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Predicting the transient response of a serpentine flow-field PEMFC I. Excess to normal fuel and air

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Abstract

A three-dimensional numerical simulation of the transient response of a polymer electrolyte membrane fuel cell (PEMFC) subjected to a variable load is presented. The model parameters are typical for a laboratory-scale cell with a serpentine flow path and a 10 cm^2 reactive area. The simulation uses a commercial computational fluid dynamics (CFD) solver modified to include the electrochemical behavior. The predictions are based on an isothermal set of equations and include transient responses of the cell in terms of local distributions of the current density and gas mole fractions. The predictions show transients in the current density that overshoot the final state value when the cell voltage is abruptly changed from 0.7 to 0.5 V for fixed excess initial stoichiometric flowrates. The fixed flowrates are excess because they correspond to stoichiometries of 2.6 and 4.4 at 0.7 V for the 0.35 A/cm^2 predicted initial current density. The percent overshoot decreases with the rate of voltage change and it is shown to change with anode gas flow rates. Also the magnitude of this overshoot and undershoot can be adjusted by changing the rate of voltage change and the operating conditions. The overshoot behavior for these excess stoichiometric flowrates is shown to depend on changes in the oxygen mole fraction distributions.

Keywords: PEM; Fuel cells; Membrane electrode assembly; Electric vehicle; Dynamic response; Overshoot

1. Introduction

The control, design, and optimum operation of polymer electrolyte membrane fuel cells (PEMFCs) will require an understanding of its dynamics when there are changes in either current, voltage, or power. These dynamics would be important for power conditioning in residential applications and for automotive systems performing in a Federal Urban Driving Scenario. While some of these dynamics could be determined from experiments, a model capable of predicting the transient response would be useful in the design flow fields and for optimization of control schemes. We are particularly interested in overshoot behavior because recent experiments in our laboratory [1–3] indicate the possibility of overshoot behavior dependent on the rate of voltage change, and stoichiometry.

As a guide for simple one-dimensional (1D) and two-dimensional (2D) models that may be developed in the future, we present here a three-dimensional (3D) solution to the isothermal, time-dependent phenomena that includes Navier–Stokes equations for the flow channel and diffusion layers of a serpentine flow field and the interaction of theses equations with anode and cathode kinetics, and the water balance throughout the cell. It is important to note that simpler models (i.e., 2D transient) could not accurately provide predictions of the serpentine flow-field. Commonly use to test membrane electrode assemblies (MEA). To obtain this solution, the 3D model of Shimpalee et al. [4,5] was extended by including the time dependent analysis of a 10-cm^2 reactive area. This set of equations, as shown below, does not account explicitly for the condensation of water vapor resulting from the local partial pressure exceeding the saturation

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pressure of water, but rather it calculates the activity of water in the gas phase and allows the analyst to manually turn off the reaction in the cells where the thickness of condensed liquid restricts mass transfer to the catalyst. Recent steady-state versions of this model [6–8] account for this water phase change and include the energy balance to predict temperature changes, but under some operational conditions liquid water does not significantly affect the performance of the cell and computational time can be saved by neglecting these phase changes. Hence, an isothermal single-phase approximation is used here.

The equations of this paper and the results discussed below can be related to previous works. For example, Um et al. [9] presented similar equations for their 3D model and applied those to their straight channel geometries. They used their own code and the equation solver was not specified. Recently Wang and Wang [10] showed dynamic study on PEMFC using commercial CFD code. However, their geometry was single straight channel flow field that is not normally used in fuel cell application, therefore the effect of pressure driven flow underneath the gas diffusion layers has been ignored. In the results presented below we also used a commercially available computational fluid dynamics (CFD) solver and we had to supply subroutines to account for the electrochemical reactions of hydrogen and oxygen for source terms in the transport equations. The complete equations are solved with a control volume based discretization of the computational domain to obtain the velocity and pressure distribution in the flow channels and the gas diffusion layers for every time interval.

In contrast to the transient analysis presented here and recent paper from reference [10], preceding modeling studies have focused on the steady state behavior of the fuel cell. Some models considered only 1D simulations [11–13], several models concentrated on 2D flow with transport of the reactants and products in the flow channels and across the membranes [14–21], and recent models put emphasis on the 3D simulations [4–10]. Some of These works have been reviewed by Shimpalee et al. [22]. One recent 1D transient model has been presented and transient measurements of the voltage as the current was changed were used to estimate parameter of a MEA. However, that model was not used to explain changing in the overshoot behavior with stoichiometry. It may also to note that the non-isothermal form of the model presented here has been verified with water balance measurement recently [7].

2. Model development

In this study, the 3D model of Shimpalee and coworkers [4,5] is extended by including the accumulation (time dependent) term. Thus, this is a transient, 3D, isothermal, single phase, and multi-species investigation of a single PEM fuel cell with twenty serpentine channels. Again, an isothermal set of equations is used to increase computational speed and to provide a basis of comparison for future work. The flow path consists of a serpentine gas channel and the details of the computational domain have been shown previously, [5,7]. Fig. 1 also shows the channel geometry and associated coordinate system. A thin membrane electrode assembly is sandwiched between anode and cathode diffusion layers. Fig. 2 shows more details of the computational domain, which consists of the anode flow channel, the anode diffusion layer, the MEA, the cathode diffusion layer, and the cathode flow channel. Fig. 2 further shows different z-locations that are used in defining source terms (see Table 1 for a list of symbols and Tables 2 and 3 for the equations used in this paper). The species considered are hydrogen, oxygen, nitrogen, and water vapor. The fuel cell operation is characterized as gas transport and transformation of one species to the other. The hydrogen from the anode flow channel is transported through the diffusion layer toward the membrane. Hydrogen molecules are dissociated to protons and electrons in the catalyst. The water that impregnates the MEA hydrates the protons and it is transported by both electro-osmosis and diffusion according to Eq. (15) of Table 3. The air mixture in the cathode channel is transported through the diffusion layer toward the membrane where oxygen reacts with protons. The water activity in the membrane is simulated by surface-

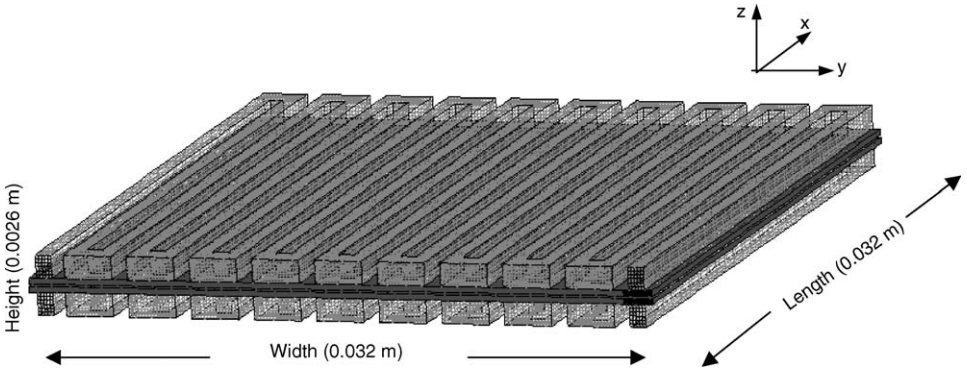

Fig. 1. The picture shows actual flow-field plate with the gas channel and its geometry model. There are 20 straight channels connected in a serpentine fashion. Anode and cathode side flow channels are symmetric and placed properly aligned on top of each other [2,3].