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Electrode structure effects on the performance of open-cathode proton exchange membrane fuel cells: A multiscale modeling approach

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ARTICLE INFO

Article history:

Received 15 November 2013

Received in revised form

5 February 2014

Accepted 28 March 2014

Available online xxx

Keywords:

PEMFC

Open-cathode

Electrode structure

Water transport

Multiscale modeling

ABSTRACT

In this paper we present a new dynamic multiscale model of an open-cathode Polymer Electrolyte Membrane Fuel Cell (PEMFC). The model describes two-phase water transport, electrochemistry and thermal management within a framework that combines a Computational Fluid Dynamics (CFD) approach with a micro-structurally-resolved model predicting the water filling dynamics of the electrode pores and the impact of these dynamics on the evolution of the electrochemically active surface area (ECSA). The model allows relating for the first time the cathode electrode structure to the cell voltage transient behavior during experimental changes in fuel cell temperature. The effect of evaporation rates, desorption rates and temperature changes on the performance of four different electrode pore size distributions are explored using steady-state and transient numerical simulations. The results are discussed with respect to water management and temperature control.

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Introduction

Energy conversion through electrochemical devices, such as fuel cells, plays an important role for the development of future sustainable energy networks. In spite of significant technological progress on the development of Polymer Electrolyte Membrane Fuel Cells (PEMFCs) for more than 50 years,

their massive commercialization for power generation in transportation is still far from being guaranteed [1,2]. Achieving their commercialization, the concomitant reduction in cost of the materials and the increase of their efficiency and stability would be the decisive breakthrough.

It should be underlined that transportation application means rough operating conditions such as highly dynamic load changes, a high number of start/stop cycles and

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<http://dx.doi.org/10.1016/j.ijhydene.2014.03.218>

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hydrothermal stresses [3]. Moreover, performance and durability goals for these systems have to be reached without external humidification [4] in order to reduce weight, size and peripheral power consumption. Thus, the study of performance degradation mechanisms of self-humidified, open-cathode systems that do not require external humidification is of great interest. The relevance of developing deeper understanding of the relation between performance and thermal system management of such a type of PEMFC is illustrated in Fig. 1 [5]. In this figure we report results obtained in a previous work of the authors [5] with the commercial 100 W, 20 cell, open-cathode PEMFC stack H-100 from Horizon Fuel Cells Technologies with an active area of 22.5 cm². The system runs of dry hydrogen with a dead-ended anode configuration and purged operation [6,7]. The stack temperature is regulated with a cooling fan directly attached to the stack housing.

Fig. 1 shows the stack voltage transient response to a stepwise increase of the stack temperature at an operation point of 0.18 A cm⁻². The spikes in the voltage signal result from periodic anode purges that were performed every 30 s. The increase in temperature results in two counteracting effects on performance. First, the improved reaction kinetics at higher temperatures leads to a significant system performance gain [8]. However, at about 50 °C the characteristic voltage response changes. Even though the voltage still increases at the beginning of a step, it does not stabilize but keeps decreasing with time. The elevated temperature intensifies the drying of the catalyst layer (CL). Since the electrolyte material in the CL requires the presence of water for the H⁺ ions to reach the so-called three-phase-contacts between reactant gas, electrolyte, and electrode catalyst, the decreasing water concentration during operation at elevated temperatures is speculated to imply the loss of active sites. The result is the observed voltage decay. The experiment shows the importance of proper thermal management and the potential for improving the system performance.

Thus, having appropriate controllers for PEMFCs operating at low relative humidities on the cathode side is crucial to speed up the integration of thermal management strategies into realistic systems for automotive applications. This necessarily undergoes developing mathematical models that capture the interplaying dynamics between water transport and thermal aspects.

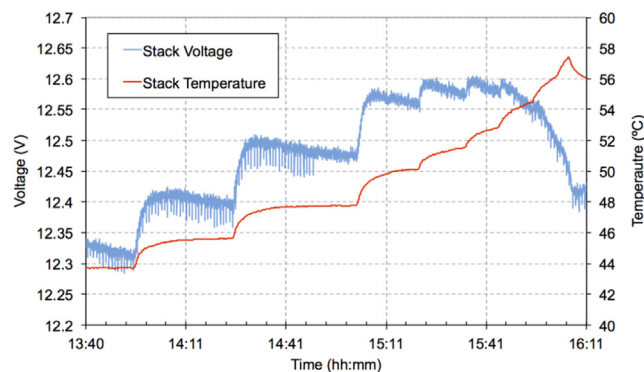


Fig. 1 – Stack temperature and voltage over time during up-stepping of the stack temperature at a constant current density of 0.18 A cm⁻² [5].

To achieve these goals, the understanding and the physical-based modeling of the water transport in the CLs is a crucial aspect, which has been the subject of numerous publications. In a pioneering work, Springer et al. [9] reported an isothermal, one-dimensional, steady-state model of a complete PEMFC. In particular, the model predicted an increase in polymer electrolyte membrane (PEM) resistance with increased current density and demonstrated the great advantage of a thinner PEM for alleviating the resistance problem. Bernardi and Verbrugge [10,11] proposed a one-dimensional mathematical model of the PEMFC for liquid water transport in porous electrodes assuming a constant liquid water volume fraction and no interactions between liquid and gas flows. A number of CL models had then been developed, including interface models, thin film models, agglomerate models, and thin film agglomerate models [12–22]. Using the agglomerate model, other researchers studied the optimum performance of PEMFC for a number of optimization parameters: type of agglomerate, CL thickness, CL porosity, distribution of Nafion[®] content, Pt loading, etc. [23–28]. Besides these models, the works of Wang and Wang [29,30] treated the CL as an individual zone with various conservation equations employed for transient modeling. Various time constants for the transient transport phenomena were proposed.

Many different two-phase flow models have been published during the last decade. Wang et al. [31] pioneered the research on this issue through analytical and numerical methods. A threshold current density was proposed to distinguish the scenarios between single- and two-phase regimes of water distribution and transport. In the subsequent works of their group, sophisticated models [32–35] were developed to simulate flooding and liquid water distribution in PEMFCs. The so-called *mature multiphase mixture formulation* with a single set of conservation equations was employed to mimic the two-phase transport process. The model of Natarajan and Van Nguyen [36,37], which considered evaporation and condensation of liquid water, also demonstrated the importance of its transport on cell performance. Wu et al. [38] discussed the different water transport modeling approaches and compared simulation results using various published expressions for liquid water saturation, relative permeability, evaporation/condensation rates and absorption/desorption rates. In most reported models the dynamics of evaporation and condensation are neglected due to the high surface area of porous media and the resulting relatively fast evaporation rate. However, the phase change model used in Ref. [38] and the respective set of parameters shows that the values for the phase change rates may change by more than two orders of magnitude and thus may have a crucial effect on liquid water distribution.

Pore network modeling (PNM) can be used to estimate relationships between reactant transport properties and the liquid water saturation in the CL with a given pore-size distribution (PSD), estimated by porosimetry experiments for instance. PNM is an efficient method to investigate multiphase transport in porous media. It was used in petroleum industry for decades and was recently applied to study water management inside the Gas Diffusion Layers (GDLs) and CLs of the PEMFC [39–41].

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