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Analytical calculation of electrolyte water content of a Proton Exchange Membrane Fuel Cell for on-board modelling applications

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HIGHLIGHTS

- Fast modelling of electrolyte water content in Proton Exchange Membrane Fuel Cells.
- Innovative diffusivity and swelling functions based on literature experiments.
- Analytical solution of water mass balance based on reasoned physical assumptions.
- Mean error below 0.26% for electrodes water content higher than 5.
- High flexibility and generalizability of the solution for on-board uses.

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ABSTRACT

This paper proposes an analytical model of the water content of the electrolyte of a Proton Exchange Membrane Fuel Cell. The model is designed by accounting for several simplifying assumptions, which make the model suitable for on-board/online water management applications, while ensuring a good accuracy of the considered phenomena, with respect to advanced numerical solutions. The achieved analytical solution, expressing electrolyte water content, is compared with that obtained by means of a complex numerical approach, used to solve the same mathematical problem. The achieved results show that the mean error is below 5% for electrodes water content values ranging from 2 to 15 (given as boundary conditions), and it does not overcome 0.26% for electrodes water content above 5. These results prove the capability of the solution to correctly model electrolyte water content at any operating condition, aiming at embodiment into more complex frameworks (e.g., cell or stack models), related to fuel cell simulation, monitoring, control, diagnosis and prognosis.

1. Introduction

Proton Exchange Membrane Fuel Cells (PEMFCs) represent one of the most promising alternatives to conventional power generation systems thanks to their flexibility, modularity, fast warmup and shut down as well as low noise and pollutant emissions [1]. Nevertheless, several drawbacks are hindering PEMFC commercialization on large scale, such as their limited durability, if compared to the reference targets already discussed by the authors in Ref. [2], as well as their high manufacturing and maintenance costs. For this reason, scientific and industrial efforts are currently oriented towards costs reduction and durability increase. In particular, it is possible to avoid (or at least limit) the occurrence of detrimental conditions, which negatively affect system performance and lifetime, by means of suitable control, diagnostic and prognostic strategies [3].

One of the most critical issues related to PEMFC operation consists in its water content management. A correct membrane hydration promotes cell ionic transport (i.e., proton transport from anode to cathode), resulting in lower cell losses. Therefore, if the electrolyte water content is reduced (i.e., less water is supplied to the membrane), proton transport resistance increases, with a consequent voltage drop. This phenomenon is renown in the literature as *drying*. On the other hand, if the water content increases too much, although the electrolyte conductivity is enhanced, the presence of a great amount of liquid water hinders the reactants (i.e. oxygen and/or hydrogen) to reach the reaction sites. This leads to a growth in the diffusion losses and to a consequent voltage reduction. This phenomenon is usually called *flooding*. Accordingly, it is clear the importance of suitable control strategies that maintain electrolyte water content within an optimal range, to balance the occurrence of the aforementioned detrimental

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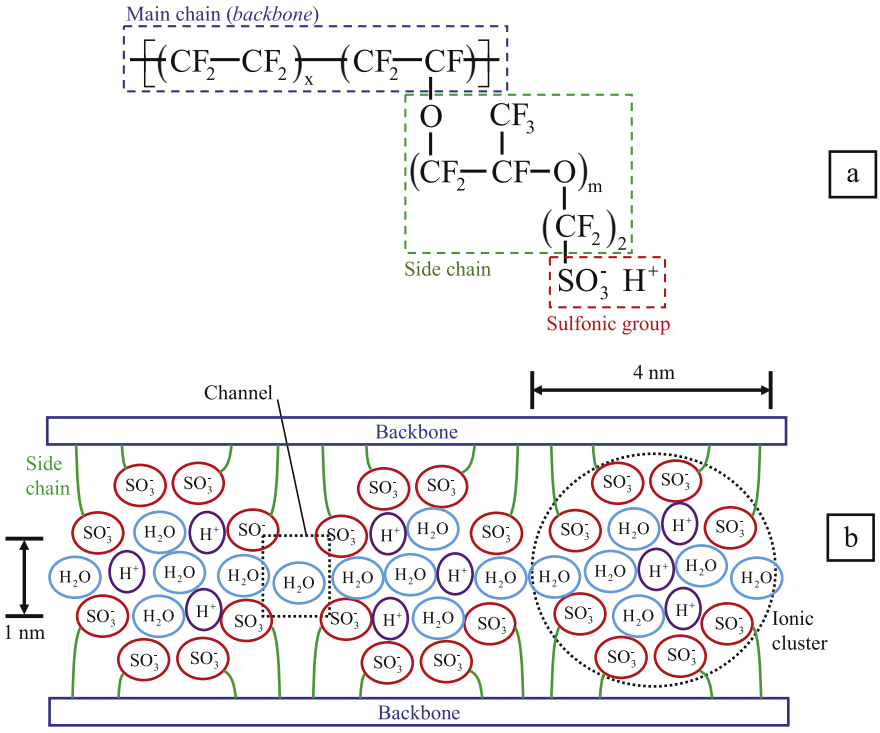

Fig. 1. Chemical structure of Nafion® (a) and cluster-network model schematic representation (b) (adapted from Refs. [15–17]).

phenomena [4]. Since a direct control of the water content is not possible, one way to ensure correct membrane hydration consists in the regulation of the humidity level at cell inlets and the cell bulk temperature.

Water transport phenomena within PEMFCs have been largely studied in the literature, due to the critical role played by water management in fuel cell performance and lifetime improvement. Many electrolyte models are currently available at various level of detail, focusing either on the sole electrolyte or on the entire fuel cell. By far, the most popular and used electrolyte model is the one developed by Springer et al. [5]. The authors developed a one-dimensional, steady-state, isothermal PEMFC model, in which two different phenomena regulate the flux of water across the electrolyte, namely electro-osmotic drag and diffusion. According to the most relevant works in the literature, this model is classified as *diffusive model*. Using a different approach, Bernardi and Verbrugge [6] developed the so-called *hydraulic model*, in which the water flux is induced by hydraulic permeation and migration. Other available models have been later developed as a variation of these diffusive and hydraulic models [7,8].

It is worth observing that solving in space and time such models usually requires great computational effort and time. Therefore, for extensive simulation purposes or real-time/on-board applications, an approximate solution is often preferred [7,9]. An example is given by the work of Mazumder [10], in which a model including water convection in the diffusive model of Springer et al. [5] is proposed. The model has been solved numerically to compute the electrolyte net water flux and average conductivity as function of electrodes humidity, electrolyte pressure drop, temperature and current density. A parametric analysis has been then performed and the results have been collected in numerical maps, which can be directly used within fuel cell models instead of complex water transport equations that require high computational time. However, although effective and easy to be implemented, such maps are strictly related to the physical properties of the considered electrolyte and their use is limited to the related technology. Therefore, the flexibility and generality of the maps is not guaranteed.

Taking into account the need for simplicity and generalizability, the purpose of this work is to develop a simplified mathematical model able to estimate the electrolyte water content of a PEMFC as a function of electrolyte physical properties and cell operating conditions (i.e., current, temperature, reactants humidity, etc.). As other literature models, the proposed one can be classified as a combination of diffusive and hydraulic models [5,6]. The model design is chosen as trade-off between computational speed and accuracy, with great attention to the correct representation of the involved water transport mechanisms [11–14]. Moreover, the model framework embeds an innovative representation of water diffusion combined with electrolyte swelling, usually neglected or greatly approximated in the literature (e.g., in Ref. [10]). According to this design, the model guarantees high simulation accuracy while offering the possibility to be easily implemented in complex on-board/real-time monitoring, diagnostic, control and prognostic algorithms. In such a way, the model may support the development and application of suitable strategies to detect in reasonable time drying and flooding and apply proper countermeasures to reduce the detrimental effects of these phenomena on cell performance and durability.

In the next sections, an overview of the electrolyte structure and main physical properties is given, followed by the analysis of the main transport mechanisms influencing electrolyte water content. The purpose of these sections is to briefly describe the basic physical phenomena and the approach followed for model design. Then, the mathematical model is detailed, addressing the considered approximations and discussing the achieved analytical solution. Afterwards, the model accuracy and reliability is investigated by comparing simulation results with those achieved with a more complex numerical solution, which requires higher computational time and it is not suitable for online applications. In the conclusions, the main advantages and drawbacks of the proposed approach are addressed, remarking the main contributions which can be given to fast fuel cell models.