

Predicting the transient response of a serpentine flow-field PEMFC II: Normal to minimal fuel and AIR

S. Shimpalee^a, W.-K. Lee^a, J.W. Van Zee^{a,*}, H. Naseri-Neshat^b

^a Department of Chemical Engineering, University of South Carolina, Columbia, SC 29208, USA

^b Department of Mechanical Engineering Technology, South Carolina State University, Orangeburg, SC 29117, USA

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Abstract

The three-dimensional (3D) transient model presented in part I is used to study the overshoot and undershoot behavior observed in a PEMFC during operation with fixed normal stoichiometric flow rates of hydrogen and air for a 1.0 V s^{-1} change in the load. In contrast to the behavior with excess flow shown in part I, the predictions show second-order responses for both decreases and increases in the load. That is, there is current overshoot when the load cell is decreased from 0.7 V to 0.5 V and there is current undershoot when the cell voltage is increased from 0.5 V to 0.7 V. The simulation of a 10 cm^2 reactive area with a serpentine flow path is used to explain this behavior in terms of the reacting gas concentrations, the flow through the gas diffusion media, the movement of water through the MEA by electro-osmotic and back diffusion forces, and the variation in the distributions of current density. The operating conditions correspond to 101 kPa, 70°C cell temperature, anode and cathode dew-points and stoichiometries of 65°C and 57°C and 1.45 and 2.42 at an initial operating voltage of 0.7 V and current density of 0.33 A cm^{-2} . The fixed flow rates correspond to stoichiometries of 1.05 and 1.73 at 0.5 V for the 0.46 A cm^{-2} predicted current density. The predictions illustrate regions where the MEA may alternate between wet and dry conditions and this may be useful to explain stability and durability of the MEA during transient operation.

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1. Introduction

Transient load changes during operation of PEMFCs with fixed gas flow rates may expose the MEA to various degrees of stoichiometry for either stationary or automotive applications. This transient operation may be a result of a sudden demand as an appliance starts or as a vehicle is accelerated or decelerated. Further these transients may be of sufficient magnitude and speed that gas flow rates cannot be adjusted by feedback control or that the capacitors in the system cannot accommodate the demand. Thus, the fuel cell by default or design may need to act as a capacitor during the power demand surge. The use of a mathematical model and a time-dependent three-dimensional (3D) equation solver is

presented here to illustrate situations where the current does not change in a typical first-order manner between steady states. In fact we have observed experimentally [1–3] and through our predictions that the current can exhibit pseudo second-order behavior with overshoots and undershoots of the current.

In part I of this series [4], we presented a time-dependent 3D model and the corresponding simulation results that showed the effect of anode stoichiometry and rate of voltage change on the transient response of a 10 cm^2 PEMFC with a serpentine flow field. That paper considered the response when the flow of gas was large, exceeding a stoichiometry of 2.6/4.4¹ for 0.7 V and 1.2/2.0 for 0.5 V (i.e.,

¹ Our notation for specifying operating conditions is to list the anode conditions first followed by the cathode. Thus, the stoic was 2.6 for the anode and 4.4 for the cathode. This relates to 160% excess hydrogen and 340% excess oxygen in the stream.

* Corresponding author. Tel.: +1 803 777 2285; fax: +1 803 777 8142.
E-mail address: vanzee@engr.sc.edu (J.W. Van Zee).

Table 1
Inlet conditions and parameters

Anode channel inlet conditions	
Velocity (m s^{-1})	1.2
Mole fraction of H_2	0.759
Mole fraction of H_2O	0.241
Dew-point temperature ($^\circ\text{C}$)	65
Cathode channel inlet conditions	
Velocity (m s^{-1})	4.5
Mole fraction of O_2	0.170
Mole fraction of N_2	0.638
Mole fraction of H_2O	0.192
Dew-point temperature ($^\circ\text{C}$)	57
Operating conditions	
Operating pressure (kPa)	101
Permeability of diffusion layer (m^2)	3.3×10^{-15}
Membrane thickness (μm)	50
Density of dry membrane (kg m^{-3})	2000
Equivalent weight of a dry membrane (kg mol^{-1})	1.1
Oxygen exchange current density (A m^{-2})	140
Hydrogen exchange current density (A m^{-2})	1000

a constant flow rate of $90 \text{ cm}^3 \text{ s}^{-1}$ and $355 \text{ cm}^3 \text{ s}^{-1}$ for the anode/cathode respectively at 101 kPa and 70°C for 0.33 A cm^{-2} at 0.7 V). The simulation used a commercial computational fluid dynamics (CFD) solver, Star-CD Version 3.2, with modified subroutines to account for the electrochemical reactions of hydrogen and oxygen and the transport of water through the membrane and catalysts layer. The complete 3D Navier–Stokes equations were solved with a control-volume-based discretization of the computational domain and the velocity and pressure distribution in the flow channels and the gas diffusion layer were obtained for every time-step.

In contrast to part I, we present here predictions to discuss the behavior when the fixed flow rates correspond to normal and maximum utilization (i.e., changes in stoichiometry from 1.45/2.42 to 1.05/1.73). That is, in an effort to expand the understanding the behavior of a PEMFC, we present here a study that focuses on changes in the cell voltage between 0.7 V and 0.5 V for a stoichiometry of 1.45/2.42 for the 0.7 V conditions (i.e., 0.33 A cm^{-2}). The operation at 0.5 V results in almost complete utilization of the hydrogen and perhaps a mass transfer limitation of the oxygen. We call this 1.05/1.73 stoichiometry a “minimal” stoichiometric condition because the cell operated a fixed voltage cannot exhibit truly starved condition (i.e., the current will adjust to the supply of fuel).

This numerical simulation uses the same transient, isothermal, 3D mass transfer model and serpentine gas-flow-channel geometry as part I. The operating conditions and model parameters of this work are shown in Table 1. The transient load profile consists of changing the cell voltage from 0.7 V at steady state to 0.5 V and from 0.5 V at steady state to 0.7 V at an average rate of 1 V s^{-1} . This rate was not linear as shown in Table 2 because we followed the output from an experimental load. As discussed in part I, the predictions were grid and time-step independent.

2. Results and discussion

Fig. 1 shows how the averaged current density changes when the cell voltages are changed from 0.5 V to 0.7 V and from 0.7 V to 0.5 V. The average is obtained by multiplying the current in each grid cell by the surface area of each cell, summing the resulting current, and then dividing this current by 10 cm^2 . Fig. 1a shows undershoot in the current density when the cell voltage is increased. The lowest averaged current density is 0.23 A cm^{-2} when the cell voltage reaches 0.685 V, and then it increases and reaches a steady-state value at 0.33 A cm^{-2} . Note that the flow condition at 0.7 V corresponds to stoichiometries of 1.45/2.42 at 0.33 A cm^{-2} and that at 0.5 V these conditions correspond to stoichiometries of 1.05/1.73 for 0.46 A cm^{-2} . This decrease of about 0.22 A cm^{-2} is comparable with the data of Ref. [1] even though the average rate of voltage change was 0.22 V s^{-1} instead of the 1.0 V s^{-1} used here. The time constants are similar due to the differences in the rate of voltage change. Fig. 1b shows overshoot behavior. The averaged current density increases from 0.33 A cm^{-2} to 0.96 A cm^{-2} when the cell voltage is 0.52 V and then the current density decreases and reaches the steady state at 0.46 A cm^{-2} . This is the same current density as that shown at 0.5 V in Fig. 1a. Note that

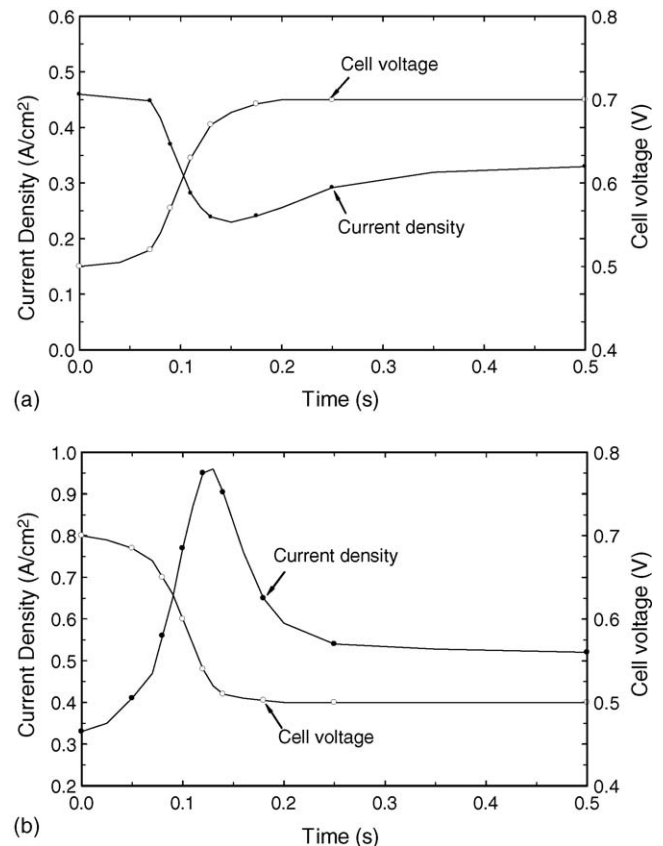


Fig. 1. (a) Averaged current density for change from 0.5 V to 0.7 V. Open circles indicate cell voltage and filled circles indicate current density and (b) averaged current density for change from 0.7 V to 0.5 V and open circles indicate cell voltage and filled circles indicate current density.

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