

IMPROVED PERFORMANCE OF MEMBRANELESS MICROFLUIDIC FUEL CELLS USING NANOSTRUCTURES: A NUMERICAL STUDY

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ABSTRACT

This work presents a numerical tool predicting the H₂ consumption of membraneless microfluidic fuel cells (MFFCs) with nanostructures on the anode. This allowed to elaborate (without and tedious fabrication cycles) that adding cubic nanostructures on the anode can improve the transport of H₂ through the electrolyte by about 1300%.

KEYWORDS: Microfluidic Fuel Cells, Nanostructures, Numerical Simulation, Lattice-Boltzmann Method

INTRODUCTION

The development of efficient power sources, that do not emit any harmful emissions, is a necessary step to reduce the worldwide impact of global warming. The realization of a MFFC, that can compete with conventional fuel cells, e.g., a proton-exchange membrane fuel cell (PEMFC), is advantageous because a MFFC is lighter and does not require a costly membrane that degrades over time [1]. A working proof of concept of a MFFC has been presented by Hashemi, et al. [1]. Unfortunately, the maximum power density of a MFFC is about 1% of that of a PEMFC. However, adding nanostructures on the anode surface could substantially improve the performance, but how to define these nanostructures is unclear and requires further investigation. A typical approach is based on trial-and-error, with many costly and tedious fabrication cycles. This work presents a tool that allows to study the performance based on numerical simulations using the lattice-Boltzmann method (LBM) solver Palabos [2].

THEORY

The MFFC can be described as a set of harmoniously cooperating components, as schematically given in Figure 1. Here, we see two channels: one containing gaseous H₂ and the other containing gaseous O₂. Both gas channels are engulfed by a liquid electrolyte that is connected through a “bridge” between the channels. Due to the surface tension working on the gas-liquid interface, only the electrolyte fills the bridge, and the two gases cannot mix. The electrolyte also allows for transport of protons from the anode to the cathode. The gases are also dissolved in the electrolyte and are, by means of diffusion, transported to the corresponding electrode, where they are consumed in the corresponding half-reaction. The MFFC will only operate when all reactants of the reactions are present, and the performance of the MFFC is limited by the mass transport of hydrogen to the anode [1]. Hence, to describe the overall performance of the MFFC, we look at the flux of H₂ that is transported to the anode in [kg/m²s]. For a flat surface, when only diffusion is considered, the steady state flux can be predicted analytically using the following equation

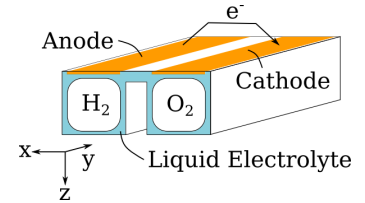


Figure 1: A schematic representation of a membraneless MFFC.

$$C_{H_2}(z) = \frac{C_{sat}}{d} z, \quad (1)$$

where C_{H_2} is the concentration at a distance z from the electrode surface, $d = 2\mu\text{m}$ is the electrolyte layer thickness, and C_{sat} is the saturation concentration.

NUMERICAL

When nanostructures are introduced on the anode, the flux of hydrogen cannot be described using Equation 1 anymore. Hence, a more sophisticated method is required. In this work we present a simulation tool using the LBM to predict the hydrogen flux based on the convection diffusion equation, i.e.,

$$\nabla \cdot (C_{H_2} \mathbf{u}) = \nabla \cdot (D \nabla C_{H_2}), \quad (2)$$

where, the velocity \mathbf{u} of the flow is obtained from the solution of the in-compressible Navier-Stokes equations. The diffusion coefficient D is set to $4.58 \times 10^{-9} \text{ m}^2/\text{s}$ for hydrogen in water at 293.15 K and 1 bar. Here, C_{H_2} is the unknown, and Equation 2 is solved using a Dirichlet boundary condition at the gas-liquid interface of $C_{\text{sat}} = 1.61514 \text{ kg/mol}^3$ at 293.15 K and 1 bar, and a Dirichlet boundary condition of $C_{\text{H}_2} = 0$ at the anode-liquid interface. The tool predicts the flux, using a first order forward finite difference approximation, accurately at $3.68 \times 10^{-6} \text{ kg/m}^2\text{s}$ for a flat surface.

Using this tool, we can now predict the hydrogen flux for complex anode surfaces. For this, we have chosen to investigate the flux on a surface with cubic nanostructures as depicted in Figure 2. These cubic nanostructures are arranged periodically at an interval of L_c and W_c in y -direction and x -direction, respectively. The cubes have a height H in z -direction, a length L in y -direction, and a width W in x -direction. For our investigation, we set the variables according to the values given in Table 1, leading to a total of $3^5 = 243$ configurations. These values were chosen in accordance with attainable manufacturing resolutions [3].

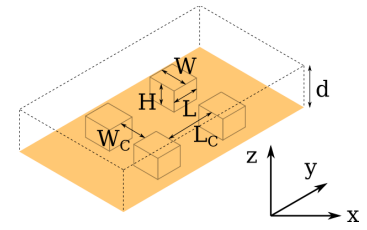


Figure 2: Cubic nanostructures on the anode surface.

Table 1. Configuration values for the cubic nanostructures.

	L_c, W_c, L, W	H
Values [nm]	250, 500, 1000	500, 1000, 1500

RESULTS AND DISCUSSION

The evaluation using the numerical tool described above allows us to evaluate the effect of the 243 considered configurations. The best performing configuration is given in Table 2 and its flux is about 13 times the flux for a flat surface. The configurations with higher height performed better than the others, indicating that diffusion is still the dominating transport mode, even in the presence of nanostructures. This also indicates that a smaller thickness of the liquid phase improves the transport of hydrogen. However, a too thin liquid phase can impair the transport of protons in the electrolyte, leading to a new bottleneck for the overall MFFC performance [1].

Table 2. Best resulting flux and corresponding configuration.

Flux [$\text{kg/m}^2\text{s}$]	L_c [nm]	W_c [nm]	L [nm]	W [nm]	H [nm]
4.917×10^{-5}	250	500	250	250	1500

CONCLUSION

A tool has been presented that can predict the H_2 transport through the electrolyte for nanostructure configurations without costly and tedious fabrication cycles. Adding cubic nanostructures to the anode can improve the transport of H_2 by about 1300%. Future work is needed to evaluate proton transport performance.

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