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Improved fuel utilization in microfluidic fuel cells: A computational study

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Abstract

Presented in this paper is a computational analysis of a membraneless microfluidic fuel cell that uses the laminar nature of microflows to maintain the separation of fuel and oxidant streams. The fuel cell consists of a T-shaped microfluidic channel with liquid fuel and oxidant entering at separate inlets and flowing in parallel without turbulent or convective mixing. Recent experimental studies have established proof-of-concept of such fuel cells and have also shown that their performance is greatly limited by poor fuel utilization. Improving fuel utilization while minimizing fuel-oxidant mixing in microfluidic fuel cells is the focus of this study. A concise electrochemical model of the key reactions and appropriate boundary conditions are presented in conjunction with the development of a computational fluid dynamic (CFD) model of this system that accounts for coupled flow, species transport and reaction kinetics. 3D numerical simulations show that the fuel cell is diffusion limited, and both microchannel and electrode geometry play key roles in system performance. Three cross-sectional geometries are investigated, and a high aspect ratio rectangular geometry results in a two-fold increase in fuel utilization compared to a square geometry with the same hydraulic diameter. By tailoring the flow rate to the axial length of the fuel cell, fuel utilization is increased to 23%. Using the numerical simulation to guide the electrode design process, an extended tapered-electrode design is proposed. Simulations of the tapered-electrode microfluidic fuel cell demonstrate a fuel utilization of over 50%.

Keywords: Membraneless fuel cell; Microfluidic fuel cell; CFD; Laminar flow; Modelling; Simulation

1. Introduction

Micro-sized power sources are needed for small, portable devices capable of operating for long periods without recharging, such as cell phones and laptop computers through to more specialized devices such as remote sensors, global positioning devices, and in vivo diagnostic medical devices. It is predicted [1] that battery technology will not keep pace with these growing portable-power demands, particularly with the next wave of wireless technology, broadband mobile computing. Microstructured fuel cells have the potential to bridge the gap between battery technology and growing portable-power demands, by providing longer duration per weight and volume, quasi-instant recharge, and constant discharge. Recent developments in the field have benefited from micromanufacturing technology and biological and chemical lab-on-a-chip concepts that have been a driving force behind the recent developments of many microfluidic devices [2]. Other emerging application areas for microfluidics include electronic cooling, aerospace, and printing [3].

Since all reactions taking place in fuel cells are surface based, the increase in the surface-to-volume ratio accompanying miniaturization leads to a fundamental improvement in power density [4,5]. There are, however, mechanical limits to the miniaturization of conventional fuel cells [6]: machining graphite bipolar plates becomes difficult, and decreasing the size of the membrane and substrate decreases their support-

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Nomenclature

A	pre-exponential factor
C_i	concentration of cell i
C_i^{mixed}	concentration of perfectly mixed solution at cell i
C_i^0	concentration of solution at cell i in the absence of mixing
D_i	diffusion coefficient
E	potential at electrode
E_a	activation energy
E_{rev}	reversible potential
F	Faraday constant
h	channel height
J_i	flux of species i
k	rate constant
n	number of electrons
N	total number of cells
P	static pressure
R	gas constant
R_{cell}	ionic resistance of electrolyte
R_i	net rate of production of species i
t	time
T	temperature
U	average fluid velocity
v	rate law
$\vec{v}$	velocity vector
Δx	diffusive mixing region width
y	distance fluid travels downstream
Y_i	local mass fraction of species i

Greek

α	charge transfer coefficient
η	overpotential
ρ	fluid density
υ	kinematic viscosity
χ	apparent reaction order

Chemical formulas

CO_2	carbon dioxide
$(COOH)_{ads}$	adsorbed COOH
e^-	electron
H^+	proton
HCOOH	formic acid
O_2	oxygen
Pt	platinum
Pt^o	occupied platinum site

ing strength. In addition, the performance of miniaturized conventional fuel cells is limited by the Ohmic polarization introduced by the membrane and related water management issues. Novel architectures are crucial for the success of microscale fuel cells [4].

Recently introduced membraneless microfluidic fuel cells [7–9] take advantage of the laminar nature of microflows to maintain the separation of fuel and oxidizer streams without the use of a membrane. A schematic of a microfluidic fuel cell and its operation are given in Fig. 1. The geometry is that of a T-intersection, or T-mixer, which is commonly used in analytical microfluidic chips. The cross-stream mixing rate in such T-intersections is diffusion limited, and many studies have focused on increasing the mixing rate in such geometries [2]. The microfluidic fuel cell, on the other hand, exploits the nature of this flow to achieve the separation of fuel and oxidant streams. The separation of fuel and oxidant is required to restrict reactions of oxidation and reduction to the appropriate electrode. Fuel is introduced at one inlet, and oxidant is introduced at the second inlet. Electrodes are placed along the walls to complete the fuel cell, and oxidation at the anode and reduction at the cathode, together provide the cell potential. The fluid facilitates protonic conduction from one electrode to the other, and the electrons generated at the anode take an external path through an applied load. The length of the reaction channel is limited by the mixing of the two streams. The operation of the fuel cell will begin to fail when the two streams become mixed to the point that oxidation and reduction are no longer restricted to the appropriate electrodes.

Choban et al. [9] were the first to demonstrate a membraneless fuel cell using formic acid and oxygen as reactants. They demonstrated that when two streams are flowing in parallel in the laminar regime, the streams remain separated, eliminating the need for a membrane. Ferrigno et al. [8] demonstrated a millimeter-scale fuel cell using vanadium as reactants. The advantage of this design is that it used the same species (vanadium) as fuel and oxidant, which can be regenerated from a mixture of the products [8]. Choban et al. [7] reported a Y-shaped microfluidic membraneless fuel cell system using formic acid and oxygen as reactants, which reached a current density of 0.4 mA cm^{-2}. The advantage of this system is that it uses acidic solutions to minimize the protonic resistance in the fluid. Both systems [7,8] were reported to be diffusion limited. In this work, a microchannel geometry with a high aspect ratio in the cross-stream direction, similar to that of Ferrigno et al. [8], is investigated, as well as a square geometry similar to that of Choban et al. [7]. Microfluidic fuel cells have several advantages over conventional fuel cells: eliminating the membrane removes related Ohmic losses, water management and sealing issues; and since the fuel and oxidant streams flow together in the same channel network, the fuel cell size is reduced, the design is simplified, and the manifolding requirements are also reduced. In addition, research in this area can capitalize on recent advances in numerical, experimental, and microfabrication techniques [10]. Microfluidic fuel cells have the further advantage of using liquid fuels, which have high energy densities compared to gaseous fuels [1], particularly important in the context of portable-power applications. However, current designs show relatively poor fuel utilization, on the order of 1% [7] to 10% [8]. Microchannel geometries and