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Water transport in gas diffusion layer of a polymer electrolyte fuel cell in the presence of a temperature gradient. Phase change effect

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ABSTRACT

The gas diffusion layer (GDL) is a crucial component as regards the water management in proton exchange membrane fuel cells. The present work aims at discussing the mechanisms of water transport in GDL on the cathode side using pore network simulations. Various transport scenarios are considered from pure diffusive transport in gaseous phase to transport in liquid phase with or without liquid–vapor phase change. A somewhat novel aspect lies in the consideration of condensation and evaporation processes in the presence of a temperature gradient across the GDL. The effect of thermal gradient was overlooked in previous works based on pore network simulations. The temperature gradient notably leads to the possibility of condensation because of the existence of colder zones within the GDL. An algorithm is described to simulate the condensation process on a pore network.

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Introduction

The gas diffusion layer (GDL) in PEMFC has several functions, [1]. The GDL contributes to make more uniform the gas supply to the active layer. The GDL must also contribute to the water management by enabling the water in excess to leave the system on the cathode side without affecting too much the oxygen access to the active layer. A key question in this context is the nature of the water within the GDL, i.e. in gaseous phase or in liquid phase. Obviously, the transfer of the water in excess in vapor phase sounds the best option if

the objective is to maintain all pores in the GDL accessible to oxygen. On the other hand, a GDL made hydrophobic generally leads to better performance. A possible effect of a hydrophobic agent makes sense only if water is present in liquid phase in the GDL. If the water transfer is in liquid phase, then as discussed in Ref. [2], it is indeed much better to make the GDL hydrophobic because this favors the formation of liquid capillary fingers occupying a small fraction of the pore space. The complementary fraction, free of water, is therefore available for the oxygen transport. Then it must be pointed out that a PEMFC typically operates at a temperature of about

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80 °C, which corresponds to a relatively high vapor saturation pressure. Furthermore, as discussed for example in Ref. [3], a temperature difference is expected across the GDL with the highest temperature on the active layer side. Since the GDL is colder on the bipolar plate side, water condensation is likely and can be another mechanism leading to the occurrence of liquid water in the GDL [4,5]. Also, because of the temperature gradient or because the relative humidity in the bipolar plate channel can be lower than 100%, evaporation is also possible. In brief, several options are possible as regards the water transport across the GDL: 1) transport in vapor phase only, 2) transport in liquid phase only, 3) transport with liquid – vapor phase change.

In this context, the present work discusses different mechanisms of water transport in the gas diffusion layer (GDL) on the cathode side from a combination of simple estimate and two-dimensional pore network simulations in relation with the water management issue. The fuel cells motivating the study are classical PEMFC but the results could be of interest for the modeling of other categories of fuel cells, e.g. Ref. [6] for example.

Pore network simulations

The modeling of transport phenomena in porous media is generally performed within the framework of the continuum approach to porous media. This approach considers volume-average transport equations and relies on the concept of length scale separation, i.e. the averaging volume should be small compared to the size of the porous domain for the Darcy's scale equations to make sense. As discussed for instance in Ref. [7], a GDL is only a few pore sizes thick. This is an example of thin porous media [8] in which the length-scale separation criterion is not satisfied. Furthermore, as also discussed in Ref. [7], the scenario of slow liquid invasion in a hydrophobic porous medium leads to a regime called the capillary fingering regime, which is fractal and thus not compatible with the volume-averaged equations. The fact that the continuum approach is highly questionable is a strong argument in favor of an alternate approach. As in several previous works, e.g. Refs. [9–11], and references therein, we use a pore network approach. In the pore network approach, the pore space is represented by a network of pores interconnected by channels. The transport of interest is directly computed at the pore network scale outside the continuum framework. For simplicity, we consider a regular two-dimensional lattice as sketched in Fig. 1. The pores correspond to the nodes of the network. The interconnecting channels between two pores correspond to the constrictions or throats of the pore space. The pores are idealized as cubic bodies and the throats are ducts of square cross-section. The pore network is constructed by assigning pore body sizes from a Gaussian distribution in the range $[d_{\text{tmin}}, d_{\text{tmax}}]$ with $d_{\text{tmin}} = 20 \mu\text{m}$ and $d_{\text{tmax}} = 34 \mu\text{m}$. The size of the porous domain is $\ell \times L$ where ℓ is the GDL thickness. As discussed in Ref. [7] representative values of L and ℓ are: $L \sim 2 \text{ mm}$ and $\ell \sim 300 \mu\text{m}$. The lateral size L corresponds to a unit cell containing a rib and two half-channels of the bipolar plate. At the bipolar plate side, one part of the GDL is in contact with a solid

phase, the rib, whereas the other part is in contact with the channel providing the oxygen. The lattice spacing (= the distance between two pores) is equal to $50 \mu\text{m}$ so that a 40×6 pore network is considered (40 is the number of pores in the lateral (in-plane) direction and 6 the number of pores across the GDL (thus in the through plane direction)).

Water transfer in vapor phase

To discuss the nature of the water transfer within the GDL, we begin with some simple analytical computations. We assume that all the water produced in the active layer as a result of the electro-chemical reaction is directed toward the GDL on the cathode side. This is a conservative estimate since a fraction of the produced water should actually go toward the anode side. The production rate (in mol/s) is classically expressed as a function of the current density in the fuel cell as,

$$Q = \frac{iA}{2F} \quad (1)$$

where F is the Faraday's constant ($F = 96485.34 \text{ C}$), i is the current density and A the cross-section surface area of the network ($A = 40 \times 50 \mu\text{m} \times 50 \mu\text{m}$ with our 2D approach).

Suppose the water transfer takes place in vapor phase by diffusion and consider for simplicity the gas as a binary mixture of oxygen and water vapor. An important parameter is then the relative humidity, denoted by RH , in the channel. The gas at the fuel cell inlet is not dry but humidified. Considering automotive applications, we can take for example $RH = 50\%$ at the inlet. As a result of water production, the relative humidity is expected to increase along the channel and can even be expected to reach almost 100% RH at the outlet of the fuel cell. Accordingly, we vary in what follows RH from about 50% to 100%. An additional simplification is to suppose that the gas is fully vapor saturated in humidity at the inlet of the GDL (the GDL inlet is the interface between the active layer and the GDL). Under these circumstances, the diffusive transport of the vapor can be expressed as,

$$J = \frac{cA}{\ell} D_{\text{app}} [\ln(1 - RH x_{\text{vsat}}(T_c)) - \ln(1 - x_{\text{vsat}}(T_{\text{al}}))] \quad (2)$$

with $c = p/RT$ where p is the total pressure ($p \sim 1.5 \text{ bar}$), R is the gas constant, ℓ is as before the thickness of the GDL ($\sim 6 \times 50 \mu\text{m}$); $x_{\text{vsat}}(T_{\text{al}})$ is the vapor mole fraction at the active layer – GDL where T_{al} is the temperature at this interface; $x_v = RH x_{\text{vsat}}(T_c)$ at the GDL/channel interface where x_v is the mole fraction of vapor and T_c is the channel temperature.

In Eq. (2), D_{app} is the apparent diffusion coefficient of the GDL. It differs from the molecular diffusion coefficient because of the presence of the porous microstructure. Using the same method as reported for instance in Ref. [12], this coefficient is computed from pore network simulations taking into account that the GDL is partially blocked by the rib as depicted in Fig. 1. Repeating the simulations for 10 different realizations of network and ensemble-averaging the results led to $D_{\text{app}}/(eD) = 0.19$ where D is the molecular diffusion coefficient of vapor ($D = 3.1 \cdot 10^{-5} \text{ m}^2/\text{s}$ at 80 °C) and $e \approx 0.65$ is the network porosity. This enables us to define the critical current density i_c beyond which it is not possible to transfer all the

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