Electrochimica Acta 261 (2018) 127–136

Contents lists available at ScienceDirect

Electrochimica Acta

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

Numerical investigation and optimization of vapor-feed microfluidic fuel cells with high fuel utilization

Yifei Wang [a, *], Dennis Y.C. Leung [a, **], Hao Zhang [b], Jin Xuan [c], Huizhi Wang [c]

[a] Department of Mechanical Engineering, The University of Hong Kong, Hong Kong, China
[b] School of Mechanical and Electrical Engineering, Jiangxi University of Science and Technology, Ganzhou, China
[c] Institute of Mechanical, Process and Energy Engineering, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, UK

ARTICLE INFO

Article history:
Received 18 May 2017
Received in revised form
1 November 2017
Accepted 19 December 2017
Available online 20 December 2017

Keywords:
Vapor-feed
Microfluidic fuel cell
Numerical modeling
Fuel boundary layer
Fuel utilization

ABSTRACT

Vapor-feed microfluidic fuel cell (VF-MFC) has various advantages against the conventional liquid-feed microfluidic fuel cell, such as simpler fluidic management, higher fuel utilization, flow rate insensitiveness, and so on. To better understand the mechanisms behind its superiority and to further optimize its performance, a 3D isothermal numerical model has been developed in this work. The computational results agree very well with the previous and present experimental data, proving the validity of the current model for the VF-MFC simulation. Through this model, it is found that the dissolved fuel in the VF-MFC is well-controlled within a thin boundary layer nearby the anode catalyst surface, which can not only satisfy the demand of anode oxidation reaction but also greatly alleviate the wastage of fuel. In this manner, the VF-MFC can achieve satisfactory power output and high fuel utilization at the same time. In addition, the boundary layer effect on electrolyte flow rate can keep the fuel concentration in the thin layer relatively stable at different flow rates, which may be the reason behind the insensitiveness of VF-MFC performance to electrolyte flow rate. To further improve its power output and fuel efficiency, effects of the fuel evaporation area and the anode open ratio have also been thoroughly investigated with the present model. It is found that an evaporation-reaction area ratio of 11.1 is sufficient for the present VF-MFC, while a smaller fuel evaporation area can lead to improved fuel utilization at the expense of lower power output. To improve both the fuel utilization and power output, the electrode area towards the channel outlet is increased while keeping the vapor entrance area constant, i.e. the anode open ratio is reduced. By this strategy, the VF-MFC can achieve 48% higher power output and elevated fuel utilization from 27.5% to 41.8%, when an anode open ratio of 1:3 is adopted.

1. Introduction

Microfluidic fuel cell (MFC) is a novel type of fuel cell, which does not need a physical membrane to separate its two electrodes and the corresponding reactants [1,2]. Instead, MFC generally employs two laminar streams, one dissolved with the fuel (i.e. the anolyte) and the other dissolved with the oxidant (i.e. the catholyte), flowing directly into its microfluidic channel and passing between its two electrodes, as shown in Fig. 1(a). Benefited from the low Reynolds number of the microfluidic flow, the vigorous convective mixing is eliminated, with only a slow diffusion process occurring at the anolyte-catholyte interface. In this manner, the fuel and oxidant are naturally separated to maintain a successful fuel cell operation.

Attributed to their simpler structure, MFCs possess many advantages compared with the conventional membrane-based fuel cells such as the proton-exchange membrane fuel cell (PEMFC). First of all, the cell cost is significantly reduced due to the elimination of the costly membrane. In addition, all the membrane-related issues can be avoided including membrane dehydration and degradation, and its sensitivity to reaction environment. Moreover, the choice of fuel, oxidant, and electrolyte species is greatly extended in MFCs, among which the dual-electrolyte configuration with acid environment on the cathode side and alkaline environment on the anode side has been demonstrated to be powerful for boosting up the power output [3–5]. Furthermore, water and heat management is inherently fulfilled by the

* Corresponding author.
** Corresponding author.
E-mail addresses: wang1fei@connect.hku.hk (Y. Wang), ycleung@hku.hk (D.Y.C. Leung).

https://doi.org/10.1016/j.electacta.2017.12.132
0013-4686/

Nomenclature

Symbols

ρ	Density (kg m^{-3})
u	Velocity (m s^{-1})
P	Pressure (Pa)
μ	Dynamic viscosity (Pa·s)
ω	Mass fraction
j	Diffusion flux (kg m^{-2} s^{-1})
S	Production/consumption rate due to electrochemical reactions (kg m^{-3} s^{-1})
M	Molar mass (kg mol^{-1})
D	Diffusion coefficient (m^2 s^{-1})
c	Molar concentration (mol m^{-3})
k	Diffusion resistance coefficient
ε	Porosity of GDL
M_n	Average molar mass of the mixture (kg mol^{-1})
σ	Conductivity (S m^{-1})
φ	Potential (V)
i	Current density (A m^{-2})
ν	Stoichiometric coefficient
n	Number of transferred electrons
F	Faraday's constant (96485 C mol^{-1})
i_0	Exchange current density (A m^{-2})
χ	Reaction order
α	Charge transfer coefficient
η	Activation overpotential (V)
R	Gas constant (8.314 J mol^{-1} K^{-1})
T	Temperature (K)
E_{eq}	Equilibrium potential (V)
Q	Charge source term (A m^{-3})

Subscript

a	Anode
c	Cathode
f	fuel
i, j, k:	Species
l	Electrolyte
o	oxidant
s	Electrode
0	Standard, reference, or boundary value
eff	effective

continuous microfluidic flow, leading to a greatly simplified fuel cell system. Nevertheless, the current MFC technology still faces many unsolved problems which have greatly impeded their further development and practical application. First, the employment of bulk aqueous solution would dramatically lower down the system energy density. In addition, the strict requirement on electrolyte flow rate control would require complex ancillary components such as micro-pumps and a stable working environment, which greatly restricts their application prospect. Furthermore, the fuel utilization is generally low since the dissolved fuel needs to diffuse to the anode catalyst layer (CL) from the bulk anolyte, which is a very slow process compared with the convective transport along the microfluidic channel. Consequently, a large portion of the fuel has no chance to be reacted, leading to low fuel utilization of less than 10% [6]. To tackle this issue, lower electrolyte flow rates are generally adopted, which, however, can degrade the cell performance by two aspects. The fuel depletion effect would be intensified on the anode side while the fuel crossover effect would be aggravated on the cathode side. As a consequence, the fuel utilization is improved at the price of sacrificed cell performance and even catalyst poisoning. This dilemma between cell performance and fuel utilization should also be solved for future MFC development.

Previously we have developed a vapor-feed MFC (VF-MFC) which has a totally different fuel delivery mode compared with the conventional liquid-feed MFC (LF-MFC) [6]. As shown in Fig. 1(b), instead of dissolving the fuel into the anolyte and feeding it to the anode from inside the channel, the VF-MFC utilizes fuel vapor from outside the channel which diffuses through the porous anode and dissolves into the flowing electrolyte. In this manner, bulk anolyte wastage is avoided, which leads to a more economic fuel delivery pattern and, consequently, a higher fuel utilization in the order of 40%. In addition, the cell performance of VF-MFC was not sacrificed. Our experimental study has already proved the advantage of VF-MFC. However, the specific mechanism behind its superiority is not clearly understood yet, which is either difficult or expensive to be explored experimentally.

Numerical modeling is a convenient and economical method for MFC research and development, which can not only reveal the deep-going mechanisms behind the experimental phenomenon but also comprehensively optimize the cell structure and operation parameters. Great efforts have been made on MFC modeling over the past decade, including the investigation of fuel utilization optimization [7–17], fuel crossover suppression [18–20], air-breathing cathode [21–23], flow-through electrodes [24–27], and other related systematic issues [28–30]. In spite of all these achievements, the current MFC modeling is mostly focused on conventional LF-MFC. To the best of our knowledge, no modeling

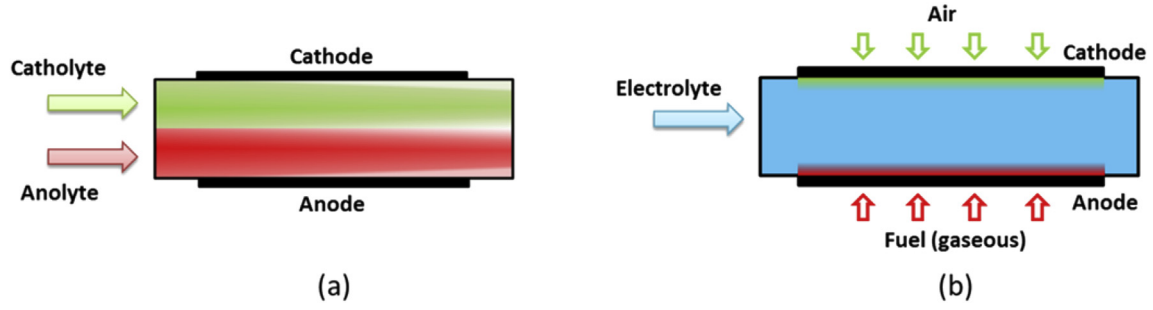

Fig. 1. Schematic diagram of two different fuel feeding modes in MFCs: (a) Liquid-feed; (b) Vapor-feed.