



# Anode partial flooding modelling of proton exchange membrane fuel cells: Model development and validation



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## ABSTRACT

A two-dimensional along-the-channel CFD (computational fluid dynamic) model, coupled with a two-phase flow model of liquid water and gas transport for a PEM (proton exchange membrane) fuel cell is described. The model considers non-isothermal operation and thus the non-uniform temperature distribution in the cell structure. Water phase-transfer between the vapour, liquid water and dissolved phase is modelled with the combinational transport mechanism through the membrane. Liquid water saturation is simulated inside the electrodes and channels at both the anode and cathode sides. Three types of models are compared for the HOR (hydrogen oxidation reaction) and ORR (oxygen reduction reaction) in catalyst layers, including Butler–Volmer (B–V), liquid water saturation corrected B–V and agglomerate mechanisms. Temperature changes in MEA (membrane electrode assembly) and channels due to electrochemical reaction, ohmic resistance and water phase-transfer are analysed as a function of current density. Nonlinear relations of liquid water saturations with respect to current densities at both the anode and cathode are regressed. At low and high current densities, liquid water saturation at the anode linearly increases as a consequence of the linear increase of liquid water saturation at the cathode. In contrast, exponential relation is found to be more accurate at medium current densities.

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## 1. Introduction

Benefiting from high energy efficiency and low emission, PEMFCs (proton exchange membrane fuel cells), play an important role in transiting a carbon intensive economy to sustainable low carbon future [1–4]. In addition, the features of PEMFCs endow a flexibility and scalability for use with batteries and CHP (combined heat and power) system for hybrid automotive and residential use [5–7], as well as energy conversion from winds to electricity [8]. Among the PEMFC family, the medium and low temperature PEMFCs are considered as promising candidates as portable and automotive power sources. However, they can experience certain operating difficulties associated with water transport and flooding during their operation, especially at a high current density [9–11].

Three phases of water co-exist in PEMFCs: as vapour and liquid in porous electrodes and channels, and as a dissolved phase absorbed by membrane and ionomer (membrane and ionomer water uptake). Among three phases, dissolved water can migrate between both electrodes through the membrane under the driving forces of EOD (electro-osmotic drag), back diffusion and hydraulic permeation [12–14]. Liquid water can be generated in terms of water vapour condensation and membrane/ionomer desorption when over-saturated. Simultaneously, liquid water is removed from the MEA (membrane electrode assembly) generally by reactant gases flowing along the channels. If water generation rate is faster than the removal rate, excess water will accumulate in the electrodes and flow channels, leading to a water flooding inside the cell. This flooding can reduce the effective porosity in the porous media and increase the pressure drop along the channel, inhibiting the gas transport to the active sites in CLs (catalyst layers), finally resulting in a decline in the cell performance [9,15,16]. Water flooding is typically observed at the cathode side due to the fact that water is produced inside the CCLs (cathode catalyst layers) by the ORR (oxygen reduction reaction).

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There have been numerous studies of water flooding at the cathode but less consideration of water transport related to the anode. However, hydrogen consumption at the anode could also result in the humidified anode reactant gas becoming supersaturated with water vapour, which can result in transfer to liquid water after condensation. Liquid water movement in hydrophilic and hydrophobic anode gas channel, as well as the effect of hydrogen inlet velocity, operating temperature and channel walls wettability, was numerically studied by Ferreira et al. [17]. Experimental studies have detected liquid water in the anode and that more liquid water was observed at a high anode relative humidity [18,19]. An in-situ detection scheme of anode flooding, developed by O'Rourke et al. [20], showed that anode flooding could be detected prior to a rapid cell voltage decline, which was considered as an early warning of cathode catalyst damage. As reported by Anderson et al. [21], AWR (anode water removal) could be used as a diagnostic tool to assess cathode water flooding in PEM fuel cells.

Catalyst layers are complex structures and are a difficult to describe and be fully understood in PEMFCs; not only due to their highly compact structure and complex composition but also because of the coupled electrochemical reactions and transport processes occurred. CLs in PEMFCs facilitate electrochemical reactions and produce water at the cathode. To describe the current density produced on each electrode in fuel cell operation, considering the water generated which can partially cover the platinum catalyst surface, (1-s) corrected B–V equation (s is the liquid water saturation, defining as the volume fraction of void space occupied by liquid water) is usually required instead of the traditional B–V equation [22–24]. The electrochemical activity may be further represented using an agglomerate model, taking into account the increase in ionomer film thickness surrounding the agglomerate due to ionomer swelling. Furthermore, by considering gas transport resistance and the reduction of porosity due to liquid water occupation, the agglomerate model can also provide a superior representation of the porous CLs in comparison with other models [25,26].

In fuel cell operation, temperature plays a significant role in achieving a high power performance. A variety of parameters, e.g. electrochemical reaction kinetics, mole fractions in gas mixture, electrolyte conductivity, rate of mass transfer, as well as liquid water saturation, are closely correlated with temperature during fuel cell operation. Within PEMFCs, the temperature distribution across the MEAs and along the flow channels can be either estimated by mathematical modelling technique or detected by experimental measurements [27–30]. Ju et al. [27] developed a three dimensional (3D), single-phase, non-isothermal model through a parametric study for GDL thermal conductivity, gas relative humidity and operating cell voltage. Wang et al. [28] measured the temperature profile within a single PEMFC with the aid of ITI (infrared thermal imaging) and found that the downstream temperature is higher than the upstream, and there was an obvious high temperature section in the outlet of oxygen. Temperature measurement were conducted by Zhang et al. [29] and Lin et al. [30] from which they found a correlation between local temperature rise and local current density, and a temperature rise at backsides of both the anode and cathode flow field plates.

However, up to now, it is still a challenge to fully couple most aspects mentioned above in modelling endeavor for a highly accurate evaluation of water flooding in a single PEMFC or stack. In this paper, we fully couple seven sub-models and apply them on a two dimensional (2D), ATC (along-the-channel) geometry for a single PEMFC: (1) agglomerate models for gas transport resistance in CLs, (2) two-phase flow models for liquid water saturation, (3) combinational diffusion models for dissolved water transport

through the membrane, (4) non-isothermal models for heat transport in MEA and channels, (5) CFD (computational fluid dynamic) models for gas transport along the channels, (6) multi-component diffusion of reactant gases in gas mixture, and (7) ionomer swelling due to non-uniform distribution of water content. The effect of liquid water on the current density are compared based on three mechanisms, including traditional B–V, (1-s) corrected B–V and agglomerate kinetics. Distributions of reactant gas, liquid water and heat within the cell are investigated. The expressions for the relationship between the liquid water saturation on each electrode and current density, as well as the liquid water saturation between anode and cathode, are regressed.

## 2. Model description

### 2.1. Assumption

Some additional assumptions were employed in this work in addition to those in the previous papers [34–38]:

1. Steady state, two-phase flow, along the channel model of a PEMFC.
2. Gas flow in the channels is laminar flow and incompressible.
3. Reactant gases enter the gas channels in a direction normal to the channel cross section.
4. Liquid water saturation in channels is continuous.
5. Gas diffusion layers and catalyst layers are isotropic.
6. No liquid water enters the channels at the inlets.
7. Same electrodes and bipolar plates are used in the anode and cathode, respectively.

### 2.2. Governing equations

The conservation equations of mass, momentum, species, energy and charges are summarized as Eqns. (1)–(4):

$$\nabla \cdot (\rho^g \mathbf{u}^g) = S_m \quad (1)$$

$$\rho^g (\mathbf{u}^g \cdot \nabla \mathbf{u}^g) = \nabla \left[ -pI + \mu^g \nabla \mathbf{u}^g + \mu^g (\nabla \mathbf{u}^g)^T - \frac{2}{3} \mu^g (\nabla \cdot \mathbf{u}^g) I \right] \quad (2)$$

$$\rho^g \mathbf{u}^g \cdot \nabla w_i^g - \nabla \cdot \left[ \rho^g \sum_{j=1}^N (1-s') D_{ij} (\nabla x_j^g - w_j^g) \frac{\nabla p}{p} + D_i^T \frac{\nabla T}{T} \right] = M_i S_i^g \quad (3)$$

$$\nabla \cdot \left[ \sum_{i=g,l} (\varepsilon \rho c_p \mathbf{u})_i T \right] - \nabla \cdot \left( \sum_{i=g,l,s} k_i \nabla T \right) = S_T \quad (4)$$

$$\sigma_s^{eff} \nabla \cdot \nabla \varphi_s + \sigma_M^{eff} \nabla \cdot \nabla \varphi_M = 0 \quad (5)$$

where  $\rho$  ( $\text{kg m}^{-3}$ ) is density,  $\mathbf{u}$  ( $\text{m s}^{-1}$ ) is velocity,  $p$  (Pa) is pressure,  $\mu$  (Pa s) is viscosity,  $M$  ( $\text{kg mol}^{-1}$ ) is molecular weight,  $D$  ( $\text{m}^2 \text{s}^{-1}$ ) is diffusion coefficient,  $D^T$  ( $\text{kg m}^{-1} \text{s}^{-1}$ ) is thermal diffusion coefficient,  $c_p$  ( $\text{J mol}^{-1} \text{K}^{-1}$ ) is specific heat capacity,  $k$  ( $\text{W m}^{-1} \text{K}^{-1}$ ) is thermal conductivity,  $T$  (K) is temperature,  $\sigma$  ( $\text{S m}^{-1}$ ) is conductivity,  $\varphi$  (V) is potential.  $w$  is mass fraction,  $x$  is mole fraction,  $\varepsilon$  is volume fraction,  $s'$  is corrected liquid water saturation and  $I$  is identity matrix. Subscript  $i$  and  $j$  represent species  $i$  and  $j$  and superscript  $g$  means gas phase.  $S$  is the source term, which is given in detail in Tables 1–3. Note that Eq. (1) to Eq. (3) were applied on reactant gas

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