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Authors

Kang, S
Kim, HS
Ha, T
[et al.](#)

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Dynamic Cell Level Modeling and Experimental Data from a Proton Exchange Membrane Fuel Cell

Sanggyu Kang, Han-sang Kim, Taehun Ha, Kyoungdoug Min*
School of Mechanical and Aerospace Engineering, Seoul National University
Seoul, Korea

Fabian Mueller, Jack Brouwer
Mechanical and Aerospace Engineering Department
National Fuel Cell Research Center, University of California, Irvine

*Corresponding author: kadmin@snu.ac.kr

ABSTRACT

A quasi three-dimensional dynamic model of a proton exchange membrane fuel cell (PEMFC) has been developed and evaluated by comparison to experimental data. A single PEMFC cell is discretized into 245 control volumes in three dimensions to resolve local voltage response, current generation, species mole fractions, temperature, and membrane hydration spatially in the PEMFC. The model can further simulate transients in electrical load, inlet flow conditions, ambient conditions, and/or other parameters to provide insight into the local dynamic performance of a PEMFC.

The quasi three-dimensional model has been validated against an experimental single cell. To compare the model, polarization constants were tuned to match one experimental operating point of the fuel cell. With this tuning, the model is shown to predict well the voltage current (V-I) behavior for the full range of cell operating current. Further, model comparison to an instantaneous increase in current indicates that the model can predict the transient electrochemical response of the PEMFC. This suggests such a model can be utilized for PEMFC system development, transient analysis of a PEMFC in general, as well as transient control design.

Keywords: PEMFC simulation, data comparison, dynamic response

INTRODUCTION

Global environmental concerns, particularly global warming and air pollution in urban areas have provided the stimulus to improve the efficiency of conventional power sources and to develop environmental friendly energy conversion technologies. One of the promising energy technologies is fuel cells. Various types of fuel cells have been developed for residential, automotive, and remote power backup, etc. Among the fuel cell types PEM fuel cell has

received much attention as a promising future power source. Its high power density, low-temperature operation, quick start-up, system robustness, transient ability, and low emissions make PEMFC very attractive especially as an automobile power sources. Powering an automobile PEMFC will be subdued to transient load conditions. Thus, it is important to investigate the dynamic respond characteristics of the PEM fuel cell. In Nernst equation, voltage is determined by current, mole fraction, temperature, pressure, membrane water content. As a result it is important to catch each characteristic during transient to understand the voltage response to load changes.

To predict the PEM fuel cell performance modeling and simulation of the PEM fuel cell have been developed [1-4]. Prior modeling work has been primarily in the form of steady state 3-D models and 1-D dynamic models. Steady state 3-D models are very useful to design and optimize the flow channel geometry with high computational cost. But it is not suitable to use for dynamic simulation of PEMFC system to build control strategies during transients. Recently 1-D dynamic model has been developed, which roughly capture water flux in the cross sectional direction. However 1-D dynamic models don't capture variation along in the flow direction.

The objective of this work is to develop a quasi-three dimensional unit PEM fuel cell model and consequently validate the model against experimental results. The model can then be used for dynamic simulation to develop the control strategies and also to investigate the effect of operating conditions on local distributions of current, temperatures, water contents, and species. Since the model is discretized in three dimensions it is possible to catch the local section where flooding occurs, and the distribution of temperature, current, mole fraction and etc during transient load conditions. In order to compare with experiment, this model is tuned to a single experimental reference point. Comparison show steady state results and dynamic simulation results well predict the experimental data.

EXPERIMENTAL SETUP

In the study, a PEM unit cell with an area of 25 cm² was used to provide the validation data. This single cell has the 7 serpentine flow paths in both of the cathode and anode. The rectangular channel depth and width is 1mm and 0.7mm, respectively. The 5 channel flow turns 7 times. The anode and cathode flow are in counter-flow configuration, which is shown in Figure 1. The MEA used in this study is based on Nafion 112. The specifications of this single cell are shown in Table 1. Figure 2 shows a schematic diagram of experimental setup. It is composed of a gas supply unit, unit fuel cell, electric loader, different sensors, personal-computer (PC) based data-acquisition system and gas chromatograph (HP 5890 series II). High-purity hydrogen and high purity dry air were used as reactant gases. Two mass flow controllers control the flow rate of hydrogen and air. The temperatures of the reactant gases were controlled by adjusting the humidifier temperature. The anode and cathode humidification temperature were set equal to the cell operating temperature [6]. A cartridge heater was used to maintain the cell temperature as a constant during the experiment, which was controlled by a PID controller.

Table 1 Specifications of cell

Description	Value
Cell Width (x)	0.0507 m
Cell height (y)	0.0507 m
Depth of anode gas channel (z)	0.001 m
Depth of cathode gas channel (z)	0.001 m
Depth of cooling channel (z)	0.001 m
Thickness of GDL (z)	0.001 m
Thickness of electrolyte (z)	7x10 ⁻⁵ m
Thickness of separator plate (z)	0.002 m

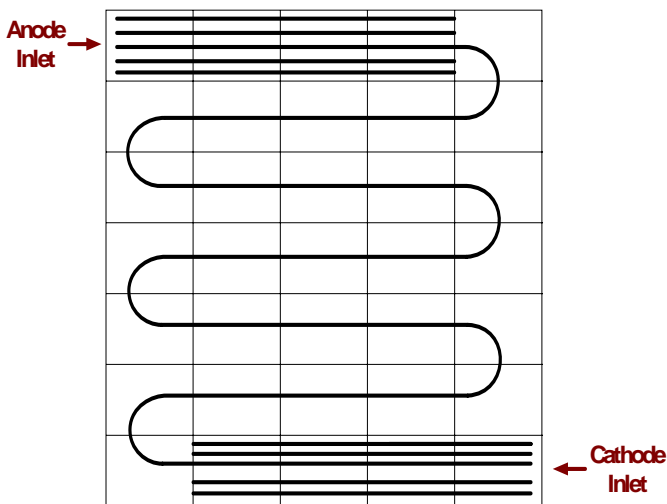


Figure 1 Schematic diagram of gas flow on cell

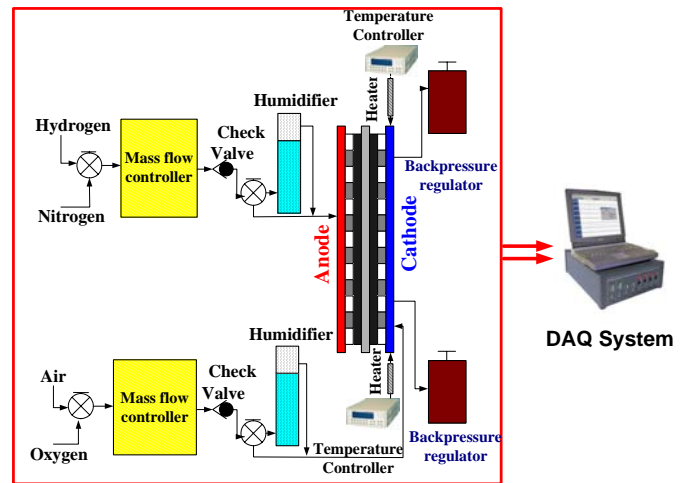


Figure 2 Schematic diagram of test equipments for GC measurements

MODEL DESCRIPTION

A dynamic model of a PEM unit cell has been developed in Matlab-Simulink®. This model is developed with spatial resolution of the dynamic characteristics of fuel cell. However, the complexity of the model is limited to the performance of a personal computer. In order to investigate the local distributions of current, temperature, and species, etc., the unit PEM fuel cell is discretized into in cross sectional direction and stream wise direction. To resolve the species distribution in the fuel cell, each unit cell is discretized into five control volumes in the cross sectional direction: anode gas, anode GDL, MEA, cathode GDL, and cathode gas as shown in Figure 3. To resolve the energy balance each unit cell is discretized into seven control volumes in the cross sectional direction: anode plate, anode, MEA with GDLs, cathode, cathode plate, coolant, and end plate. Such discretization makes it possible to capture the details of MEA behavior, such as water transport, which are critical to accurately determine polarization losses.

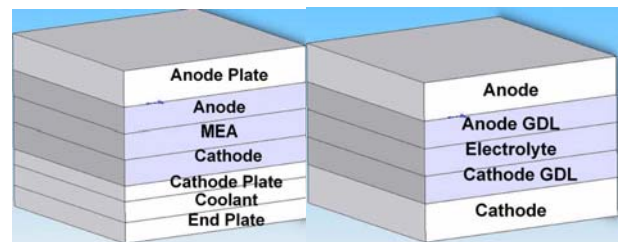


Figure 3 Control volumes for species and energy balance of PEM unit cell.

Since the experimental fuel cell contains five small channels which serpentine seven times through the fuel cell as shown in Fig 4, the fuel cell is discretized into 35 (5x7) nodes in the stream wise direction [7]. The following is a list of the general assumptions made. Details can be found in [7]

1. Control volumes are characterized by a single lumped temperature, pressure, and species mole fraction condition.

2. All gases are ideal gases.
3. No heat transfer to the environment and radiation heat transfer is neglected.
4. Each of the component models is characterized by a single state.
5. A single activation polarization equation is used to capture the effects of all physical and chemical processes that polarize the charge transfer process.
6. Quasi-steady electrochemistry is assumed.

$$h = \sum_i X_i \left(\int_{298K}^T C_{p,i} dT \right) \quad (4)$$

The temperature of the electrolyte is determined as:

$$\frac{dT_s}{dt} = \frac{Q}{\rho \times C_V \times V_{GDL+Elyte}} \quad (5)$$

More detail modeling descriptions can be found in [7]. The species transport from gas channel to GDL accounts for the convection driven by a concentration gradient and diffusion in the GDL. The mass transport coefficient at the gas channel and GDL interface is obtained based on the Reynolds analogy between heat and mass transfer;

$$c_m = \frac{Sh \cdot D_m}{L} \quad (6)$$

The diffusion coefficients for species are function of temperature and pressure and modified via the Bruggeman correlation to account for the effects of porosity and tortuosity in the GDL [8].

$$c_m = \frac{Sh \cdot D_m}{L} \quad D_m = D_o \left(\frac{T}{T_o} \right)^{3/2} \left(\frac{P_o}{P} \right) \quad (7)$$

$$D_m^{eff} = \varepsilon^{1.5} \cdot D_m$$

Water Transport

As the water content in the membrane strongly affect the ionic conductivity, the dynamic model captures the details of water behavior in the MEA. Two type of water molecule transport from anode or cathode GDL to electrolyte are considered: (1) the electro-osmotic drag, (2) back diffusion due to concentration gradient between two control volumes.

The amount of water molecules dragged from anode-electrolyte interface to cathode-electrolyte interface is modeled as being proportional to current density and the electro-osmotic drag coefficient.

$$n_{osmotic} = n_d \cdot \frac{i}{F} \quad (8)$$

Osmotic drag coefficient, n_d , is calculated from the membrane water content, λ , which depends on the water activity, a [1].

$$n_d = 0.0029\lambda^2 + 0.05\lambda - 3.4 \cdot 10^{-19} \quad (9)$$

$$\lambda = \begin{cases} 0.043 + 17.81k - 39.85k^2 + 36k^3 & \text{for } 0 < k \leq 1 \\ 14 + 1.4(k-1) & \text{for } 1 \leq k \leq 3 \end{cases}$$

With the water activity is calculated by:

$$k = \frac{X_{H_2O} P}{P_{sat}} \quad (10)$$

The water diffusion due to the concentration gradient between GDLs and electrolyte control volume is calculated by

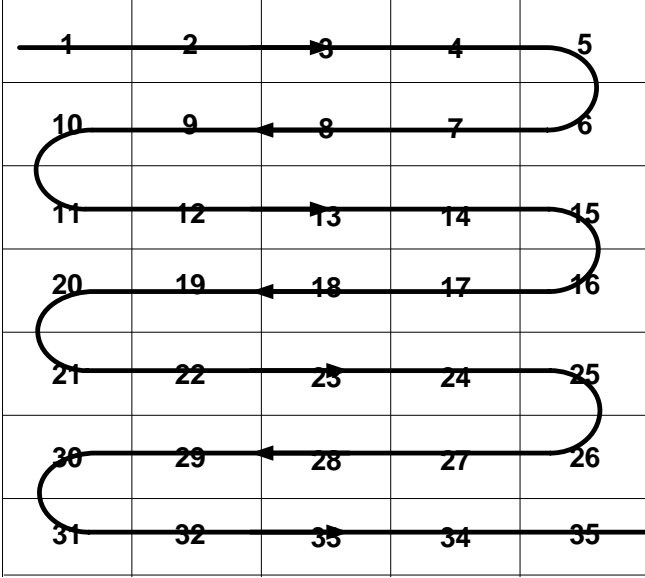


Figure 4 Schematic diagram of Nodal PEM Fuel Cell

Gas conservation

Gas channel mole fractions through out the cell are determined from the following equation.

$$\frac{dX_{out}}{dt} = \frac{1}{N} (N_{in}^{&N} X_{in} - N_{out}^{&N} X_{out} + \sum \Phi) \quad (1)$$

The amount of moles in the GDL is determined as:

$$\frac{dN}{dt} = \sum \Phi + \sum \Psi + \sum \Theta + R_i \quad (2)$$

where Φ is the species diffusion flux from adjacent Bulk control volume. And Ψ is the water diffusion flux from adjacent electrolyte volume, and Θ is the water osmotic flux between GDL control volumes. In general, osmotic flux is transferred from anode GDL to cathode GDL, and water diffusion flux is toward anode GDL from cathode GDL.

Energy conservation

The temperature through out the gas channel is determined from this energy conservation. Enthalpy flux and the heat transfer from the MEA and bipolar plate is important thing to calculate the energy transfer in the gas flow model:

$$\frac{dT_{out}}{dt} = \frac{1}{NC_V} (\sum N_{in}^{&N} h_{in} - \sum N_{out}^{&N} h_{out} + \sum \mathcal{Q}) \quad (3)$$

With the enthalpy determined as:

$$R_{diffusion} = D_w \frac{dc}{dx} \quad (11)$$

The diffusion coefficient of water in the electrolyte, D_w , is calculated from the empirical equation [1]:

$$D_w = D_\lambda \cdot \exp\left[2416\left(\frac{1}{303} - \frac{1}{T}\right)\right] \quad (12)$$

$$D_\lambda = \begin{cases} 10^{-6} & \text{for } \lambda < 2 \\ [1 + 2(\lambda - 2)] \cdot 10^{-6} & \text{for } 2 \leq \lambda \leq 3 \\ [3 - 1.67(\lambda - 3)] \cdot 10^{-6} & \text{for } 3 < \lambda < 4.5 \\ 1.25 \cdot 10^{-6} & \text{for } 4.5 \leq \lambda \end{cases}$$

It is assumed that the water is produced in the cathode GDL which is calculated by

$$R_{water} = M_{H_2O} \cdot \frac{nI}{2F} \quad (13)$$

Electrochemical Model

The fuel cell voltage in the model is calculated by subtracting activation polarization and ohmic polarization from the Nernst potential. The Nernst equation is solved for the anode and cathode GDL partial pressures, and the reversible potential dependence was accounted for by solving the dependence of Gibbs free energy on temperature. Since the partial pressure of H_2 , O_2 , and H_2O evaluated in the GDL are used in the Nernst equation a concentration polarization was excluded.

$$V_{cell} = V_{Nernst} - \eta_{act} - \eta_{ohm} \quad (14)$$

$$V_{Nernst} = -\frac{\Delta G(T)}{nF} + \frac{R_u T}{nF} \ln\left(\frac{P_{H_2} \cdot P_{O_2}^{\frac{1}{2}}}{P_{H_2O}}\right) \quad (15)$$

Activation Polarization

The rate of reaction of oxygen reduction is much slower than hydrogen oxidation. Thus a cathode activation polarization, in the form of Tafel's equation was utilized [9].

$$V_{act} = a \ln \frac{i}{i_o}, \quad a = \frac{R_u T}{2\alpha F} \quad (16)$$

Ohmic Polarization

The ohmic polarization is due to the electrical resistance of the electrodes and collector plate and ionic resistance in the polymer membrane. The ohmic voltage drop is modeled proportionally to current by ohms law:

$$V_{ohm} = i \cdot \frac{t}{\Omega} \quad (17)$$

Where the conductivity in the membrane is modeled as by Springer et al. [14] for the membrane conductivity:

$$\Omega = (c_1 \lambda - c_2) \cdot \exp\left[350\left(\frac{1}{303} - \frac{1}{T}\right)\right] \quad (18)$$

RESULTS AND DISCUSSIONS

Validation

The quasi-three dimensional PEM fuel cell model developed in this study simulates the polarization curve of unit PEM fuel cell. One reference data point shown in Table 2 was selected to tune several unknown parameters in the model, and once established, the same parameter values were used for all other conditions. Figure 5 shows the polarization curve comparison between simulation and experiment. Simulation results well predict the experimental data.

Table 2 Operating condition of the reference point

Humidity	60 %	Temperature	70 °C
H2 flow rate	0.18 slm	O2 utility	0.73 slm
Current	0.584 A/cm2	Cell Voltage	0.466 V
Pressure.	110 kPa		

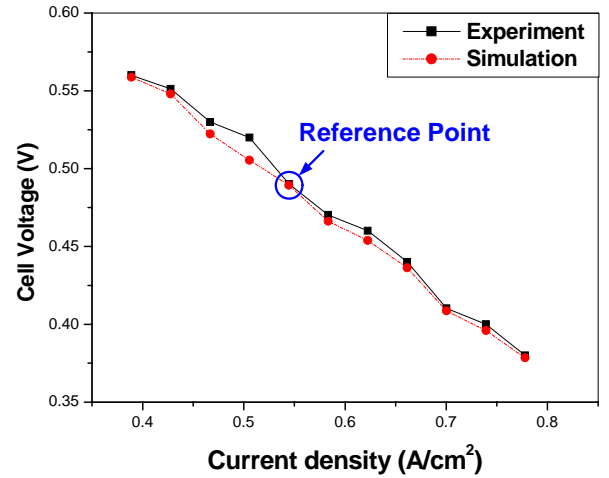


Figure 5 Comparison polarization curve between experiment and simulation

Secondly, the simulation result of dynamic system response to a lowering of the system current from 20 amps to 10 amps was compared to the experimental data. The temperature of the unit cell, anode and cathode gases was 70 °C and relative humidity of both anode and cathode was 60 percent. Measured current of the unit PEM fuel cell is shown in Figure 6. Until 1,121 seconds, the system was operated as a steady state at current of 20 amps and then the current was linearly reduced to 10 amps during 90 seconds. The dynamic model was first allowed to reach steady state at current of 20 amps before the lowering the system current was applied.

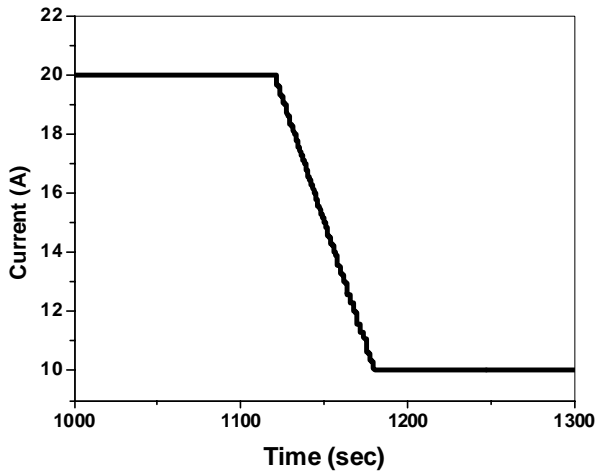


Figure 6 Cell current during the transient

The cell voltage is compared in Figure 7. During the transient state the simulated cell voltage agree well with the experimental results. As the system current is decreased, the system voltage is almost monotonically increased from 0.38 V to 0.55 V due to decrease in ohmic and polarization losses. As the unit cell has large thermal capacitance and its temperature is controlled by the electric heater, the temperature effect on cell performance is negligible. Corresponding cell power is shown in Figure 8. The trend of declination is similar with current. The power is decreased from 10.735 to 6.361 during the transient

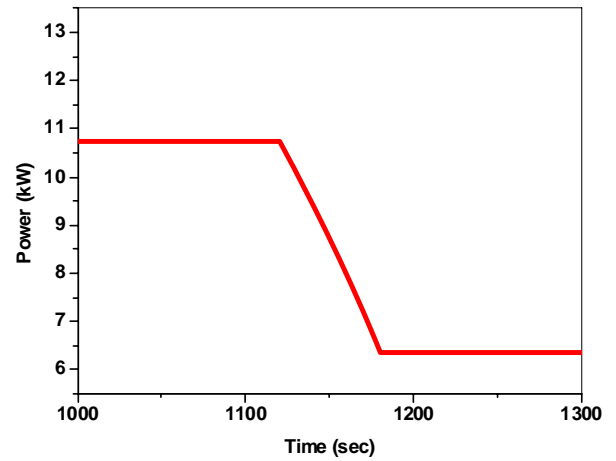


Figure 8 Cell power variation during the transient

Simulation Result

One of the main features of this model is the ability to capture the local current, temperature, and species distributions at steady or transient states. Local current distribution at cell current of 15 amps corresponding to time of 1151 seconds in Figure 6 is shown in Figure 9. The line which was drawn in the Figure 9 is the boundary of each cell model node. The arrow indicates the hydrogen flow direction. Air flow direction is opposite to the hydrogen flow due to counter-flow type. Local current density is gradually increased along the anode gas stream and reaches the maximum at left-bottom corner and then is decreased along the anode outlet. Membrane water content shown in Figure 10 is fairly uniform except near the anode outlet due to low relative humidity of the cathode gas inlet. This means that MEA is uniformly hydrated over the whole cell area, except near the anode outlet

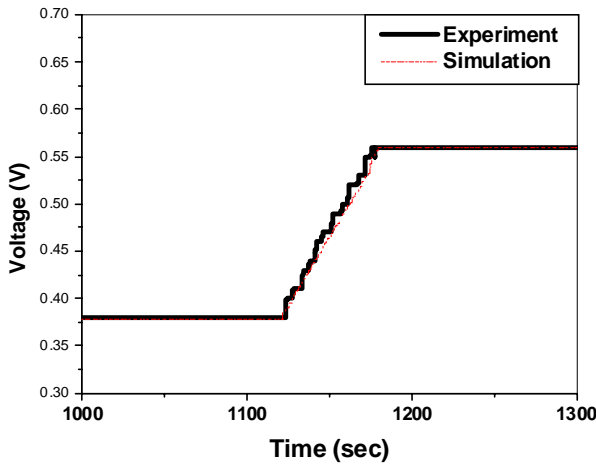


Figure 7 Cell voltage variation during the transient

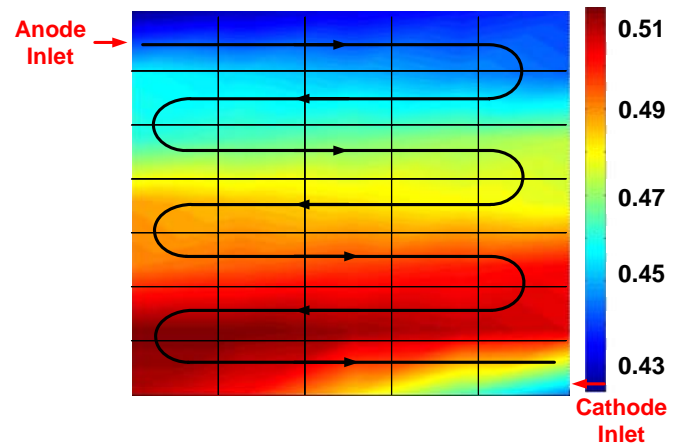


Figure 9 Local current density distribution at transient state, temperature of 70 °C and relative humidity of 60 %

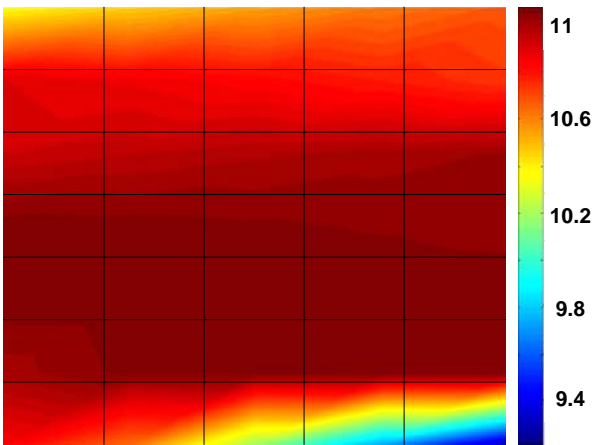


Figure 10 Membrane water content distribution at transient state, temperature of 70 °C and relative humidity of 60 %

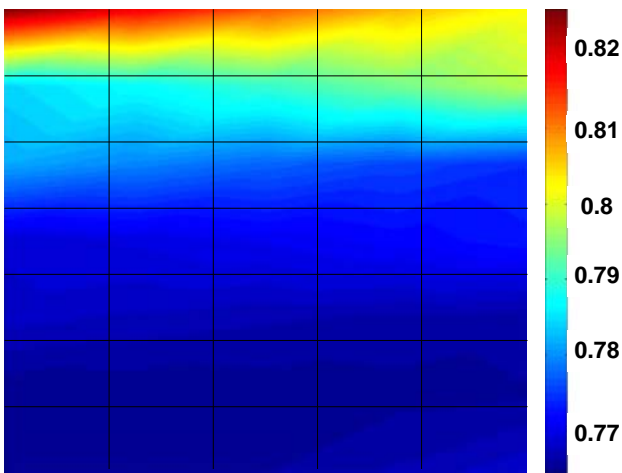


Figure 11 Anode H₂ mole fraction at transient state, temperature of 70 °C and relative humidity of 60 %

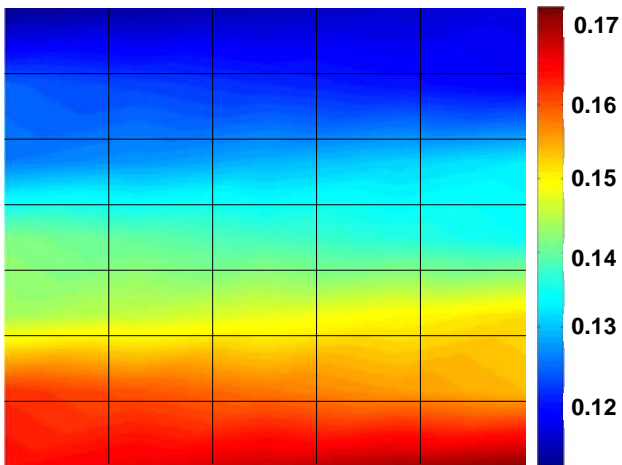
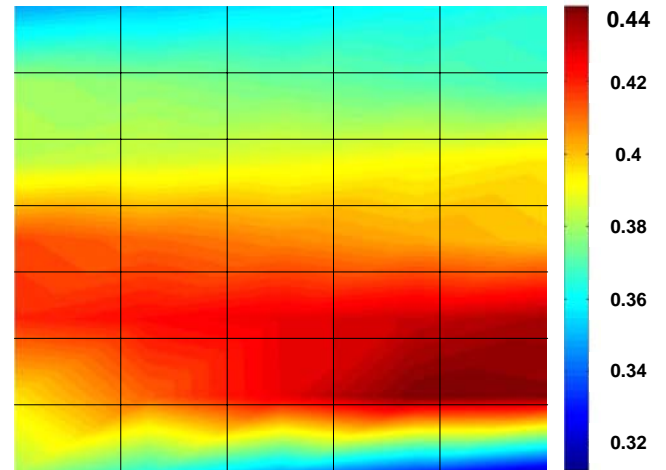


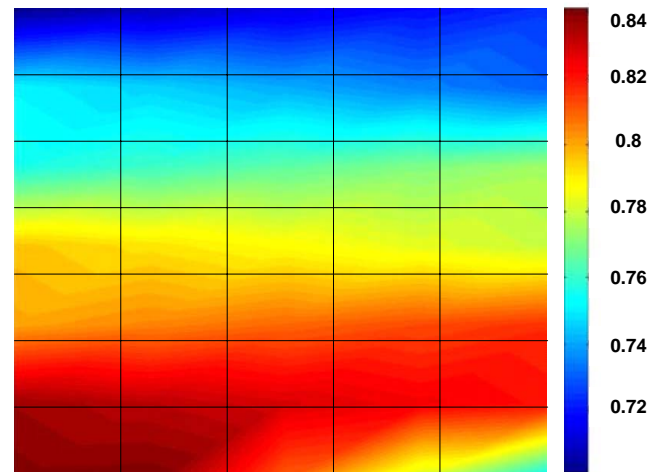
Figure 12 Cathode O₂ mole fraction at transient state, temperature of 70 °C and relative humidity of 60 %

The hydrogen mole fraction is quite uniform along the cell as shown in Figure 11. Oxygen mole fraction substantially decreases along the air flow direction from the cathode inlet. This is due to oxygen reduction reaction and H₂O production at the cathode side of the MEA. Over all the oxygen mole fraction in the cathode decreased about 65 % along the air stream. This explains why the local current density is minimal at the anode inlet area due to low oxygen mole fraction.

Figure 13 shows the local current distributions with different cell current density. The local current distribution at high current is more uniform than low current, but the general current distribution shape is very similar. Location of the maximum current density is moved close to the cathode inlet as the current is increased.



(a) Current 10 A



(b) Current 20 A

Figure 13 Local current density distributions at steady state, temperature of 70 °C and relative humidity of 60 %

CONCLUSIONS

A quasi-three dimensional dynamic model of a PEM fuel cell stack has been developed. A single cell is discretized into five control volumes for species and seven control volumes for energy balance in the cross sectional direction, and in 35 nodes

in the stream wise direction. With such discretization it is possible to capture local current, temperature, species mole fraction, relative humidity through out the fuel cell.

A comparison of current-density voltage polarization curve between experiment and simulation shows that the system model well predicts the experimental system. Transient simulation of this model is also well matched with the experimental results to within a few percent. Furthermore, from stream wise discretization, the current distribution and species mole fraction, temperature and flooding can be captured during transient. Also the model can be used to investigating the control strategies during the transients. This suggests such a model can be utilized for transient analysis of a PEMFC and transient control development.

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