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A new approach to modelling water flooding in a polymer electrolyte fuel cell

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ABSTRACT

The distribution and migration of liquids in various layers of a PEFC is commonly modelled by the 3D flow equations. Given the fact these layers are very thin, there are major problems with such models, including heavy computational efforts and doubts in their applicability to the gas diffusion layer (GDL). Recently, a new approach for modelling multiphase flow through a stack of thin porous layers has been developed [Qin and Hassanizadeh, Int. J. Heat Mass Transfer 70 (2014) 693–708]. In this approach, which is called "*reduced continua model*", each layer is modelled as a 2D domain with governing equations formulated in terms of thickness-averaged properties. The mass exchange between layers is prescribed by a new constitutive equation. The aim of this paper is to illustrate the implementation of the reduced continua model and show its advantages in modelling liquid water flooding in the GDL and micro porous layer (MPL) of a PEFC. We find that, in comparison to the Richards model, the reduced continua model predicts quite similar water dynamics in the MPL, but a lower steady-state water saturation in the GDL, particularly under the channel area. We provide a quantitative indication of the enormous computational efficiency of the reduced continua model as compared to the Richards model. Finally, the sensitivity studies of major material parameters of the reduced continua model have been provided.

Introduction

Two-phase flow through multilayers of thin porous media is an important process in a number of industrial applications and hygiene products. One of the typical applications is the polymer electrolyte fuel cell (PEFC), which has received much attention over the past two decades [1–4]. They convert chemical energy in fuels (e.g. H_2) to electricity by means of electrochemical reactions, with the advantages of high efficiency, low/zero emission, and quick startup [5].

Usually, hundreds of PEFC units are connected in series, as a stack, to provide useful power. A schematic representation of a PEFC unit is shown in Fig. 1a. It consists of a cathode side (where air is delivered) and an anode side (where hydrogen is delivered), separated by a solid electrolyte membrane as an electrical insulator [3]. Each side consists of one bipolar plate (BP), one gas diffusion layer (GDL), one micro porous layer (MPL), and one catalyst layer (CL). Several intricate transport processes can occur in an operating PEFC, such as reactant diffusion in the gas phase, air–water flow, heat transfer, as well as electron and proton conduction [5]. An optimum water

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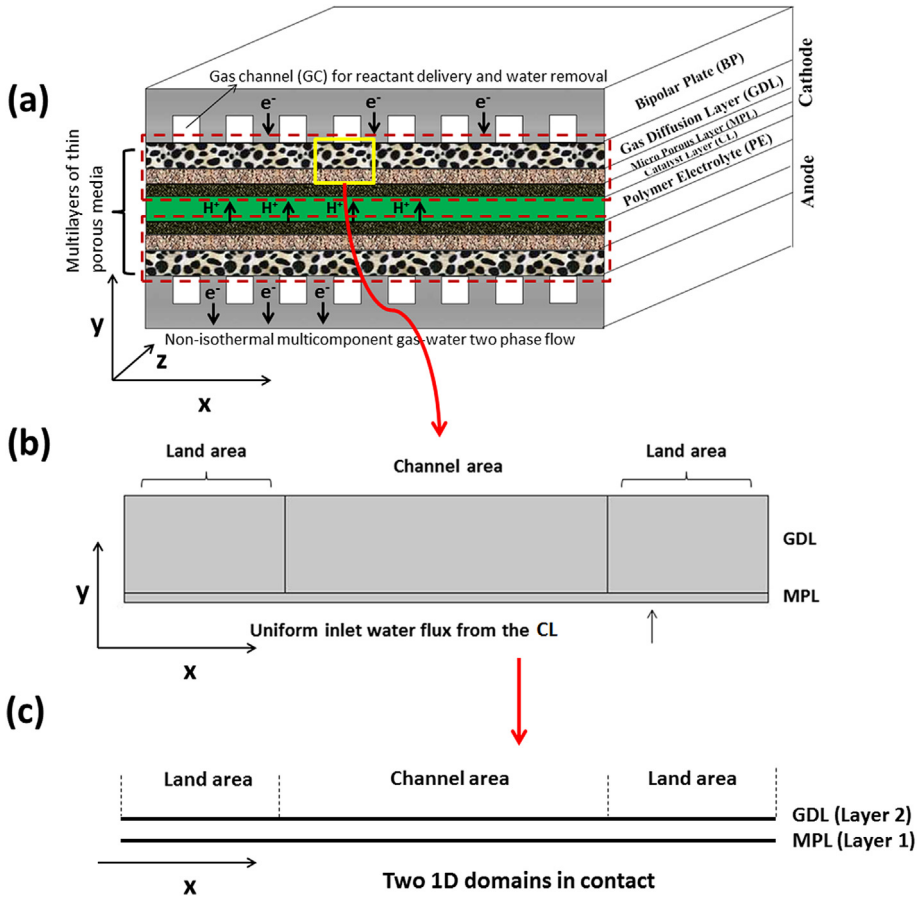

Fig. 1 – (a) Schematic representation of a PEFC unit; (b) simplified 2D computational domain used in the traditional Richards model; and (c) two 1D computational domains used in the reduced continua model.

balance is critical to the operation of PEFCs. On one hand, the solid membrane needs to attain high water content for effective ionic conduction; on the other hand, too much water accumulating in the system would result in reactant transport limitation and cell degradation [6–10]. Normally, such a situation is termed as '*liquid water flooding*' in PEFCs.

In an operating PEFC, water is produced partly from the humidification of inlet reactants and partly from electrochemical reactions in the cathode CL. At high current densities and/or in humid environments, all diffusion layers (GDL, MPL, and CL) and GCs can become flooded, particularly on the cathode side [11]. In general, liquid water movement in a PEFC can be categorized into three subprocesses, namely: (1) liquid water production and transport in CL; (2) liquid water transport in MPL and GDL; (3) liquid water emergence at GDL-GC interface and its subsequent movement in GC. In modeling these water transport processes, a number of difficulties have been encountered with traditional Darcy-based models. First, it is a major challenge to model imperfect physical contact interfaces between neighboring porous layers with quite different material properties; e.g. between MPL and CL [12–14]. Second, there is no satisfactory approach for coupling liquid water dynamics in GC and the description of water transport in GDL [15–17]. This problem is commonly referred to as the two-phase interface treatment between free flow and porous media flow. Last but not least, it is very questionable whether three dimensional (3D) Darcy-based models are applicable to these extremely thin porous layers. It is known that most macroscale PEFC models [2, 9, 10, and 16] are formulated in terms of averaged quantities, which are defined over an averaging domain known as the representative elementary volume (REV). A major requirement of this REV is that its size must be much larger (10–15 times) than the pore size, but much smaller than the modeling domain size [18]. This criterion cannot be satisfied in the fibrous GDL as its thickness is only 10–15 times its mean pore size. Based on the pore-scale pore-network modeling of water transport in a GDL, Rebai and Prat [19] illustrated the poor predictions of traditional Darcy-based models. In addition, 3D modeling of these interacting thin porous layers often requires heavy computational efforts, which have hindered the stack-level modeling of PEFCs.

It is interesting to point out that the conventional concept of REV does apply to the MPL, although it is even thinner than the GDL. This is because the mean pore size of MPL is several hundred nanometers [3], which is about hundred times smaller than its thickness (around 30 microns). This allows the identification of an appropriate REV. Thus, we define '*a physically thin porous layer*' as a porous layer for which the REV length scale requirements are not satisfied along the layer