Pore network modelling of condensation in gas diffusion layers of proton exchange membrane fuel cells

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ABSTRACT

A pore network model (PNM) is exploited to simulate the liquid water formation by vapour condensation in the gas diffusion layer (GDL) on the cathode side considering the spatial temperature variations within the GDL. The computed distributions are markedly different from the ones computed in previous works assuming capillarity controlled invasion in liquid phase from the catalyst layer and found to be in quite good agreement with several experimental observations. The proposed model opens up new perspectives for understanding the water transfer in protons exchange membrane fuel cells and the associated water management and aging issues.

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1. Introduction

In spite of many studies, the exact mechanisms of water transfer in the various layers forming a proton exchange membrane fuel cell (PEMFC) are not fully understood. This also holds for the gas diffusion layers (GDL).

As discussed in [1], different mechanisms can be invoked as regards the transfer across the GDL of the water generated by the electrochemical reaction in the catalyst layer (CL): transfer in vapour phase, transfer in liquid phase with negligible liquid–vapour phase change phenomena, transfer with evaporation – condensation mechanisms. This is so because we actually do not know whether the water formed in the CL enters the GDL in liquid phase, in vapour phase or as a mix of both phases. This fundamental question is schematically illustrated in Fig. 1. Although detailed in-situ visualizations of liquid phase distributions in a GDL are possible using for example mini PEMFC dedicated for X-ray tomography, e.g. [2], it is difficult to infer from the visualizations the exact mechanisms at play. We can therefore distinguish two assumptions. Assumption #1 consists in assuming that water enters the GDL in liquid phase. Assumption #2 consists in assuming that water enters the GDL in vapour phase. Since it is difficult to

decide from the available experimental data which assumption is the most relevant, additional useful insights can be sought from modelling and numerical simulations.

As for other problems involving multiphase flows in porous media, many techniques have been used in relation with PEM fuel cells. The most frequent one is based on the classical continuum approach to porous media and involves the generalized Darcy's law and the concepts of capillary pressure curves and relative permeabilities. Although widely used, notably in CFD commercial codes, the relevance of this classical approach has been questioned, e.g. [3], because this type is modelling is not well adapted to simulate the capillary forces dominated regime prevailing in GDL. There is also a problematical lack of length scale separation since the thickness of a GDL is typically less than 10 pore sizes. Owing to these limitations, alternative approaches have been developed. These notably include the direct simulations, such the ones based on Lattice Boltzmann Methods, e.g. [4], Monte Carlo simulations [5] and the simulations based on pore network models (PNM). The computational times of the latter over domains of comparable sizes, i.e. containing the same number of pores, are typically orders of magnitude smaller than for the two other methods. For this reason as well as the general simplicity of this approach, the present study is based on a PNM approach.

PNMs have become a somewhat popular tool to study transfer phenomena in GDL, e.g. [6–23]. It must be noted that these studies are all more or less explicitly based on assumption #1, i.e. all the

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Nomenclature

a	lattice spacing, m		U	electrical tension, V
c	gas phase mole concentration, mol/m^3		V_p	pore volume, m^3
d	throat width, m		x_v	vapour mole fraction
D	vapour diffusion coeff., m^2/s			
D^*	vapour diffusion effective coefficient, m^2/s		*Greek symbols*	
F	Faraday constant, C		β	partition coefficient
g	throat diffusive conductance, mol/s		δ	GDL thickness, m
H_{ch}	channel height, m		ε	porosity
h_{lv}	reaction enthalpy, J/mol		Φ	heat flux, W/m^2
i	current density, A/cm^2		λ	thermal conductivity, W/m/K
L	GDL lateral size, m		λ^*	effective thermal conductivity, W/m/K
L_c	channel width, m		η	nucleation parameter
L_r	rib width, m		χ	pore volume correction factor
$\mathbf{n}$	unit normal vector			
p_v	vapour partial pressure, Pa		*Subscripts*	
p_{vs}	saturation vapour pressure, Pa		bp	bipolar plate
P_{ref}	gas phase total pressure, Pa		c	compressed
Q	water injection flux, mol/m^2/s		ch	channel
R	gas constant, J/kg/K		p	pore
RH	local relative humidity, %		uc	uncompressed
RH_{ch}	channel relative humidity, %		v	vapor
T	temperature, K		$//$	in plane
T_{bp}	bipolar plate temperature, K		$\perp$	through plane

water coming from the adjacent catalyst layer enters the GDL in liquid phase and flows through the GDL in liquid phase. Assumption #1 of liquid water invasion is also made in [24], but with the consideration of an additional phenomenon, the possible evaporation of the liquid within the GDL, see also [1]. In brief, to the best of our knowledge, no previous study based on PNM has explicitly considered assumption #2 as central assumption. In contrast with the aforementioned studies, the present work is based on assumption #2, i.e. we explore the situation where water enters the GDL in vapour phase from the CL.

As we shall see, the occurrence of water in the GDL under assumption #2 is then due to the condensation of the water vapour.

Modelling the condensation process in a GDL using PNM or related approaches is not completely a novelty. For instance, one can cite the qualitative studies reported in [25,26] limited to 2D simulations and without explicit consideration of the temperature variations across the GDL, a key aspect, however, for the simulation of condensation, and our recent paper [1], where a condensation algorithm was presented and briefly illustrated through a few simulations in a 2D pore network only. The fact that previous PNM studies dealing with condensation are scarce and somewhat skimpy is somewhat surprising since condensation is considered as an essential process by several authors, e.g. [26–34].

The objective of the present article is therefore to present and analyse PNM simulations of liquid water formation by
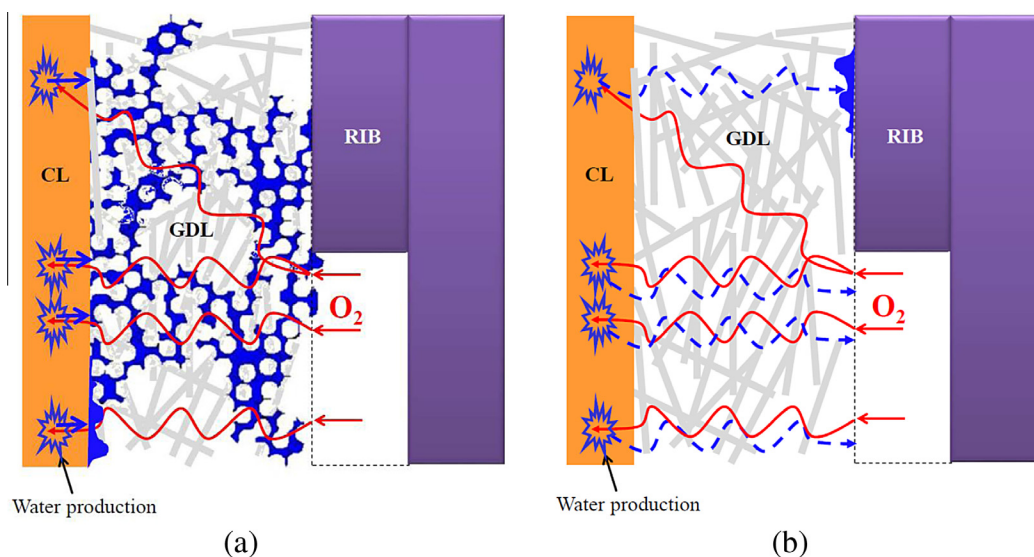

Fig. 1. Schematic of the two main situations regarding the phase, liquid or vapour, of the water entering the GDL from the catalyst layer (CL); (a) assumption #1: water enters the GDL in liquid form (in blue), (b) assumption # 2: water enters the GDL in vapour form (blue dashed lines). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)