Pore trapping mechanisms in two-phase flows through fuel cells porous media

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Abstract

The peak performances in fuel cells are strongly limited by flooding of the electrodes. Flooding occurs as a consequence of the intense electrochemical reaction in the cell, when, at high current density, a high amount of water is produced and trapped in the gas diffusion layers (GDLs). The trapped water blocks the pores of the fibrous GDLs and impedes the uniform diffusion of fuel gas along the cell area. Therefore, a fast removal of water from the porous layer is demanded. How to enhance such a mechanism in order to improve the water management remains still an open question. In the present study we address this problem with an innovative bottom-up approach: by means of Lattice-Boltzmann simulations, we investigate the effects of the microstructure at the pore-scale on the two-phase flows dynamics, in order to optimise the GDLs design and obtain an efficient water management at the macroscale. Results show that, during imbibition, the wetting phase can be trapped at the pore throat, impeding liquid removal. The trapping mechanism is primarily governed by the thermodynamic energy barriers induced by the pore expansions, in a complementary way to Haines jump during drainage. This undesired phenomenon is exacerbated in hydrophobic media during imbibition. These findings suggest a possible new route for innovative design of gas diffusion layers in fuel cells applications.

Introduction

The need to find new solutions for a future sustainable mobility makes fuel cells increasingly attractive. Nevertheless, many technological issues still must be addressed in order to improve their technological and economical competitiveness in the mobility sector. (Sørensen & Spazzafumo 2018) In particular, a key challenge is the development of an efficient water management of the cell. Several efforts have been made for achieving effective water management, e.g. through the application of hydrophobic treatments to the fibre surfaces composing GDLs or by means of a complex three-dimensional architecture of the cells (Yoshida & Kojima 2015). However, the fundamental mechanisms governing two-phase flows at the pore-scale are still not completely understood. For instance, recent experiments have revealed non-Darcian mechanisms of two-phase flows in porous media, often characterised by intermittent behaviours of the flow dynamics (Haines jump) (Berg 2013). To what extent, these intermittent behaviours and complex mechanisms can affect water management in fuel cells is still not understood.

In the present study, we explore the dynamics of two-phase flows in fuel cells porous media via an original bottom-up approach: on the basis of the study of the fundamental behaviour of the fluid at the pore-scale, with the aim of extracting the optimum design parameters of the GDL and improve the water management in the cell.

Numerical Method

Simulations of liquid imbibition are performed by means of a Lattice-Boltzmann Shan-Chen model. We firstly investigate the two-phase flow dynamics in a simplified two-dimensional domain composed of straight parallel fibres, see Fig. 1 (b), with a liquid volume subjected to a pressure gradient. Secondly, we study the imbibition mechanisms in a more complex porous structure, formed by randomly distributed and randomly transversally oriented fibres, see Fig. 3 (b) and (c).

Results and Discussion

Preliminary results show that a slight variation of the contact angle can impede liquid penetration, trapping the liquid in the pore, as well depicted in Fig. 1 (a). We investigate this interesting result (which cannot be described by Darcy's or Lucas-Washburn's laws) by looking at the thermodynamic balance of the system. We estimate the Helmholtz free energy variation dF during imbibition as (Berg 2013):

$$dF = -\sum_{i=1}^{2} p_i dV_i + \gamma dA_{lg} \qquad (1)$$

with p_i and V_i the pressure and volume of the i-th phase, γ the surface tension and A_{lg} the liquid-gas surface area. Equation 1 is applied to the control volume represented in Fig. 1
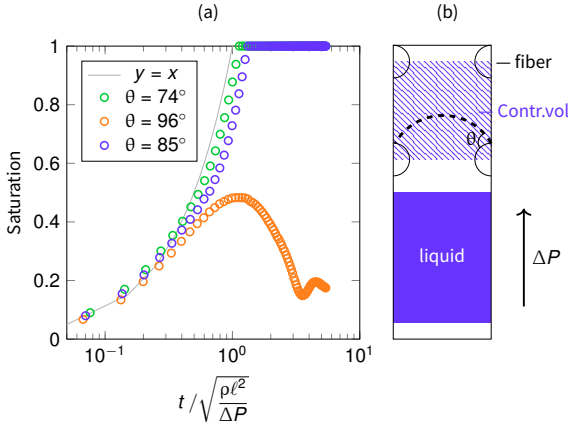
Figure 1: (a) The saturation variation in time; time has been non-dimensionalised with the characteristic imbibition time, with ℓ the liquid volume length. (b) Sketch of the two-dimensional domain. Dashed line: liquid-gas area expansion at the throat exit.

(b) and rewritten in dimensionless form:

$$dF^* = \frac{dF}{P_c V_f} = -dSat + \frac{\gamma}{P_c V_f} dA_{lg} \qquad (2)$$

where Sat and V_f are the saturation and the total fluid volume of the control volume, and P_c is the capillary pressure. For imbibition to be thermodynamically sustainable, it must be $dF^* \leq 0$. Figure 2 shows that the two terms in Eq 2 counterbalance each other in the first times. The capillary pressure sustains liquid penetration and counterbalances the increase of the liquid-gas area at the throat exit (see e.g. Fig. 1 (b)), so that $dF^* \sim 0$ with varying saturation. In the hydrophilic case, after having reach the maximum liquid-gas area expansion, the capillary pressure suddenly drops and a new minimum of the free energy is reached. On the contrary, in the hydrophobic case, liquid penetration does not occur at long times. A possible explanation is that, in order for the liquid to penetrate, the hydrophobicity constraints the fluid to further increase the liquid-gas surface area; an increment that the fluid is not able to energetically sustain, therefore liquid retracts and remains trapped at the pore throat.
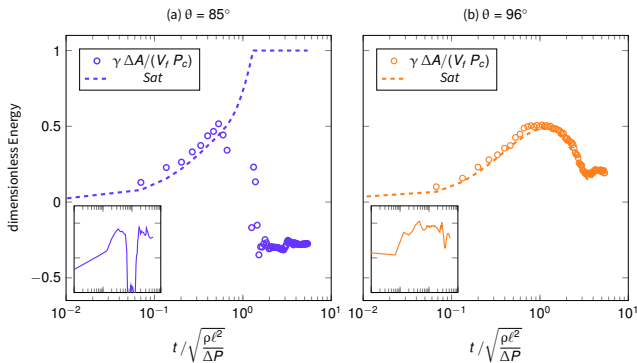

Figure 2: The two term of Eq. 2 representing the dimensionless energy for a contact angle of 85° (a) and 96° (b). Insets: capillary pressure vs. time.

Since the trapping probability depends both on the fibre

wettability and on the pore throat diameter, in more complex media liquid would penetrate the big pore throats and it would be trapped in smaller throats, with the trapping probability increasing with the hydrophobicity. Figure 3 shows an example of the liquid pore trapping occurring in hydrophobic media composed of randomly transversally oriented fibres.

Conclusions

The mechanism of liquid pore trapping in fibrous porous media is studied by means of Lattice-Boltzmann simulations at the pore-scale. Results reveal the mechanism of trapping and pore blockage in hydrophobic porous media. The liquid-gas surface area plays a pivotal role in determining the trapping probability in porous media composed of fibres. This new finding opens up the root for an innovative design of gas diffusion layer in fuel cells with improved performances in terms of water management.
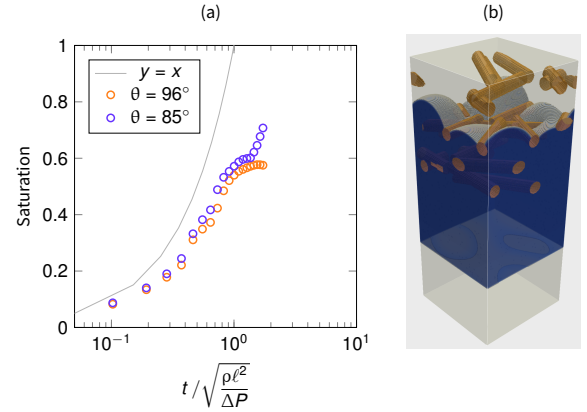
Figure 3: (a) The saturation variation in time during imbibition in the three-dimensional fibrous media. (b) The trapping of liquid in the hydrophobic medium is also visible in the snapshots of simulations at dimensionless time $t^* = 2$.

Acknowledgments

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