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## A numerical study on microfluidic fuel cell: Improving fuel utilization and fuel operation concentration

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### Abstract

In this work, a simulation study of MFC based on counter-flow structure was implemented. The results indicate that the counter-flow channel enables effective suppression on fuel diffusion mixing thus intensifies fuel utilization. However, the potential loss caused by resistance of electrolyte hinder the performance significantly. Decrease in flow rate leads to enhancement on fuel utilization in spite of improving diffusion loss at the same time.

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### 1. Introduction

By harnessing laminar flow characteristic of microfluidic under low Reynolds number, the costly exchange membrane can be removed in microfluidic fuel cell (MFC), which makes MFC an attracting energy source for portable electricity consumers[1]. From first presentation of MFC in 2002[2], MFCs grounded on different structures and fuels were reported[1]. Especially after the gas diffusion electrode (GDE) was adopted[3], the performance of MFC gradually becomes competent as an energy source.

However, the low fuel utilization and low energy density problem that MFC suffers blocks extensive application of MFC [4, 5]. MFC with counter-flow microchannel was raised to overcome the fuel utilization issue[6], and this kind of structure was predicted to achieve over-limiting current potential[7]. In this study, a three-dimensional numerical model couples CFD with electrochemical kinetics and mass transfer was developed to investigate the performance of counter-flow MFCs.

### 2. Methodology

#### 2.1 Physical problem statement

The geometry of this model is depicted in Fig.1a. Dimension of channel is 2mm×1mm in  $w \times h$ , and electrode is 6.5mm in length. Formic acid supported with sulfuric acid (0.5 M) as electrolyte was used as anolyte, while sulfuric acid (0.5 M) dissolved with saturated oxygen (0.25 M) served as oxidant. In anode, electro-oxidation of formic acid occurs

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While oxygen reduction reaction (ORR) taking place at GDE cathode



## 2.2 Numerical model

The interactions involved in MFC governed by the following equations

$$\nabla \cdot (\rho u) = 0 \quad (3)$$

$$\rho(u \cdot \nabla)u = \nabla \cdot \left[ -pI + \mu(\nabla u + (\nabla u)^T) - 2/3\mu(\nabla \cdot u)I \right] \quad (4)$$

$$-\sigma \Delta \phi = \nabla \cdot i \quad (5)$$

$$u \cdot \nabla c_i = \nabla \cdot (D \nabla c_i) + S_i \quad (6)$$

The energy conservation equation of MFC is excluded in this model because the temperature variation within the cell normally below 1K and can be neglected[8]. The reaction rates for each species  $S_i$  are related to the local electrochemical reaction

$$S_i = \nu_i \nabla \cdot i / (nF) \quad (7)$$

$$i = i_0 \left( c_i / c_{ref} \right) \cdot \left( \exp(0.5F\eta/(RT)) - \exp(-0.5F\eta/(RT)) \right) \quad (8)$$

$$\eta = \phi_s - \phi_l - E_{eq} \quad (9)$$

## 2.3 Boundary conditions and numerical procedure

The inlet flow rate and outlet pressure was set to solve the hydrodynamics equations while non-slip condition was set at walls. Inflow concentrations were also used to determine the concentration distribution. All the involved parameters for model input are listed in Table 1. COMSOL Multiphysics 4.3b was applied to resolve the differential equations. Structural grids were conducted to discretize the geometry domain. Grid independence check was carried out to assure the precision of calculations.

Table 1 Key input parameters

Parameter	Intendment	Unit	Value	Refs.
$\rho$	Density	kg/m <sup>3</sup>	1000	[9]
$\mu$	Viscosity	Pa·s	8.9×10 <sup>-4</sup>	[9]
$u$	Flow rate	m s <sup>-1</sup>	-	-
$p$	Pressure	Pa	-	-
$I$	Tensor	-	-	-
$\phi$	Potential	V	-	-
$\nu$	Stoichiometric number	-	-	-
$\sigma_l$	Conductivity of electrolyte	S m <sup>-1</sup>	20	[10]
$\sigma_s$	Conductivity of electrode	S m <sup>-1</sup>	1.15×10 <sup>4</sup>	[11]
$c_i$	Concentration	mol L <sup>-1</sup>	-	-
$D_f$	Diffusivity of fuel	m <sup>2</sup> s <sup>-1</sup>	1.37×10 <sup>-9</sup>	[12]
$D_o$	Diffusivity of oxygen	m <sup>2</sup> s <sup>-1</sup>	2.42×10 <sup>-9</sup>	[9]
$F$	Faradic constant	C mol <sup>-1</sup>	96485	-
$R$	Universal constant	J K <sup>-1</sup> mol <sup>-1</sup>	8.3145	-
$T$	Temperature	K	298	-
$i$	Local current density	mA cm <sup>-2</sup>	-	-
$i_{0,a}$	Exchange current density of anode	mA cm <sup>-2</sup>	2×10 <sup>-3</sup>	Assumed

$i_{0,c}$	Exchange current density of cathode	$\text{mA cm}^{-2}$	$8 \times 10^{-4}$	Assumed
$C_{f,ref}$	Reference concentration of fuel	$\text{mol L}^{-1}$	1	[13]
$C_{o,ref}$	Reference concentration of oxidant	$\text{mol L}^{-1}$	0.25	[13]

### 3. Results and discussion

#### 3.1 Model validation

A model of MFC with same dimensions and operation conditions as the one from Jayashree's work[14] was built. The validation of this model was examined by comparing the J-V performance of each electrode between simulation and experiments[14]. As shown in Fig. 1b, the results present good agreement to the measured values, which confirms the effectiveness of this model.

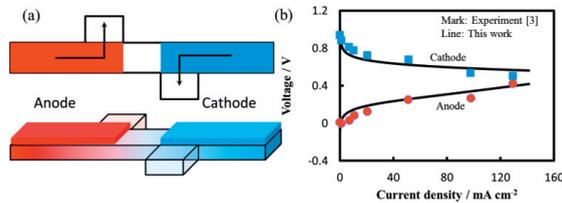


Fig.1. (a) Schematic of counter-flow MFC; (b) polarization curves of anode and cathode

#### 3.2 Cell performance

The overall performance of counter fuel cell is shown in Fig. 2 as well as classification of each potential loss. The current performance of counter-flow MFC is  $27 \text{ mA cm}^{-2}$  in short circuit current density and  $3.8 \text{ mW cm}^{-2}$  as maximum power density. The results indicate that ohmic loss reaches as high as  $0.4 \text{ V}$ , which is triple as normal co-laminar MFC[10]. Since the electrodes were placed in parallel rather than oppositely, resistance of electrolyte will be hundreds of ohms. Therefore, for the counter-flow structure that is sensitive to resistivity, applying high conductive media or structure is important for improving performance.

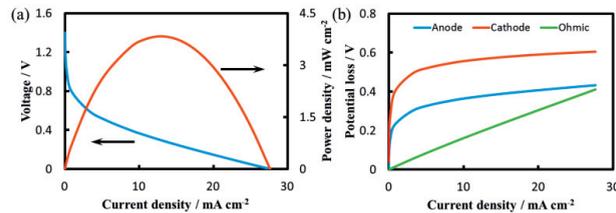


Fig. 2. (a) Curves of J-V and P-V at  $12 \mu\text{L min}^{-1}$  fed with 1M fuel; (b) each potential loss involved in MFC

#### 3.3 Fuel concentration effect on cell performance

Herein, concentrated fuel was harnessed to obtain high energy density and its effect on counter-flow MFC was investigated. As indicated in Fig. 3a, the concentration profiles against flow rate were presented. The diffusion region becomes distinct and moves to oxidant outlet along with flow rate increasing, which will cause fuel leakage at oxidant outlet. Fuel loss in oxidant outlet caused by diffusion mixing of different fed concentration is shown in Fig. 3b. For 1 M fuel inflow, fuel loss at oxidant outlet mainly owes to the fuel leakage at high flow rate. But with flow rate decreasing, fuel loss reduces because most of fuel was consumed before transfer to oxidant outlet. While for higher fuel concentration like 5 M, minimum diffusion mixing can be obtained at about  $12 \mu\text{L min}^{-1}$ , further decreasing flow rate will accelerate diffusion mixing. At flow rate less than  $12 \mu\text{L min}^{-1}$ , the suppression against fuel diffusion effect from convection of oxidant stream becomes feeble, and then the unspent fuel can provide enough concentration difference to drive formic acid diffuse to oxidant outlet. Curves of fuel utilizations of different concentration against flow rate are indicated in Fig. 3c. Enhanced fuel utilization can be obtained for fuel in range from 1M to 10M. Although diffusion mixing will be accelerated by concentrated fuel, it still affects little to the whole utilization.

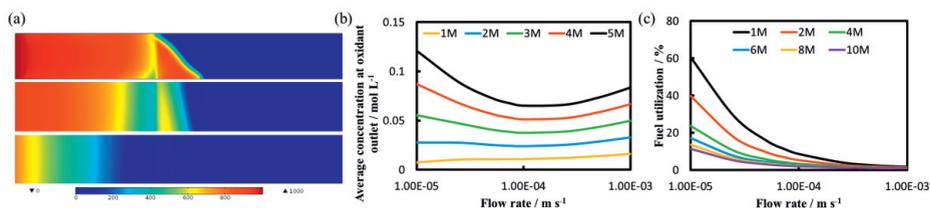


Fig. 3. (a) Concentration distribution of 1M formic acid, from top to bottom is  $1 \times 10^{-3} \text{ m s}^{-1}$ ,  $1 \times 10^{-4} \text{ m s}^{-1}$ ,  $1 \times 10^{-5} \text{ m s}^{-1}$ ; (b) fuel diffusion loss at oxidant outlet; (c) fuel utilization of various concentrations.

#### 4. Conclusion

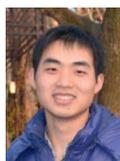
In this paper, a numerical study was conducted to investigate the performance of MFC based on counter-flow comprehensively. The potential loss owes to ohmic resistance can be triple as co-laminar structure and hinders the current performance significantly. High fuel utilization can be achieved with flow rate reducing.

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#### Biography

Hao Zhang is a PhD student from East China University of Science and Technology. During his PhD study, he worked as a Research Assistant in Ability R&D Energy Research Center, City University of Hong Kong for 10 months. His research interests focus on microfluidic technology for energy conversion and sustainable energy.