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Water equilibria and management using a two-volume model of a polymer electrolyte fuel cell

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Abstract

In this paper, we introduce a modified interpretation of the water activity presented in Springer et al. [T.E. Springer, T.A. Zawodzinski, S. Gottesfeld, Polymer electrolyte fuel cell model, J. Electrochem. Soc. 138 (8) (1991) 2334–2342]. The modification directly affects the membrane water transport between the anode and the cathode (two electrodes) of the polymer electrolyte membrane (PEM) fuel cell in the presence of liquid water inside the stack. The modification permits calibration of a zero-dimensional isothermal model to predict the flooding and drying conditions in the two electrodes observed at various current levels [D. Spernjak, S. Advani, A.K. Prasad, Experimental investigation of liquid water formation and transport in a transparent single-serpentine PEM fuel cell, in: Proceedings of the Fourth International Conference on Fuel Cell Science, Engineering and Technology (FUELCELL2006-97271), June 2006]. Using this model the equilibria of the lumped water mass in the two electrodes are analyzed at various flow conditions of the stack to determine stable and unstable (liquid water growth) operating conditions. Two case studies of water management through modification of cathode inlet humidification and anode water removal are then evaluated using this model. The desired anode water removal and the desired cathode inlet humidification are specified based upon (i) the water balance requirements, (ii) the desired conditions in the electrodes, and (iii) the maximum membrane transport at those conditions.

Keywords: PEMFC; Water management; Anode water removal; Water dynamics

1. Introduction

Due to the significant influence of water [3,4] on the performance of the polymer electrolyte membrane fuel cell (PEMFC), many models have been developed to capture its spatial distribution within a fuel cell stack. These computational fluid dynamics (CFD) models are then used to optimize the cell flow field (width, length, orientation, etc.) and materials (hydrophobicity, porosity, thickness, etc.). Once the optimum fuel cell is designed, CFD models [5] can again, theoretically, be used to select the right number of cells to be combined in a stack in order to avoid large cell-to-cell variations. Although the above fuel cell design process is visionary, it is still far from being realized. Ultra large-scale models [6] have so far been used to simulate medium size single cells with fixed geometry and materials interconnection.

Once the fuel cell is designed the only remaining degrees of freedom for water management are the mass flow rates entering and leaving the electrodes of the fuel cell stack. The actuating mechanisms for controlling water flow rates, for example, anode and cathode inlet humidification, oxygen excess ratio (OER), and anode recirculation, are not spatially distributed, but allow control only in the stack manifolding, which in turn constitutes the boundary control to the electrodes. Water management of the fuel cell stack with these actuators cannot be used to control the spatial distribution of water in the stack (from cell to cell and within the stack material). Nevertheless, one can start by controlling the mass of water in the two lumped volumes that correspond to the anode and the cathode electrodes and augment this methodology with diagnostic mechanisms that detect maldistribution of water through cell to cell variability or large pressure variations [7]. It is through the water management in the electrodes that we hope to control the humidity conditions at the catalyst where the reaction happens.

In this paper, the capabilities of physically actuated system variables to achieve water balance in the stack are evaluated

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Nomenclature

p	pressure (Pa)
m	mass (kg)
y	vapor mass fraction
W	flow rate (kg s^{-1})
T	temperature (K)
I_{st}	stack Current (A)
N	molar flux (mole s^{-1} cm^{-2})
$\bar{M}$	molecular weight (kg mole^{-1})
R	gas constant (J kg^{-1} K^{-1})
λ	water content
a_w	water activity
ϕ	relative humidity
ω	humidity ratio
$\tilde{k}$	flow coefficient (kg s^{-1} Pa^{-1})

Superscripts and subscripts

a	anode
c	cathode
m	membrane
st	stack
v	vapor phase
l	liquid phase
H_2O	water
H_2	hydrogen
O_2	oxygen
N_2	nitrogen
gen	generated
rem	water removed
in	inlet
out	outlet
sat	saturated

using a zero-dimensional, isothermal, lumped parameter PEMFC stack model similar to [8]. In this low order model, water (both liquid and vapor) accumulates in the lumped volumes of the two electrodes. Additional components in the stack that can potentially store water, such as gas diffusion layer (GDL) and membrane, are neglected. Moreover, the model assumes instantaneous transition from vapor to liquid phase if the partial pressure of water vapor exceeds the saturation pressure. Finally, an ideal thermal control is assumed that maintains constant temperature throughout the stack.

Clearly, the stack model with these assumptions will not capture any spatial distribution. Instead, this low order model focuses on important lumped phenomena, such as, anode flooding at lower current densities [2,9] and anode drying at higher current densities [10]. In order to capture the phenomenon of anode flooding, the model presented in [12,11] is modified to allow liquid water on the cathode side of the membrane to influence membrane water transport.

The low order model facilitates the stability analysis of the water equilibria arising from employing various popular water management techniques, such as controlling humidity of inlet flow or anode water removal using recirculation [14,13]. This step is important since only stable equilibria can be achieved via feedforward maps (look-up tables) that use the information of the current drawn to determine, for instance, the appropriate level of anode water removal [15] or cathode inlet humidification [16,17].

We demonstrate a methodology to achieve water management using (i) cathode inlet humidification, and (ii) anode water removal, as actuating mechanisms. Other mechanisms, namely, anode humidification and cathode water removal through high oxygen excess ratio, might be necessary when operating at very low or very high currents. The use of these mechanisms will need more investigation than the one that can be allotted in this paper.

The paper is structured as follows: the stack model related to water management is discussed in Section 2. The water dynamics in the anode and the cathode and their interaction under different operating conditions are discussed in Section 3. The model predictions of stack flooding and drying characteristics without active water management are discussed in Section 4. In Section 5, different water management strategies involving cathode inlet humidification and anode water removal are identified and their ability to achieve particular water conditions are investigated independently of specific actuating components. Section 6 summarizes the results in the paper.

2. Model for water management analysis

In this section, we first present the membrane water transport model [1] with a modification to the typical interpretation of water activity used in [11,12,18]. The proposed modification enables the prediction of liquid water accumulation in the anode at low current densities, which is important for mobile fuel cell applications due to the frequent operation at low loads. Then, we integrate this modified membrane water transport model with anode and cathode mass balance equations to develop the two-volume fuel cell model.

2.1. Membrane water transport

The water transport through the membrane from the anode to the cathode, W_{memb}, is given by

$$W_{memb} = \bar{M}_{H_2O} A_{fc} n_{cells} (N_{drag} - N_{diff}), \quad (1)$$

where A_{fc}(cm^2) denotes the active fuel cell area, n_{cells} the number of cells in the stack and $\bar{M}_{H_2O}$ the molecular weight of water. The molar flux per unit cell from the anode to the cathode due to the electro-osmotic drag is N_{drag} (mole s^{-1} cm^{-2}), while N_{diff} (mole s^{-1} cm^{-2}) is the molar flux per unit cell from the cathode to the anode due to the difference in water concentration on the anode and cathode sides.

These fluxes depend upon the stack current, I_{st}; the membrane water content, λ_m; and the amount of water present on the anode and cathode sides [1,11]. The molar flux due to electro-osmotic