

## Optimization Study of Proton Exchange Membrane Fuel Cell Performance

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### Abstract

A mathematical model of the proton exchange membrane (PEM) fuel cell type, based on physical-chemical knowledge of the phenomena occurring inside the cell, was developed to study the performance at different operation variables. The effects of different operating parameters on the performance of PEM fuel cell studied using pure hydrogen on the anode side and air on the cathode side. Results with different fuel cell operating temperatures, different operating pressures and various combinations of these parameters were obtained. The possible mechanisms of the parameter effects and their interrelationships are discussed. The modeling results are compared with known experimental results. The comparison shows good agreements between the modeling results and the experimental data.

**Key words:** Optimization, Proton exchange, Fuel cell.

### Introduction

Recently, there has been growing concern about acid emissions, carbon dioxide, and other air quality matters, which have made renewable technologies an attractive option. Fuel cell technology is expected to play an important role in meeting the growing demand for distributed generation. In an ongoing effort to meet increasing energy demand and to preserve the global environment, the development of energy systems with readily available fuels, high efficiency and minimal environmental impact is urgently required (Barbir and Gomez, 1997). A fuel cell system is expected to meet such demands because it is a chemical power generation device that converts the chemical energy of a clean fuel (e.g., hydrogen) directly into electrical energy. Still a maturing technology, fuel cell technology has already indicated its advantages, such as its high-energy conversion efficiency, modular design and very low environmental intrusion, over conventional power generation equipment (Wright, 2004). Among all kinds of fuel cells,

proton exchange membrane fuel cells (PEMFCs) are compact and lightweight, work at low temperatures with a high output power density, and offer superior system startup and shutdown performance (Johnson et al., 2001; Wang et al., 2003). These advantages have sparked development efforts in various quarters of industry to open up new field of applications for PEMFCs, including transportation power supplies, compact cogeneration stationary power supplies, portable power supplies, and emergency and disaster backup power supplies.

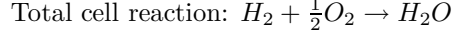
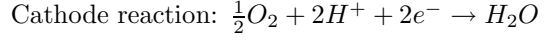
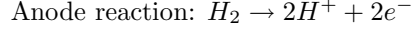
Two key issues limiting the widespread commercialization of fuel cell technology are better performance and lower cost. PEMFCs performance is limited by polarizations. A good understanding of the effect of design and operating conditions on the cell potential is required in order to reduce polarization. The performance of PEM fuel cells is known to be influenced by many parameters, such as operating temperature, pressure and discharge current. In order to improve fuel cell performances, it is essential to understand these parametric effects on fuel cell

operations. To understand and improve the performance of PEMFCs, researchers have developed several mathematical models to explain the behavior of potential variation with the discharge current. Mathematical modeling is a powerful tool for improving the performance of fuel cell stacks. Two main modeling approaches can be found in the literature. The first approach includes mechanistic models, which aim to simulate the heat, mass transfer and electrochemical phenomena encountered in fuel cells (Mann et al., 2000; Andrew and Xianguo, 2001). The second approach includes models that are based on empirical equations, which are applied to predict the effect of different input parameters on the voltage-current characteristics of the fuel cell, without examining in depth the physical and electrochemical phenomena involved in fuel cell operation (Lee et al., 2004). Some models are characterized by a high complexity, with several partial differential equations to be taken into account (Berning and Djilali, 2003; Mingruo et al., 2004). This high complexity creates problems of simulation times, parameter identifications, etc., especially when they are to be enclosed in a larger system, such as an electric vehicle.

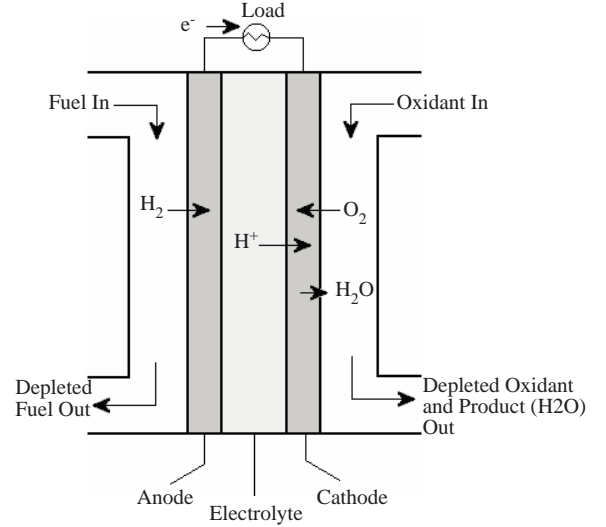
The purpose of this paper, therefore, is to develop a mathematical model for investigating the performance optimization of a PEM fuel cell that, although simplified and containing some semi-empirical equations, is still based on the chemical-physical knowledge of the phenomena occurring inside the cell. Model validation against the experimental data given by Chahine et al. (2001) is presented.

## Background

The fundamental structure of a PEMFC fuel cell can be described as 2 electrodes (anode and cathode) separated by a solid membrane acting as an electrolyte (Figure 1). Hydrogen fuel flows through a network of channels to the anode, where it dissociates into protons that, in turn, flow through the membrane to the cathode and electrons that are collected as electrical current by an external circuit linking the 2 electrodes. The oxidant (air in this study) flows through a similar network of channels to the cathode where oxygen combines with the electrons in the external circuit and the protons flowing through the membrane, thus producing water. The chemical reactions occurring at the anode and cathode electrode of a PEM fuel cell are as follows:



The products of this process are water, DC electricity and heat.



**Figure 1.** Schematic diagram of a proton exchange membrane fuel cells.

## Mathematical Model

Useful work (electrical energy) is obtained from a fuel cell only when a current is drawn, but the actual cell potential ( $V_{cell}$ ) is decreased from its equilibrium thermodynamic potential ( $E$ ) because of irreversible losses. When current flows, a deviation from the thermodynamic potential occurs corresponding to the electrical work performed by the cell. The deviation from the equilibrium value is called the overpotential and has been given the symbol ( $\eta$ ). The overpotentials originate primary from activation overpotential ( $\eta_{act}$ ), ohmic overpotential ( $\eta_{ohmic}$ ) and diffusion overpotential ( $\eta_{diff}$ ).

Therefore, the expression of the voltage of a single cell is

$$V_{cell} = E + \eta_{act} + \eta_{ohmic} + \eta_{diff} \quad (1)$$

The reversible thermodynamic potential of the chemical reactions,  $H_2+O_2$ , previously described, is given by the Nernst equation:

$$E = E^\circ - \left[ \left( \frac{RT}{nF} \right) \ln \left( \frac{P_{H_2O}}{P_{H_2} \times \sqrt{P_{O_2}}} \right) \right] \quad (2)$$

where the reversible standard potential  $E^\circ$  of an electrochemical reaction is defined as

$$E^\circ = -\frac{\Delta G^\circ}{nF} \quad (3)$$

Activation overpotential arises from the kinetics of the charge transfer reaction across the electrode-electrolyte interface. In other words, a portion of the electrode potential is lost in driving the electron transfer reaction. Activation overpotential is directly related to the nature of the electrochemical reactions and represents the magnitude of activation energy, when the reaction propagates at the rate demanded by the current. The activation overpotential occurring at the electrodes of a PEMFC is given by Eq. (4), which is known as the Tafel equation.

$$\eta_{act} = \left(\frac{RT}{\alpha nF}\right) \ln(i_o) + \left(\frac{RT}{\alpha nF}\right) \ln(i) \quad (4)$$

Ohmic overpotential results from electrical resistance losses in the cell. These resistances can be found in practically all fuel cell components: ionic resistance in the membrane, ionic and electronic resistance in the electrodes, and electronic resistance in the gas diffusion backings, bipolar plates and terminal connections. This could be expressed using Ohm's Law equations such as

$$\eta_{ohmic} = -iR^{internal} \quad (5)$$

Diffusion overpotential is caused by mass transfer limitations on the availability of the reactants near the electrodes. The electrode reactions require a constant supply of reactants in order to sustain the current flow. When the diffusion limitations reduce the availability of a reactant, part of the available reaction energy is used to drive the mass transfer, thus creating a corresponding loss in output voltage. Similar problems can develop if a reaction product accumulates near the electrode surface and obstructs the diffusion paths or dilutes the reactants. The diffusion overpotential can be expressed as

$$\eta_{diff} = \left(\frac{RT}{nF}\right) \ln\left(\frac{i_l - i}{i_l}\right) \quad (6)$$

The thermodynamic efficiency of the fuel cell  $E_{fc}$  can be determined as the ratio of output work rate  $W_{gross}$  to the product of the hydrogen consumption rate  $\dot{m}_{H_2}$  and the lower heating value of hydrogen  $LHV_{H_2}$  (Cownden et al., 2001).

$$E_{fc} = \frac{W_{gross}}{\dot{m}_{H_2} \cdot LHV_{H_2}} \quad (7)$$

Once the output voltage of the stack is determined for a given output current, the gross output power is found as:

$$W_{gross} = I \cdot V_{cell} \quad (8)$$

The output current is correlated with the hydrogen mass flow rate by the equation (Cownden et al., 2001)

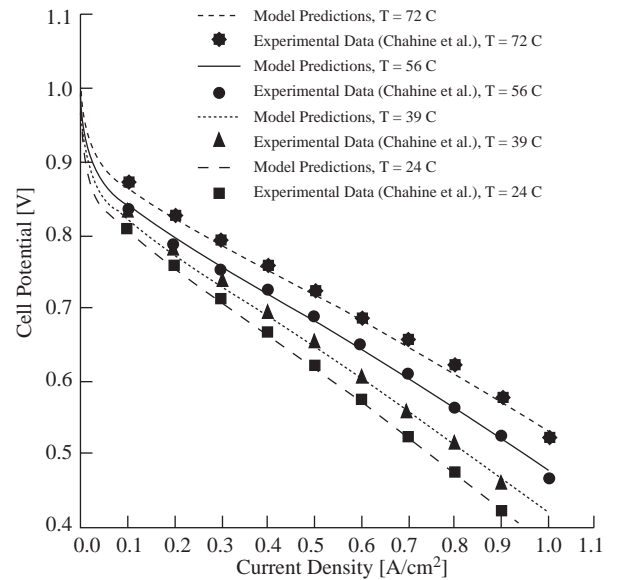
$$\dot{m}_{H_2} = \frac{I \cdot MW_{H_2}}{2F} \quad (9)$$

Thus, the thermodynamic efficiency of the fuel cell can be simplified as follows:

$$E_{fc} = \frac{2V_{cell}F}{MW_{H_2} \cdot LHV_{H_2}} \quad (10)$$

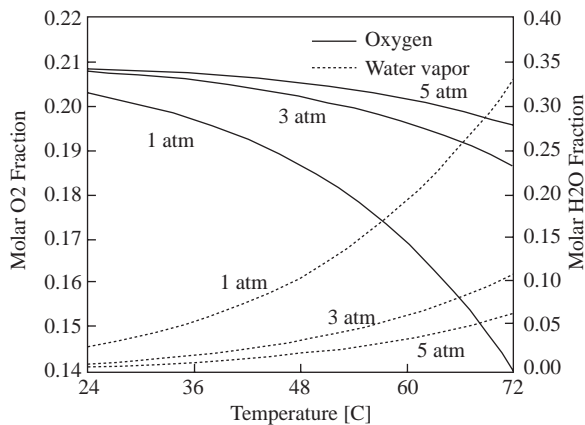
## Results and Discussion

Model validation involves the comparison of model results with experimental data, primarily for the purpose of establishing confidence in the model. To validate the mathematical model presented in the preceding section, comparisons were made to the experimental data given by Chahine et al. (2001) for a single cell operated at different temperatures and at a reactant pressure of 3/3 atm. Figure 2 compares the computed polarization curves with the measured ones. The calculated curves show good agreement with the experimental data for all temperatures.



**Figure 2.** Comparison between the model predictions and experimental results of Chahine et al. (2001).

The resulting inlet gas composition of the cathode side gas stream for different pressures is shown in Figure 3. Clearly, at an operation pressure of 1 atm the effect of the temperature on the inlet composition is much stronger than at elevated pressures. At 72 °C for 1 atm pressure, almost 33% (molar) of the incoming cathode side gas stream consists of water vapor and only around 14% is oxygen. It was already noted in Figure 3 that the change in the inlet gas composition is particularly strong in the range from 1 to 3 atm. Above 3 atm the composition changes only slightly with pressure.

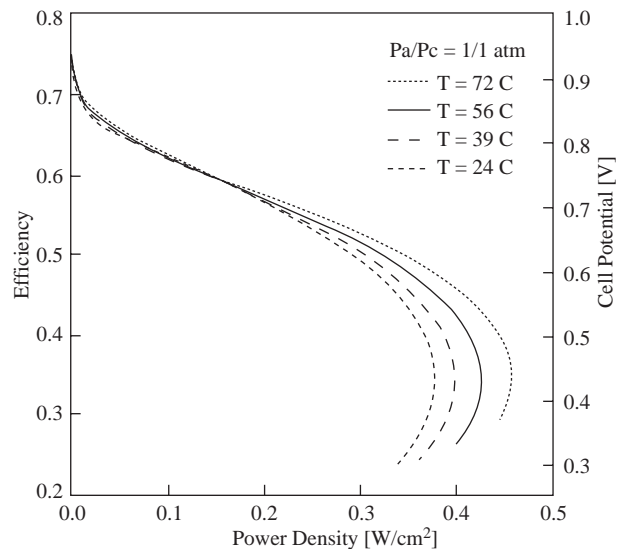


**Figure 3.** Molar inlet composition of the cathode side gas stream as function of temperature and different values of reactant pressures.

Performance curves with different cell temperatures are presented in Figure 4. The performance of the fuel cell increases with the increase cell temperature. The exchange current density increases with the increase in fuel cell temperature, which reduces activation losses. Another reason for the improved performances is that higher temperatures improve mass transfer within the fuel cells and result in a net decrease in cell resistance (as the temperature increases the electronic conduction in metals decreases but the ionic conduction in the electrolyte increases). This may explain the improvement in performance (Wang et al., 2003).

Performance curves with different operating pressures are presented in Figure 5. The pressures of the anode and cathode sides were kept the same. The performance of the fuel cell improves with the increase in pressure. The higher open circuit voltage at the higher pressures can be explained by the Nernst equation. The overall polarization curves shift positively as the pressure increases. Another reason for the improved performances is the partial pressure

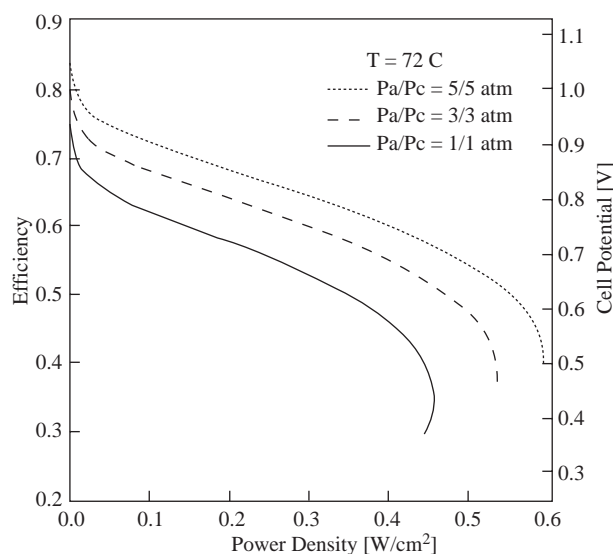
increase in the reactant gases with increasing operating pressure (cf. Figure 3). Changes in operating pressure have a large impact on the inlet composition and hence on the power density, as shown in Figure 5. The maximum power density shifts positively with increasing pressure because the rate of the chemical reaction is proportional to the partial pressures of the hydrogen and oxygen. Thus, the effect of increased pressure is most prominent when using air. In essence, higher pressures help to force the hydrogen and oxygen into contact with the electrolyte. This sensitivity to pressure is greater at high currents.



**Figure 4.** Relationship between fuel cell efficiency and power output for different values of cell temperature.

The fuel cell efficiency is directly proportional to the cell potential, as shown in Eq. (10); therefore, efficiency is also a function of power density. Figures 4 and 5, therefore, have both voltage and efficiency on the “y” axis. The efficiency at maximum power is much lower than that at partial loads, which makes the fuel cells very attractive and efficient for applications with highly variable loads where most of the time the fuel cell is operated at low load and high efficiency. The fuel cell’s nominal efficiency is therefore an arbitrary value, ranging anywhere between 0.3 and  $\sim 0.6$ , which can be selected for any fuel cell based on economic rather than on physical constraints. For example, for a fuel cell at a reactant pressure of 1 atm and 72 °C cell temperature, one may select a maximum operating point at 0.5 V and

0.89 A/cm<sup>2</sup>, resulting in 0.44 W/cm<sup>2</sup> and an efficiency of 0.4. However, one may get the same power output by selecting 2 cells, connected in series, operating at 0.71 V and 0.31 A/cm<sup>2</sup> each. Obviously, the latter would be twice as expensive, but it would be more efficient (0.57), and therefore would consume less fuel. This example clearly illustrates that the efficiency of a fuel cell may be “bought” by adding more cells, and it is driven by economic factors, such as the cost of individual cells, cost of hydrogen and the resulting cost of generated power.



**Figure 5.** Relationship between fuel cell efficiency and power output for different values of reactant pressures.

Returning to Figures 4 and 5, the maximum power occurs at approximately 0.4 to 0.5 V, which corresponds to a relatively high current. At the peak point, the internal resistance of the cell is equal to the electrical resistance of the external circuit. However, since efficiency drops with increasing voltage, there is a tradeoff between high power and high efficiency. Fuel cell system designers must select the desired operating range according to whether efficiency or power is paramount for the given application.

## Conclusion

A mathematical model based on physical-chemical knowledge of the phenomena occurring inside the cell of a PEMFC was developed and the effect of operation conditions on cell performance was investigated.

The mathematical model of electrochemical reactions and current distribution as presented herein is shown to be able to: (1) understand the many interacting, complex electrochemical and transport phenomena that cannot be studied experimentally; (2) identify limiting steps and components; and (3) provide a computer-aided tool for the design and optimization of future fuel cell engines with much higher power density and lower cost.

The effect of temperature on the inlet gas composition is particularly strong in the range from 1 to 3 atm. Above 3 atm the composition changes only slightly with pressure. Changes in operating pressure have a large impact on the inlet composition and, hence, on fuel cell performance.

For most applications, and particularly for steady operation, a fuel cell does not have to be operated at its maximum power, where the efficiency is lowest. When a higher nominal cell potential is selected, the cost of additional cells is offset by savings on fuel cost.

The results of the present study indicate that operating temperature and pressure can be optimized, based on cell performance, for given design and other operating conditions.

## Nomenclature

$E$	thermodynamic potential (V)
$E^\circ$	standard potential (V)
$E_{fc}$	thermodynamic efficiency
$F$	Faraday's constant (96487 C/mol)
$i$	current density (A/cm <sup>2</sup> )
$i_o$	exchange current density (A/cm <sup>2</sup> )
$i_l$	limiting current density (A/cm <sup>2</sup> )
$I$	current (A)
$LHV_{H_2}$	lower heating value of hydrogen (J/kg)
$\dot{m}_{H_2}$	hydrogen mass flow rate (kg/s)
$MW_{H_2}$	molecular mass of hydrogen (kg/mol)
$n$	number of electrons per reacting ion or molecule
$P_a, P_c$	total pressure of anode and cathode, respectively (atm)
$P_{H_2}, P_{O_2}, P_{H_2O}$	partial pressure of hydrogen, oxygen and water (atm)
$R$	gas constant (8.314 J/mol K)
$R^{internal}$	total internal area specific resistance ( $\Omega cm^2$ )

$T$	cell temperature (K)	$\eta_{act}$	activation overpotential
$V_{cell}$	cell voltage (V)	$\eta_{diff}$	diffusion overpotential
$W_{gross}$	gross output power (W)	$\eta_{ohmic}$	ohmic over potential
$\Delta G^{\circ}$	Gibbs energy change for the reaction under standard conditions (J/mol)		

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