

## Dynamic Thermal Model for Proton-Exchange Membrane Fuel Cell

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### ABSTRACT

In this paper, a mathematical model is developed to simulate the transient phenomena in a polymer electrolyte membrane fuel cell (PEMFC) system. Large transient changes are expected for practical application such as transportation vehicles due to acceleration and deceleration. Simple models are usually unable to capture these transient dynamics. For control purposes, a fuel cell model must include the dynamics of flow and pressure in the anode and cathode channels and mass/heat transfer transients. The proposed model can predict the transient response of cell voltage, temperature of the cell, hydrogen/oxygen out flow rates and cathode and anode channel pressures under sudden change in load current. It is implemented in SIMULINK environment. The model is tested by simulating a transportation-size fuel cell with 85 kW maximum power output. Results for maximum power and multi-step input current that simulate start up-shut down cycle are shown. The predicted power, pressure and temperature are matching the published data for the fuel cell. The model will be very useful for the optimal design and real-time control of PEM fuel cell systems in practical automotive or stationary applications.

### INTRODUCTION

Since the introduction of PEM fuel cells as a power source, various modeling techniques at different levels of complexity have been used to model membrane electrode assembly (MEA). Mechanistic methods [1-3] are aimed at modeling multispecies diffusion in the diffusion layer of the electrode, the reaction kinetics in the catalyst

layers, and proton and water transport through the membrane. These models are based on complex partial differential equations and many physical parameters are needed before any solution is attempted, which reduces the scope of application of these models to small fuel cell systems.

On the other hand, large fuel cell systems needs a less complicated model with fewer parameters. Empirical modeling by representing fuel cell voltage as a function of various fuel cell parameters is a reliable and computationally efficient method [4,5]. This method is based on benchmark experimental studies.

Due to the need to hydrate membranes of the fuel cell, water is introduced into the cell by passing the reactants through humidifiers before entering the cell. Monitoring the hydration level of the membrane is an important issue that has to be considered. The dynamic modeling of fluid flow and heat transfer in the fuel cell is a crucial step in order to predict and control fuel cell performance. This is usually requires non-steady state and transient behaviors due to sudden load change.

Many authors attempted developing a fuel cell system-level model [6-8]. Pukrushpan *et al.* [6] developed a constant temperature model that includes compressor, supply and return manifolds. Their model lacks heat transfer and thermal transients. Consideration of thermal transients was implemented by Xue *et al.* [7]. He applied his model to a small fuel cell sytem. Cooling effects was implemented implicitly, i.e., heat transfer coefficients were assumed. Vasu and Tangirala [8] developed an explicit cooling models, where the heat transfer coefficients can be calculated assuming cooling channels dimensions.

The goal of this study is to develop a control-oriented system-level dynamic model of PEMFC that incorporates the temperature, gas flow, membrane hydration, inlet gas humidification effects, and cooling effects. The model is tested by modeling an 85 kW fuel cell.

### DYNAMIC MODELING APPROACH

In this research, we develop a dynamic model of PEMFC using control volume approach with lumped parameters. The fuel cell model is divided into five sub-models; namely, the anode channel, the cathode channel, membrane, thermal model, and voltage model. Hydrogen is humidified with water and then enters the anode channel. Part of the hydrogen and water vapor diffuse into the MEA, where the hydrogen dissociates into protons and electrons at the anode catalyst layer, while the water vapor diffuses through the anode electrode into the membrane and further diffuses into the cathode side through the membrane with the aid of protons. At the cathode side, the oxygen is humidified and enters the cathode channel. Part of the oxygen and vapor diffuse into the MEA where the oxygen dissociates and combines with the protons and electrons to form water at the cathode catalyst layer, and the remaining water diffuses either into the cathode channel or back into the anode channel.

### ANODE MODEL

The mass conservation equations for the anode species are written as

$$\frac{dm_{H_2}}{dt} = \dot{m}_{H_2,in} - \dot{m}_{H_2,out} - \dot{m}_{H_2,reacted} \quad (1)$$

$$\frac{dm_{H_2O_{an}}}{dt} = \dot{m}_{H_2O_{an},in} - \dot{m}_{H_2O,m} - \dot{m}_{H_2O(v)_{an,out}} \quad (2)$$

where the anode inlet mass flow rates are

$$\dot{m}_{H_2,in} = \lambda_{H_2} \dot{m}_{H_2,reacted} \quad (3)$$

$$\dot{m}_{H_2O_{an},in} = \Omega_{an,in} \dot{m}_{H_2,in} \quad (4)$$

where  $\lambda_{H_2}$  is the hydrogen excess ratio, and  $\Omega_{an,in}$  is the anode inlet flow humidity ratio.

The reacted hydrogen rate is

$$\dot{m}_{H_2,reacted} = M_{H_2} n_{fc} I_{st} / (2F) \quad (5)$$

where  $M_{H_2}$  is molecular masses of hydrogen and,  $n_{fc}$  is the number of fuel cells,  $I_{st}$  is the stack current, and  $F$  is the faraday constant. The anode outlet mass flow rate is calculated from nozzle equation as

$$\dot{m}_{an,out} = c_{nzl,an} \frac{p_{an}}{\sqrt{T}} \left( \frac{p_{amb}}{p_{an}} \right)^{\frac{1}{\gamma}} \times \sqrt{\frac{2\gamma}{\gamma-1} \left[ 1 - \left( \frac{p_{amb}}{p_{an}} \right)^{\frac{\gamma-1}{\gamma}} \right]} \quad (6)$$

where  $c_{nzl,an}$  is the anode nozzle constant,  $T$  is the stack temperature,  $p_{an}$  is the anode pressure, and  $p_{amb}$  is the ambient pressure. The species at the outlet are determined by

$$\dot{m}_{H_2,out} = \dot{m}_{an,out} / (1 + \Omega_{an}) \quad (7)$$

$$\dot{m}_{H_2O(v)_{an,out}} = \Omega_{an} \dot{m}_{an,out} / (1 + \Omega_{an}) \quad (8)$$

### CATHODE MODEL

The mass conservation equations for the cathode species are written as

$$\frac{dm_{O_2}}{dt} = \dot{m}_{O_2,in} - \dot{m}_{O_2,out} - \dot{m}_{O_2,reacted} \quad (9)$$

$$\frac{dm_{N_2}}{dt} = \dot{m}_{N_2,in} - \dot{m}_{N_2,out} \quad (10)$$

$$\frac{dm_{H_2O_{ca}}}{dt} = \dot{m}_{H_2O_{ca},in} + \dot{m}_{H_2O_{ca},gen} + \dot{m}_{H_2O,m} - \dot{m}_{H_2O(v)_{ca,out}} - \dot{m}_{H_2O(l)_{ca,out}} \quad (11)$$

where the inlet mass flow rates are

$$\dot{m}_{O_2,in} = \lambda_{O_2} \dot{m}_{O_2,reacted} \quad (12)$$

$$\dot{m}_{N_2,in} = \frac{1 - x_{O_2}}{x_{O_2}} \dot{m}_{O_2,in} \quad (13)$$

$$\dot{m}_{H_2O_{ca},in} = \Omega_{ca,in} (\dot{m}_{O_2,in} + \dot{m}_{N_2,in}) \quad (14)$$

$$\dot{m}_{O_2,in} = \lambda_{O_2} \dot{m}_{O_2,reacted} \quad (15)$$

where  $x_{O_2}$  is the oxygen mass fraction in dry mixture,  $\lambda_{O_2}$  is the oxygen excess ratio, and  $\Omega_{ca,in}$  is the cathode inlet flow humidity ratio.

The reacted oxygen and generated water rates are

$$\dot{m}_{O_2,reacted} = M_{O_2} n_{fc} I_{st} / (4F) \quad (16)$$

$$\dot{m}_{H_2O,ca,gen} = M_{H_2O} n_{fc} I_{st} / (2F) \quad (17)$$

where  $M_{O_2}$  and  $M_{H_2O}$  are molecular masses of oxygen and water,  $n_{fc}$  is the number of fuel cells,  $I_{st}$  is the stack current, and  $F$  is the faraday constant. The cathode outlet mass flow rate is calculated from nozzle equation as

$$\dot{m}_{ca,out} = c_{nzl,ca} \frac{p_{ca}}{\sqrt{T}} \left( \frac{p_{amb}}{p_{ca}} \right)^{\frac{1}{\gamma}} \times \sqrt{\frac{2\gamma}{\gamma-1} \left[ 1 - \left( \frac{p_{amb}}{p_{ca}} \right)^{\frac{\gamma-1}{\gamma}} \right]} \quad (18)$$

where  $c_{nzl,ca}$  is the cathode nozzle constant,  $T$  is the stack temperature,  $p_{ca}$  is the cathode pressure  $p_{amb}$  is the ambient pressure. The species at the outlet are determined by

$$\dot{m}_{O_2,out} = x_{O_2} \dot{m}_{ca,out} / (1 + \Omega_{ca}) \quad (19)$$

$$\dot{m}_{N_2,out} = x_{N_2} \dot{m}_{ca,out} / (1 + \Omega_{ca}) \quad (20)$$

$$\dot{m}_{H_2O(v),ca,out} = \Omega_{ca} \dot{m}_{ca,out} / (1 + \Omega_{ca}) \quad (21)$$

$$\dot{m}_{H_2O(l),ca,out} = \begin{cases} 0 & \phi < 1 \\ \max(\dot{m}_{H_2O,ca,in} + \dot{m}_{H_2O,ca,gen} + \dot{m}_{H_2O,mem} - \dot{m}_{H_2O(v),ca,out}, 0) & \phi = 1 \end{cases} \quad (22)$$

where  $\phi$  is the relative humidity. The details of the thermodynamics calculation are described in the Appendix.

### MEMBRANE MODEL

This model calculates the rate of mass flow across the membrane. It is function of the stack current and relative humidity of the reactants in the anode and the cathode flow channels. Water transport is due to two effects, namely: (i) electro-osmotic

drag where the water molecules are dragged from the anode to the cathode side by protons; (ii) back diffusion due to the concentration gradient of water across the membrane. The expressions are as follows:

$$\dot{m}_{H_2O,m} = M_{H_2O} A_{fc} n_{fc} \times \left( \frac{n_d I_d}{F} - D_w \frac{C_{v,ca} - C_{v,an}}{t_m} \right) \quad (23)$$

where  $A_{fc}$  is active cell area,  $n_d$  is the electro-osmotic drag coefficient,  $D_w$  is the water diffusion coefficient,  $C_{v,an}$  and  $C_{v,ca}$  are anode and cathode water concentrations. The details of membrane model are given in the Appendix.

### VOLTAGE MODEL

The stack voltage is calculated as

$$V_{st} = n_{fc} V \quad (24)$$

where

$$V = E - V_{act} - V_{ohm} - V_{conc} \quad (25)$$

where  $E$  is the open-circuit voltage,  $V_{act}$ ,  $V_{ohm}$  and  $V_{conc}$  are the voltage drops due to activation loss, ohmic loss and concentration loss, respectively. Their empirical relations are listed in the Appendix.

### THERMAL MODEL

Applying energy equation to the fuel cell stack, the following equation is obtained

$$m_{st} C_{p,st} \frac{dT}{dt} = \dot{Q}_{reac} + \Delta \dot{H}_{sens} - P_e - \dot{Q}_{HT} \quad (26)$$

where  $m_{st}$  is the stack mass,  $C_{p,st}$  is the stack specific heat,  $\dot{Q}_{reac}$  is the rate of chemical energy of reaction,  $\Delta \dot{H}_{sens}$  is the change in sensible enthalpy of flow,  $P_e$  is the electrical power output of the stack, and  $\dot{Q}_{HT}$  is the heat transfer from stack to surroundings and coolant.

The heat of reaction is given by

$$\dot{Q}_{reac} = \dot{m}_{H_2,reacted} Q_{H_2,LHV} \quad (27)$$

where  $Q_{H_2,LHV}$  is the lower heating value of hydrogen.

The sensible enthalpy change for the flow is given by

$$\begin{aligned} \Delta \dot{H}_{sens} = & (\dot{m}_{H_2,in} C_{p,H_2} + \dot{m}_{H_2O,an,in} C_{p,H_2O(v)}) \\ & \times (T_{an,in} - T_0) \\ & + (\dot{m}_{O_2,in} C_{p,O_2} + \dot{m}_{N_2,in} C_{p,N_2} \\ & + \dot{m}_{H_2O,ca,in} C_{p,H_2O(v)}) (T_{ca,in} - T_0) \\ & - (\dot{m}_{H_2,out} C_{p,H_2} + \dot{m}_{H_2O,an,out} C_{p,H_2O(v)}) \\ & + \dot{m}_{O_2,out} C_{p,O_2} + \dot{m}_{N_2,out} C_{p,N_2} + \dot{m}_{H_2O(v),ca,out} C_{p,H_2O(v)} \\ & + \dot{m}_{H_2O(l),ca,out} C_{p,H_2O(l)} (T - T_0) \end{aligned} \quad (28)$$

where  $T$  is the stack temperature,  $T_0$  is the reference temperature (273 K),  $T_{an,in}$  is the anode inlet temperature,  $T_{ca,in}$  is the cathode inlet temperature.

The heat transfer is the summation of natural convection ( $\dot{Q}_{nc}$ ), radiation ( $\dot{Q}_{rad}$ ), and cooling ( $\dot{Q}_{cool}$ ) as

$$\dot{Q}_{HT} = \dot{Q}_{nc} + \dot{Q}_{rad} + \dot{Q}_{cool} \quad (29)$$

where

$$\dot{Q}_{nc} = (h_{nc,V} A_{nc,V} + h_{nc,H} A_{nc,H}) (T - T_{amb}) \quad (30)$$

$$h_{nc,V} = Nu_{H_{st}} k / H_{st} \quad (31)$$

$h_{nc,V}$  and  $h_{nc,H}$  are the natural convection heat transfer coefficients for vertical and horizontal plates, respectively and  $T_{amb}$  is the ambient temperature. Nusselt number ( $Nu_{H_{st}}$ ) for a vertical plate is given by

$$Nu_{H_{st}} = \left[ \frac{0.825 + 0.387 Ra_{H_{st}}^{1/4}}{(1 + (0.492/Pr)^{0.5625})^{1/4}} \right]^2 \quad (32)$$

where  $Ra$  is Rayleigh number and  $Pr$  is the Prandtl number.

Similarly the heat transfer coefficient for horizontal plate is obtained as [9]

$$h_{nc,H} = Nu_L k / L \quad (33)$$

where

$$Nu_L = 0.54 Ra^{1/4} \quad (34)$$

The reference length ( $L$ ) for this relation is calculated as  $L = A_{st,H} / P_{st,H}$  where  $A_{st,H}$  is the horizontal area of the stack and  $P$  is the perimeter.

The radiation heat transfer rate is determined by

$$\dot{Q}_{rad} = \varepsilon \sigma A_{rad} (T^4 - T_{amb}^4) \quad (35)$$

The cooling heat transfer rate is determined from the change in coolant temperature as

$$\dot{Q}_{cool} = \dot{m}_{clt} C_{p,clt} (T_{clt,out} - T_{clt,in}) \quad (36)$$

The outlet coolant temperature is given by

$$\begin{aligned} T_{clt,out} = & T - (T - T_{clt,in}) \\ & \times \exp\left(-\frac{h_{fc} A_{clt}}{\dot{m}_{clt} C_{p,clt}}\right) \end{aligned} \quad (37)$$

where

$$A_{clt} = n_{fc} n_{clt} n_{cls} P_{clt} n_{cl} L_{clt} \quad (38)$$

$$h_{fc} = Nu_{D_H} k / D_H \quad (39)$$

where  $D_H$  is the hydraulic diameter, and Nusselt number is determined from [9]

$$Nu_{D_H} = \begin{cases} 3.66 & Re \leq 2300 \\ \frac{f}{8} (Re - 1000) Pr & Re > 2300 \end{cases} \quad (40)$$

where  $Re$  is Reynolds number and  $f$  is the friction factor given by

$$f = \frac{1}{(0.79 \log(Re) - 1.64)^2} \quad (41)$$

## RESULTS

The simulated fuel cell data is listed in Table 1. It is Ballard Mark 902 fuel cell used for transportation applications. Max current is 300 with max power of 85 kW. Max operating temperature is 85°C and operating pressure is 1 to 3 bar. Two simulation runs were performed, namely, the rated power case and a start up-shut down cycle with multi-current steps to simulate a real drive cycle.

Partial pressures of anode and cathode species are shown in Figs. 1 & 2. At the beginning, Pressure starts building up very fast in cathode channel, then, it increases at a smaller rate until it reaches steady state at 300 s. The anode pressure builds up at a slow rate and it reaches steady state at 300 s. The nozzle constants are calibrated such that the pressure at both cathode and anode pressures are near to the limit of the operational range of the fuel cell (3 bar) and the difference between cathode and anode pressure is small, which is required to protect the membrane. Although, the inlet hydrogen is 100% humidified, the relative humidity in the anode channel does not exceed 82%. This is due to water

transport from anode to cathode channel. Cathode relative humidity reaches one very fast and it remains at that value. This indicates that the membrane hydration level is satisfactory.

Table 1. Simulation Parameters

parameter	value
<b>Stack</b>	
$n_{fc}$	381
$A_{fc}$ [ $cm^2$ ]	280
$L_{st}$ [m]	0.805
$W_{st}$ [m]	0.375
$H_{st}$ [m]	0.25
$m_{st}$ [kg]	96
$C_{p,st}$ [kJ/kg K]	1.1
<b>Anode</b>	
$V_{an}$ [ $m^3$ ]	0.005
$p_{an,in}$ [bar]	1.01325
$\phi_{an}$	1
$\lambda_{H_2}$	1.01
$C_{nzl,an}$	$4.5 \times 10^{-9}$
<b>Cathode</b>	
$V_{ca}$ [ $m^3$ ]	0.01
$P_{ca,in}$ [bar]	1.01325
$\phi_{ca}$	0.7
$\lambda_{O_2}$	2
$C_{nzl,ca}$	$1 \times 10^{-5}$
<b>Membrane</b>	
$t_m$ [cm]	0.01275
$\rho_m$ [ $kg/cm^3$ ]	0.002
$M_m$ [kg/mol]	1.1
<b>Coolant</b>	
$T_{cli,in}$ [K]	300
$V_{cni}$ [mm/s]	2.6
Coolant Channel cross section[mm]	3×3
$n_{cli,chns}$	20
<b>Ambient</b>	
$T_{amb}$ [K]	288
$p_{amb}$ [bar]	1.01325
$\rho_{amb}$ [ $kg/m^3$ ]	1.2204

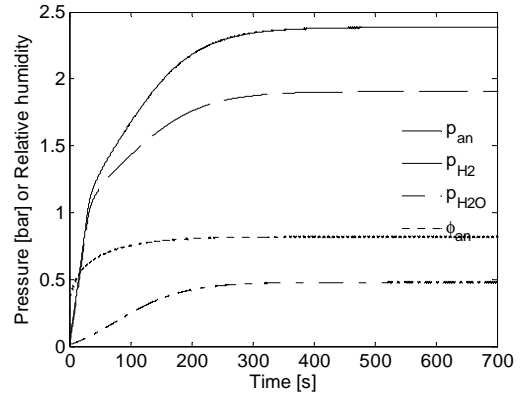


Fig. 1. Anode species partial pressures

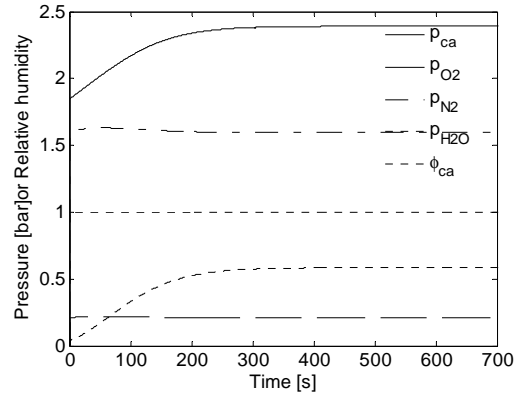


Fig. 2. Cathode species partial pressures

Figs. 3&4 demonstrate the mass change inside anode and cathode respectively. Steady state is reached at 300 s, which is compatible with pressure results. Since excess ratios for hydrogen and oxygen are greater than one, both gases build up their masses inside the anode and cathode volume.

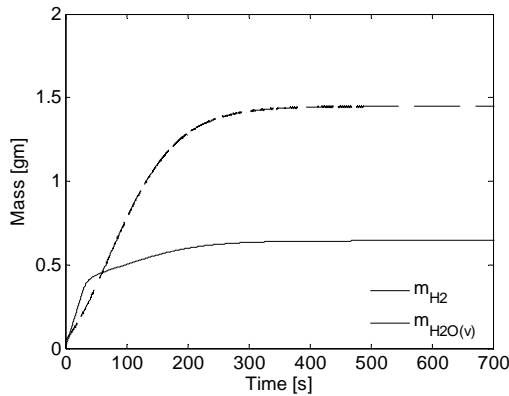


Fig. 3. Anode species masses

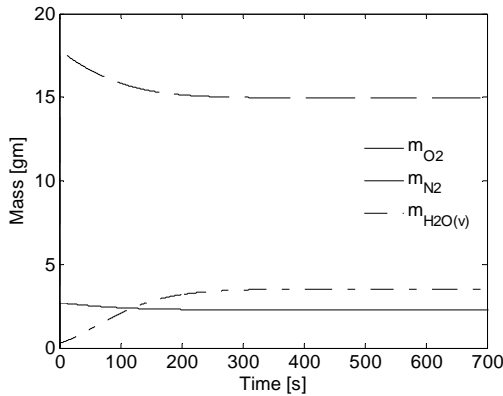


Fig. 4. Cathode species masses

Looking at temperature transient behavior at Fig. 5, it is realized that the fluid transient behavior follows the thermal transient. The steady state power (84.6 kW) and temperature (85.7°C) are in agreement with the published data of the simulated fuel cell. Stack voltage and current are shown in Fig. 6. Steady state stack voltage is 282 corresponding to a single cell voltage of 0.74 V.

The results of the second case that simulates the dynamic performance during start up-shut down cycle are shown in Figs. 7-12. For this case, the inlet hydrogen and oxygen flows are varied according to the load current, i.e., we assume that there is a control algorithm that adjusts hydrogen and oxygen flows based on the load current. The load current changes in a multi-step (0-100-200-300-200-100-0). After each step there is a transient followed by steady state. Comparing Fig. 7 and Fig. 8, The difference

between anode and cathode pressures remains small. Since, hydrogen and oxygen remains inside the fuel cell when it is shut down, the final voltage is different from the start voltage as shown in Fig. 12. The power obtained at 100 A is 33 kW, while the power at 200 A is 60 kW. No published data is available for such load currents.

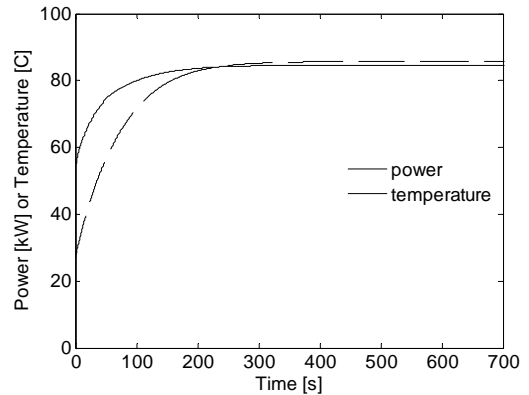


Fig. 5. Stack power and temperature

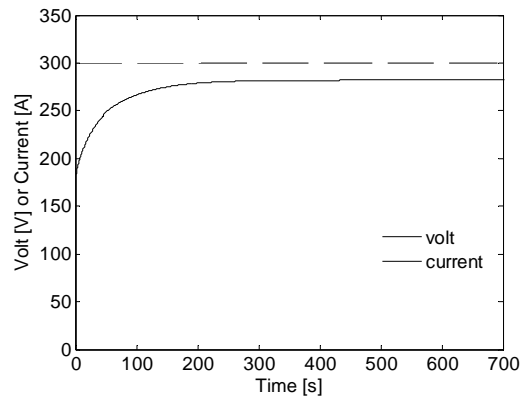


Fig. 6. Stack voltage and current

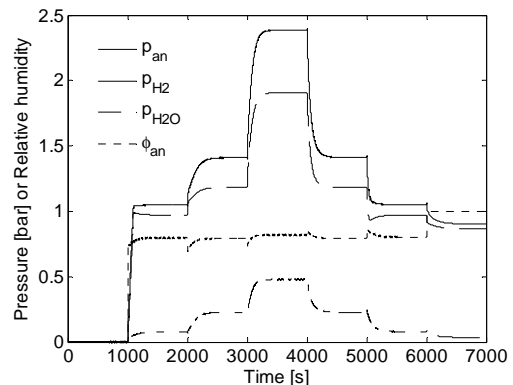


Fig. 7. Anode species partial pressures for start up-shut down cycle

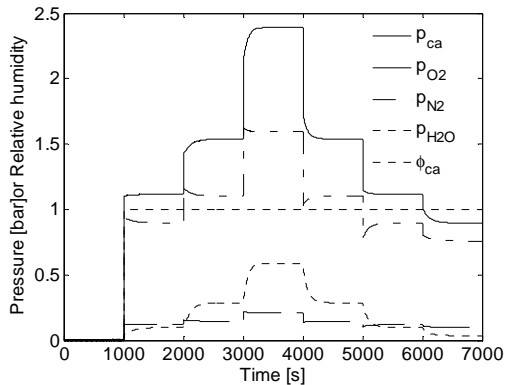


Fig. 8. Cathode species partial pressures for start up-shut down cycle

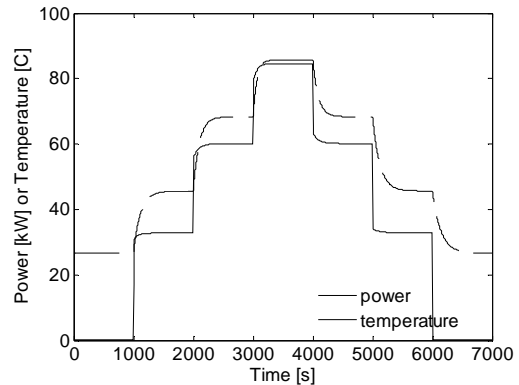


Fig. 11. Stack power and temperature for start up-shut down cycle

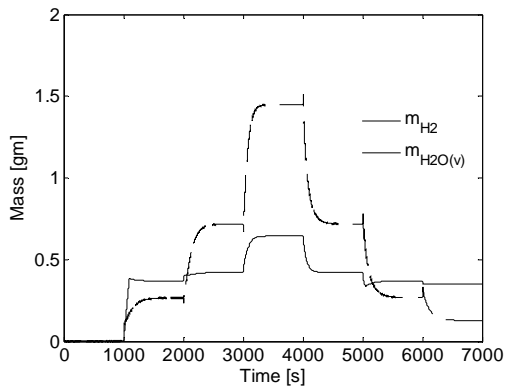


Fig. 9. Anode species masses for start up-shut down cycle

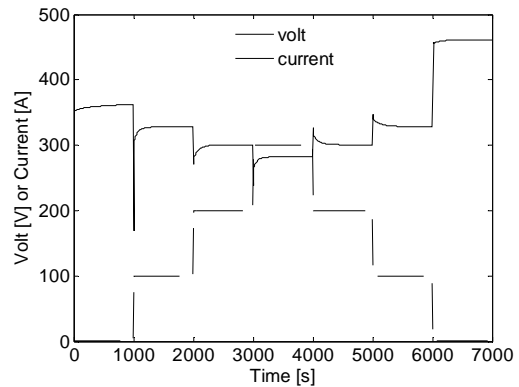


Fig. 12. Stack voltage and temperature for start up-shut down cycle

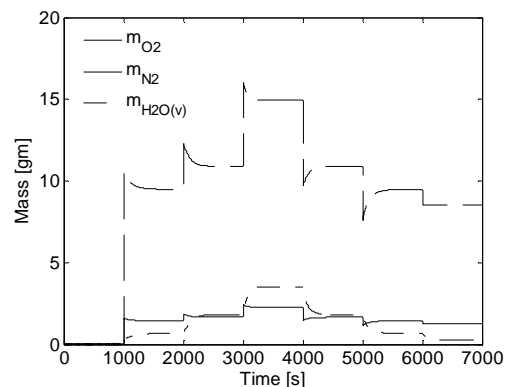


Fig. 10. Cathode species masses for start up-shut down cycle

## SUMMARY/CONCLUSIONS

A transient mathematical model for PEM fuel cells has been developed. The model incorporates fluid flow, heat transfer, and empirical voltage modeling. Explicit heat transfer formulae are used to determine the heat transfer coefficients and the cooling rate. The model is capable of predicting both steady state and unsteady performance of the fuel cell. The model was successfully tested by predicting the performance of an automotive fuel cell with 85 kw maximum power. For future studies, the model will be used to control the fuel cell.

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## DEFINITIONS/ABBREVIATIONS

### Symbols

$A$	area
$A_{fc}$	active fuel cell area
$c_{nzt}$	nozzle constant
$C_p$	specific heat constant
$C_v$	concentration
$\Delta H$	enthalpy change
$D_w$	water diffusion coefficient
$E$	open-circuit voltage
$f$	Friction factor
$F$	Faraday constant
$H_{st}$	stack height
$I$	current
$k$	conductivity
$L$	length
$\dot{m}$	mass flow rate
$M$	molecular weight
$n_d$	electro-osmotic drag coefficient
$n_{fc}$	number of fuel cells
$Nu$	Nusselt number
$p$	pressure
$P$	power or perimeter
$Pr$	Prandtl number
$\dot{Q}$	heat transfer rate
$Ra$	Rayleigh number
$Re$	Reynolds number
$t$	time
$t_{mem}$	membrane thickness
$T$	temperature
$T_0$	reference temperature (273 K)
$V$	voltage
$x$	mass fraction

### Greek Symbols

$\gamma$	specific heat ratio
$\Omega$	humidity ratio
$\phi$	relative humidity
$\sigma$	Stefan-Boltzman constant
$\varepsilon$	emissivity
$\lambda$	excess ratio

### Superscripts and subscripts

$act$	activation
$amb$	ambient
$an$	anode
$ca$	cathode
$clt$	coolant
$cnl$	channels
$cool$	cooling
$e$	electrical
$fc$	fuel cell or forced convection
$gen$	generated



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<i>HT</i>	heat transfer
<i>l</i>	liquid
<i>LHV</i>	lower heating value
<i>mem</i>	membrane
<i>v</i>	vapor
<i>nc</i>	natural convection
<i>ohm</i>	ohmic
<i>rad</i>	radiation
<i>reac</i>	reaction
<i>sens</i>	sensible
<i>st</i>	stack

## APPENDIX

### ANODE

Water vapor partial pressure is obtained from the ideal gas equation as

$$p_{H_2O(v)} = m_{H_2O(v)} R_{H_2O} T / V_{an} \quad (A.1)$$

The relative humidity is calculated from

$$\phi_{an} = \min(p_{H_2O(v)} / p_{sat}, 1) \quad (A.2)$$

Anode species partial pressures and total pressure are determined as

$$\begin{aligned} p_{H_2O(v)} &= \phi_{an} p_{sat} \\ p_{H_2} &= m_{H_2} R_{H_2} T / V_{an} \\ p_{an} &= p_{H_2} + p_{H_2O(v)} \end{aligned} \quad (A.3)$$

Anode humidity ratio is calculated as

$$\Omega_{an} = M_{H_2O} p_{H_2O(v)} / (M_{H_2} p_{H_2}) \quad (A.4)$$

### CATHODE

Water vapor partial pressure is obtained from the ideal gas equation as

$$p_{H_2O(v)} = m_{H_2O(v)} R_{H_2O} T / V_{ca} \quad (A.5)$$

The relative humidity is calculated from

$$\phi_{ca} = \min(p_{H_2O(v)} / p_{sat}, 1) \quad (A.6)$$

Cathode species partial pressures and total pressure are determined as

$$\begin{aligned} p_{H_2O(v)} &= \phi_{ca} p_{sat} \\ p_{O_2} &= m_{O_2} R_{O_2} T / V_{ca} \\ p_{N_2} &= m_{N_2} R_{N_2} T / V_{ca} \\ p_{ca} &= p_{O_2} + p_{N_2} + p_{H_2O(v)} \end{aligned} \quad (A.7)$$

Humidity ratio and mass fractions are obtained as follows:

$$p_{air,dry} = p_{ca} - p_{H_2O(v)} \quad (A.8)$$

$$\Omega_{ca} = M_{H_2O} p_{H_2O(v)} / (M_{air} p_{air,dry}) \quad (A.9)$$

$$m_{air,dry} = m_{O_2} + m_{N_2} \quad (A.10)$$

$$x_{O_2} = m_{O_2} / m_{air,dry} \quad (A.11)$$

$$x_{N_2} = m_{N_2} / m_{air,dry} \quad (A.12)$$

## MEMBRANE

$$\dot{m}_{H_2O,m} = M_{H_2O} A_{fc} n_{fc} \left( \frac{n_d i_d}{F} - D_w \frac{C_{v,ca} - C_{v,an}}{t_m} \right) \quad (A.13)$$

$$D_w = D_\lambda \exp \left( 2416 \left( \frac{1}{303} - \frac{1}{T} \right) \right) \quad (A.14)$$

$$D_\lambda = \begin{cases} 10^{-6} & \lambda_m < 2 \\ 10^{-6} (1 + 2(\lambda_m - 2)) & 2 \leq \lambda_m < 3 \\ 10^{-6} (3 - 1.67(\lambda_m - 3)) & 3 \leq \lambda_m < 4.5 \\ 1.25 \times 10^{-6} & \lambda_m \geq 4.5 \end{cases} \quad (A.15)$$

$$\lambda_m = \frac{\lambda_1 + \lambda_2}{2} \quad (A.16)$$

For  $i \in [an, ca]$

$$\lambda_i = \begin{cases} 0.043 + 17.81 a_i - 39.85 a_i^2 + 36 a_i^3 & 0 < a_i \leq 1 \\ 14 + 1.4(a_i - 1) & 1 < a_i \leq 3 \end{cases} \quad (A.17)$$

The water content of the membrane is  $\lambda_{an}$

$$n_d = 0.0029 \lambda_{an}^2 + 0.05 \lambda_{an} - 3.4 \times 10^{-19} \quad (A.18)$$

$$C_{v,i} = \rho_m \lambda_i / M_m \quad (A.19)$$

## VOLTAGE

Voltage for one cell is written as

$$V = E - V_{act} - V_{ohm} - V_{conc} \quad (A.20)$$

where

$$\begin{aligned} E &= 1.229 - 8.5 \times 10^{-4} (T - 298.15) \\ &+ 4.3085 \times 10^{-5} T [ \log(p_{H_2}) \\ &+ .5 \log(p_{O_2}) ] \end{aligned} \quad (A.21)$$

$$V_{act} = 0.9514 + T [-0.00312 - 7.4 \times 10^{-5} \log(C_{O_2}) + 0.000187 \log(i_d)] \quad (A.22)$$

$$C_{O_2} = p_{O_2} / (5.08 \times 10^6 \exp(-498/T)) \quad (A.23)$$

$$V_{ohm} = i_d R_m t_m \quad (A.24)$$

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$$i_d = \frac{I_{st}}{n_{fc}} \quad (\text{A.25})$$

$$R_m = 181.6 \left[ 1 + 0.03 i_d + 0.062 \left( \frac{T}{303} \right)^2 i_d^{2.5} \right] \quad (\text{A.26})$$
$$/ \left[ (14 - 0.634 - 3 i_d) \exp \left( 4.18 \frac{T - 303}{T} \right) \right]$$

$$V_{conc} = i_d \left( \frac{c_2 i_d}{2.2} \right)^2 \quad (\text{A.27})$$

$$p = \frac{p_{O_2}}{0.1173} + p_{sat}$$

$$c_2 = (7.16 \times 10^{-4} T - 0.622) p \quad (\text{A.28})$$
$$+ (-1.45 \times 10^{-3} T + 1.68) \quad \text{if } p < 2$$

$$c_2 = (8.66 \times 10^{-5} T - 0.068) p$$
$$+ (-1.6 \times 10^{-4} T + 0.54) \quad \text{if } p > 2$$