INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 40 (2015) 7817–7828

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A single domain approach to modeling the multiphase flow within a flowing electrolyte – direct methanol fuel cell

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ARTICLE INFO

Article history:
Received 2 September 2014
Received in revised form
6 November 2014
Accepted 14 November 2014
Available online 13 January 2015

Keywords:
Single domain model
Multiphase
Fuel cell
DMFC
Flowing electrolyte

ABSTRACT

In this study, the well-known Multiphase Mixture Model (MMM) was improved with a new single domain approach which was used to model the flow behaviour and performance of a Flowing Electrolyte - Direct Methanol Fuel Cell (FE-DMFC). Emphasis was placed on the methanol and water crossover fluxes. Unlike the existing methods, the proposed method only requires the mixture variables, thereby decoupling the requirement for information about the gaseous state. This new approach was demonstrated by describing the physics of the fuel cell under base line operating conditions, as well as different cathode humidifications. The observed trends were found to be consistent with experimental and modeling results in DMFC literature. The model suggests that the flowing electrolyte channel (FEC) effectively washes unreacted methanol out of the system, yielding a negligible methanol crossover flux at the cathode catalyst layer. Furthermore, it was determined that the convection caused by the back-pressure within the FEC is an important factor to consider; since this effect is sufficiently strong to cause water to flow from the FEC to the anode. The model also suggests that decreasing the cathode humidification increases both the methanol and water crossover fluxes as well as the ohmic resistance within the membranes and FEC. This result suggests that some liquid water within the cathode could be beneficial for the fuel cell, to decrease these losses.

Introduction

Direct methanol fuel cells (DMFCs) are considered to be a promising technology for low power and portable applications [1,2]. However, two of the greatest challenges associated with this technology are the crossover of methanol and water, and the two-phase flow within the anode and cathode. The increased cathode activation polarization and catalyst degradation caused by methanol crossover has been estimated to

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http://dx.doi.org/10.1016/j.ijhydene.2014.11.103

account for more than 30% of the total losses for most DMFC configurations [3]. Whereas, the two-phase flow and crossed over liquid water to the cathode hinders the flow of fuel and oxidant to their respective catalyst layers (CLs), thus decreasing the performance.

Several groups have modeled the two-phase behaviour in DMFCs and two of the most common approaches are the multi-fluid model [4–6] and the multiphase mixture model (MMM) [7–10]. These models are either formulated as a multi-domain or a single domain model. In the multi-domain approach, each layer within the fuel cell is treated separately and coupled through interfacial conditions. This approach is likely the most numerically stable of the two approaches but likely demonstrates slower convergence. In the single domain approach, the governing equations are formulated in such a way where the entire fuel cell is treated in the same manner and the governing equations for all layers are solved simultaneously [11,12]. As such, the single domain approach removes the need for any interfacial conditions. This approach is very convenient for fuel cell modeling, and has since become an attractive option. Since current formulations of the single domain approach require information concerning the gaseous phase (to measure the activity of the membranes), this method is somewhat inconvenient for the MMM [12,13].

Due to the dominant nature of the losses associated with methanol crossover, much research has been placed on reducing or eliminating methanol crossover. One approach was proposed by Kordesch and his team with the flowing electrolyte fuel cell [14,15]. In this case, the anode and cathode of the DMFC are separated by an ionically conductive fluid (liquid electrolyte) such as diluted sulfuric acid, as shown in Fig. 1. This flowing electrolyte washes away any methanol that attempts to crossover, thus protecting the cathode from any parasitic current loss. In the case where the electrolyte is simply flown through the DMFC once, it is known as a flowing electrolyte – direct methanol fuel cell, or FE-DMFC. The advantage of this kind of fuel cell is that it can theoretically function as a DMFC without a mixed potential at the cathode.

Several single phase hydrodynamic studies [16–19] and single phase models for the FE-DMFC have been proposed [20–22]. However, to the authors' knowledge, none have examined the multiphase effects within this fuel cell. Due to the attractiveness of the single domain approach, a new formulation is proposed, where only mixture variables are required, thereby decoupling the need for information regarding the gaseous phase and allow for the direct application of the MMM. The proposed formulation has been applied to model the multiphase flow within the FE-DMFC in detail, and validated against in-house experimental results. This new approach was also demonstrated over the base line operating conditions and various inlet cathode humidifications. In each case, the underlying physics of this fuel cell will be discussed with emphasis placed on the methanol and water crossover fluxes. The modeling results are compared against trends in DMFC experimental and modeling literature.

Overview of model

As discussed in the Introduction, current FE-DMFC models are single phase. This limits the realism of the results as well as what can be examined. Furthermore, the results obtained, over-predict the performance of the fuel cell. Therefore, in this section, a more comprehensive and flexible multiphase model is developed to allow for a more accurate estimation of

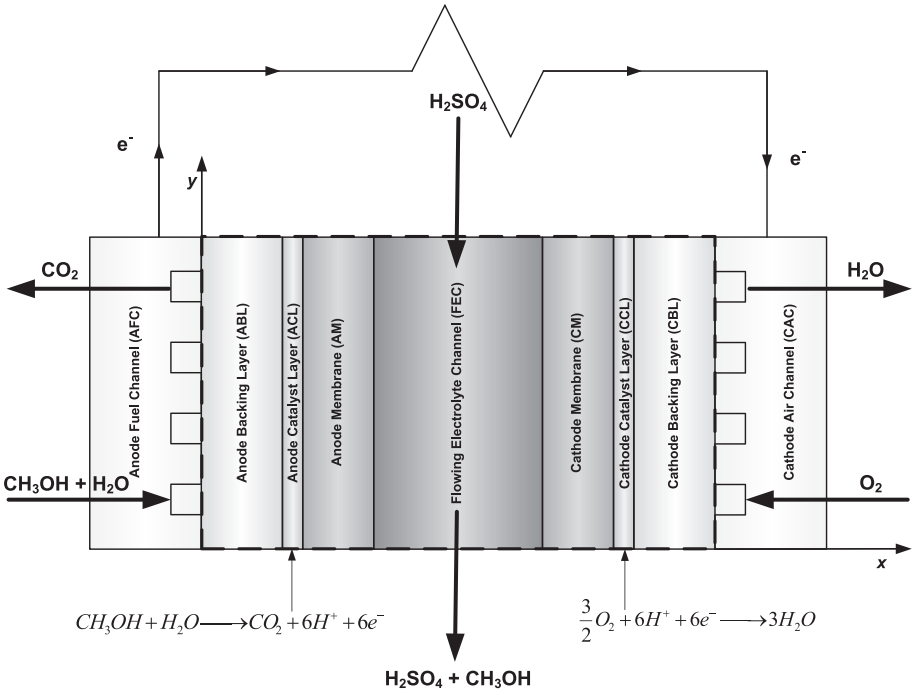

Fig. 1 – Schematic of a flowing electrolyte-direct methanol fuel cell (FE-DMFC). The dashed box and the *x* and *y* axes represent the computational domain and the *x* and *y*-directions for the model. Modified from Ouellette et al. [22].