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Numerical study of the effect of the channel and electrode geometry on the performance of microfluidic fuel cells

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ABSTRACT

Using COMSOL Multiphysics 3.5, 3D numerical models of different microfluidic fuel cells have been developed in this paper to determine the effect of different modifications which have been implemented in the microfluidic fuel cell since its advent. These modifications include the channel geometry aspect ratio and electrode configuration, the third flow between the anolyte and catholyte in the channel (i.e., multi-stream laminar flow), and multiple periodically placed inlets. To be consistent with the convention, the output power of the device is normalized by the electrode surface area; however, the power density calculations are also performed through normalization by the device volume. It is shown that the latter method is more realistic and providing more information from the design point of view since the ultimate goal in designing the microfluidic fuel cell is to fabricate a compact, yet powerful device. Finally, a novel design of the microfluidic fuel cell with a tapered channel is suggested and compared to the non-tapered geometry through the polarization curves. The steps which have been taken in COMSOL to obtain these polarization curves are clearly and thoroughly explained. The Butler–Volmer equation was implemented to incorporate for the electrochemical reactions at the electrodes. The "Conductive Media DC" module, in COMSOL, is used to model the electric fields within the fuel cell. The concentration distributions of the reactant species are obtained using the "Incompressible Navier–Stokes" and "Convection and Diffusion" modules. Solving these equations together predicts the current density for given cell voltage values. The results demonstrate the cell voltage losses due to activation, ohmic and concentration overpotentials. It is shown that for a fixed value of the cell voltage (say 0.45 V), the fuel cell with multiple periodically placed inlets has the highest fuel utilization (i.e., 62.3%); while the "Simple square" geometry depicts 13.8% fuel utilization at this potential. Thus, the multiple-inlets design is particularly suitable for low-voltage applications which require high current. Also, the results of the tapered geometry proposed in this paper show that tapering the channel enhances the polarization curve comparing to the square cross-section geometry with extended electrodes. In essence, the fuel utilization of the "Extended square" geometry is increased from 15.4% to 57.6% by tapering the channel. This is due to the fact that the mixing region growth rate is restricted in the tapered geometry, and hence the electrodes on the top and bottom walls of the channel can be more extended toward the centre of the channel before the crossover occurs.

1. Introduction

Recently, there has been a growing demand for small but high power sources of energy for portable devices which are expected to function for long periods of time without the need for recharging [1] (such as global positioning systems, laptops and mobile phones). The current battery technology can hardly keep up with this growing power demand [2]. A recent comparison between Li-ion batteries and fuel cells has shown that the latter has much higher power density, and hence more potential to respond to the future market [2]. Since the reactions in fuel cells are surface based, miniaturization of fuel cells, which increases the surface-to-volume ratio, leads to even further improvements in the power density [3,4]. Thus, miniaturized fuel cells are capable of bridging the gap between the battery technology and the high power density required for the portable applications. A prodigious amount of research has been conducted on the miniaturization of the conventional fuel cells [5–7]. Although the energy density of the miniaturized fuel cell increases as its size continues to shrink, several technological and mechanical challenges (e.g., issues related to water and heat management, the ohmic overpotential caused by the membrane, and machining of the graphite bipolar plates) still remain [6,8]. These challenges limit the further decrease in the size, and hence

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Nomenclature

A	cross-sectional area of the charge transfer
D	diffusion coefficient
$E_{REVERSIBLE}$	reversible potential
F	Faraday constant
H	height of the channel
R	universal gas constant
R_f	ohmic resistance for ionic transport
S	consumption rate of reactant species
T	cell temperature
U	average flow velocity
ai_0	exchange current density
c	local concentration of the reactants
d	distance between the anode and cathode
e	mole number
i	rate of the electrochemical reaction
n	number of electrons transferred in the reaction
p	pressure
v	velocity
x	distance fluid travels down the channel
α	charge transfer coefficient
δ	inter-diffusion region width
η	activation overpotential
μ	viscosity
ρ	density
σ	ionic conductivity
ϕ_e	local potential in the electrolyte
ϕ_s	solid phase voltage

limit the increase in the power density of the miniaturized fuel cells.

Recently, a novel design and structure of the fuel cell, called the microfluidic fuel cell, has been introduced to overcome the above limitations of the miniaturized fuel cells. Fig. 1 presents the schematic of a typical Y-shaped microfluidic fuel cell. In such systems, the fuel and oxidant are introduced into a microchannel through separate inlets and form a side-by-side co-laminar flow between the electrodes, which are typically positioned along the channel. Laminar flow maintains separation of the fuel and oxidant. This eliminates the need for the membrane and overcomes the membrane-related issues (such as the ohmic overpotential and water management) mentioned for the miniaturized fuel cells. Due to the laminar nature of the flow in these systems, the transport phenomenon is diffusion limited, and hence the channel geometry plays an important role. As the fuel and oxidant streams travel down the channel the inter-diffusion region (i.e., mixing region) is established and grows due to the transportation of reactants from their own side to the other side through diffusion. This mixing region limits the amount of the reactants that can be potentially

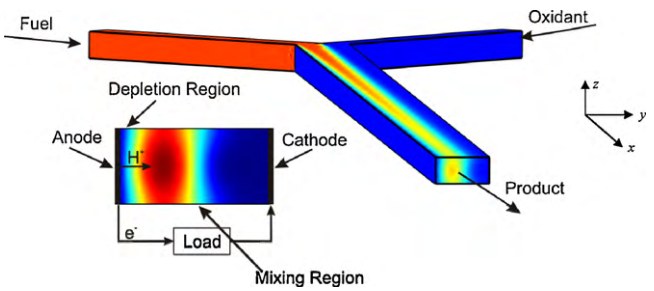

Fig. 1. A schematic of a typical Y-shaped microfluidic fuel cell.

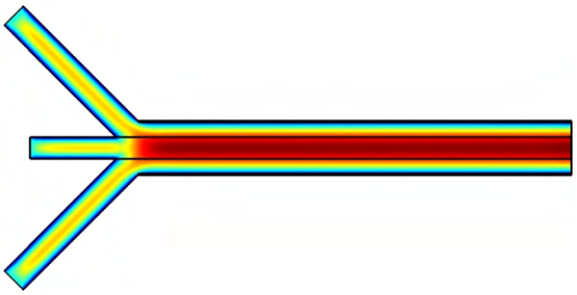

Fig. 2. A schematic of a microfluidic fuel cell with the third electrolyte stream (this schematic shows the velocity field in the microfluidic fuel cell).

available to the electrodes. This will also limit the extension of the electrodes from the wall toward the middle of the channel (which is desirable since it increases the active surface area) due the crossover issue [1]. At the same time, there is a concentration boundary layer forming on each electrode as the fluid is traveling toward the end of the channel. This concentration boundary layer (also known as depletion layer) is acting as a resistance for the reactants to reach to the active surfaces. It is desirable to have a thin depletion layer all over the electrodes.

Bazylak et al. [1] examined three different channel cross-sections with different aspect ratios, obtained the fuel and oxidant distribution, and calculated the fuel utilization. They found that the rectangular cross-sections have higher fuel utilization compared to the square ones. Chang et al. [9] also conducted a numerical analysis for a fixed flow rate and a fixed channel cross-section aspect ratio (i.e., height to width ratio). They reported that the reduction of cross-sectional area results in higher fuel cell performance. They also observed that for a constant cross-sectional area, the high aspect ratio results in a higher cell performance. The improved performance can be associated with two facts: (1) the higher the channel height, the higher the Peclet number (i.e., $Pe = UH/D$ which represents the convective to diffusive transport). The higher the Peclet number the faster the depletion regions are filled with fresh reactants, so higher current is produced by the cell; (2) in high aspect ratio geometries, the anode and cathode electrodes are closer to each other; therefore, the resistance to proton transfer in the electrolyte (Eq. (1)) is reduced [10]:

$$R_f = \frac{d}{\sigma A} \tag{1}$$

In this equation, R_f is the ohmic resistance for ionic transport, d represents the distance between the anode and cathode, σ refers to ionic conductivity and A is the cross-sectional area of the charge transfer.

Besides the channel aspect ratio and the electrode configurations, there have been a few more geometrical modifications suggested over the past few years [1,11–13]. For instance, Sun et al. [11] proposed a multi-stream laminar flow microfluidic fuel cell which is basically the same as a typical membraneless Y-shaped microfluidic fuel cell except with three inlets. Fig. 2 presents this design. The third stream is inserted between the fuel and oxidant streams to keep the anolyte and catholyte separated as they travel down the channel. The effect of inserting the third flow is similar to reducing the width of the channel, as it presses the concentration boundary layers against the electrodes which are on the side walls. This speeds up the electrochemical reactions since these reactions are a function of concentration gradient at the electrodes. In addition to the above advantage, the overall ionic resistance between the anode and cathode can be decreased if the third stream electrolyte has high proton conductivity (e.g., changing the sulfuric acid concentration in the third electrolyte affects its ionic conductivity).