It results in heterogeneous current distribution in the electrode that reduces the performance of the fuel cell. Thus, one of the most challenges in the design of passive fuel cells is how to feed the electrode with reactants and remove the products from the electrode appropriately.

The objective of the present paper is to numerically study the transport phenomena in a passive mode cathode of a PEM fuel cell that operates without external forced flows. The porous cathode is attached to a perforated current collector. It breathes the fresh air through the perforations and routes out the electric current through its solid counterpart. A set of conservation equations of mass, momentum, species and charge is developed. The Darcy law describes the fluid flow characteristics in the porous cathode. The Stefan–Maxwell equations illustrate the multi-species diffusion in the porous cathode. The Butler–Volmer equation depicts the electrochemical reaction on the surfaces of

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Nomenclature

c_i	mole concentration of the species i (mol m^{-3}), $c_i = \left[\frac{\omega_i}{M_i} / \sum_j \frac{\omega_j}{M_j} \right] \frac{P}{RT}$
$D_{\text{H}_2\text{O}}$	diffusivity of water vapor ($\text{m}^2 \text{s}^{-1}$)
D_{O_2}	diffusivity of oxygen ($\text{m}^2 \text{s}^{-1}$)
F	Faraday's constant
i_{ct}	current density (A m^{-2})
M	molecular weight (kg mol^{-1})
n	mass flux ($\text{kg m}^2 \text{s}^{-1}$)
p	pressure (Pa)
$p_{i,m}$	possibility of the electrolyte in the connection of the catalyst layer
$p_{i,s}$	possibility of the catalyst in the connection of the catalyst layer
R	universal gas constant ($\text{W mol}^{-1} \text{K}^{-1}$)
T	temperature (K)
\mathbf{u}	velocity vectors (m s^{-1})
x, y, z	coordinate system, Fig. 1 (m)

Greek symbols

α	symmetric factor
ε	cathode porosity
ϕ_l	potential of the ionic conductor (electrolyte-phase) (V)
ϕ_s	potential of the electric conductor (catalyst-phase) (V)
η_t	total overpotential across the computational module (V)
κ	permeability (m^2)
μ	dynamic viscosity (m s^{-2})
ρ	density (kg m^3)
σ_l	ionic conductivity of the membrane phase (S m^{-1})
σ_s	electric conductivity of the catalyst-phase (S m^{-1})
τ	tortuosity
v_l	volume fraction of the ionic conductor (electrolyte-phase) in the cathode
v_s	volume fraction of the electronic conductor (catalyst-phase) in the cathode
ω	mass fraction

the porous cathode. A finite-element based computational fluid dynamics (CFD) [14,15] methodology is employed to solve the multi-physics transports in the air-breathing cathode of a PEM fuel cell. Emphasis is placed on the effect of the total overpotential on the species/electron co-transports in a porous cathode of a PEM fuel cell. The relation between the current distributions and the mass transports are discussed in detail. The informative results obtained by the present study can help in understanding of the local gas transports and electrochemical characteristics in an air-breathing PEM fuel cell. Also, they can provide a solid

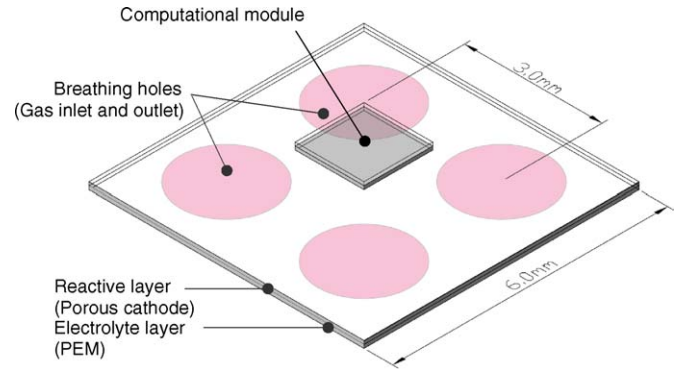


Fig. 1. Fuel cell cathode with a perforated current collector.

basis for optimizing the geometry of the passive PEM fuel cell stack.

2. Model descriptions

2.1. Governing equations

Fig. 1 shows a typical geometry of a self-breathing cathode of a PEM fuel cell with perforated current collectors, which is often seen in mini- or micro-fuel cells [16,17]. The pink circular zones on top surfaces of the module are the cathode inlets that are open to the ambient, while the rest of the top surfaces sit flush against the current collector. Due to the perforation layout, a 3D model is needed to simulate the mass transport, current and reaction distributions. For memory and time saving, a unit cell shown in Fig. 2 is considered in the present study. The unit cell is $1.5 \text{ mm} \times 1.5 \text{ mm}$ in surface, and the gas inlet/outlet hole has a radius of 1.0 mm . Both the reactive layer and the electrolyte layer are $75 \mu\text{m}$ thick. The origin of the coordinate system is set to the remote corner of the unit cell, as shown in Fig. 2.

The upper rectangular domain is a porous structure that contains the feed gas mixture, an electronically conducting material (catalyst) and an ionically conducting material (electrolyte). The oxygen reduction reaction takes place in the reactive layer. It can be represented by the following equations.

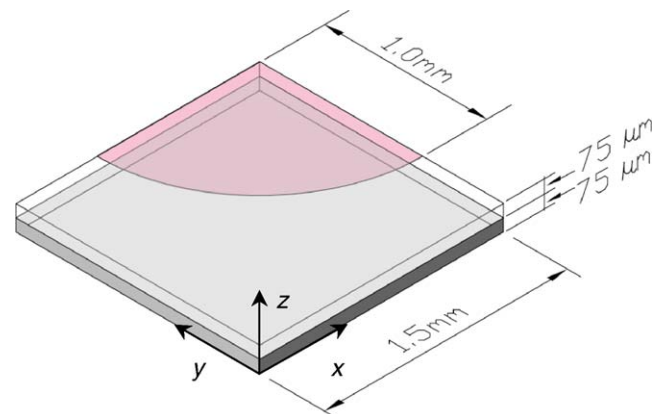


Fig. 2. Dimensions and the coordinate system of the computational module.

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