Optimal Control and Design of Functionality to Improve Efficiency and Lifetime of Proton Exchange Membrane Fuel Cell

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OPTIMAL CONTROL AND DESIGN OF FUNCTIONALITY TO IMPROVE EFFICIENCY AND LIFETIME OF PROTON EXCHANGE MEMBRANE FUEL CELL

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Abstract
This work is devoted to identify operating conditions to maximize the life of power supply, meet the required power output and improve fuel consumption efficiency. We devise a framework for designing fuel cell power supplies for field sensor networks, which have important applications in environmental monitoring, wildlife preservation, in disaster monitoring and in border security. The high efficiency, low emission and zero noise pollution features of fuel cells have made them a promising clean power source.

Especially, proton exchange membrane fuel cells are promising alternative to conventional fossil fuel system, because they are clean, quiet and operate high efficiencies. However, challenges remain in achieving long lives due to shortage factors such as degradation and hydrogen storage. These shortages mainly depend on the operating conditions of PEM FC, load, start/stop cycles, working temperature, humidity etc.

Keywords: Power supply, Fuel cells, high efficiency, PEMFC, degradation processes of PEMFCs, optimal controls for PEMFCs

Introduction
Fuel cells offer the possibility of zero-emissions power production by using hydrogen as a fuel to generate electrical energy through a chemical reaction.

Various types of fuel cells have been developed over the last few decades such as Alkaline fuel cell (AFC), Direct Methanol fuel cell (DMFC), Phosphoric Acid fuel cell (PAFC), Molten Carbonate fuel cell (MCFC), Solid Oxide fuel cell (SOFC), and Proton Exchange Membrane (PEM) fuel cell.

PEM fuel cells are low temperature fuel cells that use a solid polymer in the form of a solid phase proton conducting membrane as an electrolyte which eliminate the need to contain corrosive liquids. PEM fuel cells have many advantages over the other fuel cell types; including low temperature operation, high power density, fast start up, system robustness, flexibility of fuel type (with reformer) and reduced sealing, corrosion, shielding or leaking concerns.

PEM fuel cells are candidates for a wide range of portable and stationary power applications which include transport as a major application, stationary and portable power generator and electronic devices.

Besides using the PEM fuel cell as a standalone power generator, the PEM fuel cell can be implemented with a renewable energy system for energy storage application.

Generally, The PEM fuel cell could be prepared as a single cell for small power requirement or as a cell stack where many cells are combined together to achieve the voltage and power output level required for the application. In spite of the excellent features as a power source, PEM fuel cell technology still faces serious challenges in terms of cost, durability and performance.

In general, the Fuel cells are slightly bigger than batteries with same capacity. However, in order to meet the full requirements of portable applications, the developers of PEM fuel cells have to reduce the size and weight of fuel cells.

As a power source, the mechanical durability of fuel cell is considered as a key performance factor particularly for transport applications. The mechanical durability of the fuel cell can be enhanced through design and develop a bipolar plate with high mechanical strength and high corrosion resistance. Metals-based flow plates provide several advantages over the traditional graphite flow plates from the durability point of view. The main drawback of the metallic flow plates is that they normally corrode in the PEM fuel cell environment.
In addition to corrosion problem of the flow plates, the membrane degradation during long-term operations of the PEMFC forms another durability concern in this technology. PEMFC is an electrochemical device that produces electrical power through a chemical reaction between a fuel such as hydrogen and oxygen. A fuel, hydrogen is delivered into anode side and an oxygen into the cathode side. Accordingly, at the anode side, the hydrogen is ionized to form protons (H⁺) which can across electrolyte, whereas at the cathode oxygen is reduced and forms water with protons (H⁺) that are transported through the proton conductive membrane. The sub-reactions and overall reaction can be expressed by the following equations:

Anode: \( \text{H}_2 \rightarrow 2\text{H}^+ + 2\text{e}^- \)
Cathode: \( \frac{1}{2}\text{O}_2 + 2\text{H}^+ 2\text{e}^- \rightarrow \text{H}_2\text{O} \)
Overall: \( \frac{1}{2}\text{O}_2 + \text{H}_2 \rightarrow \text{H}_2\text{O} \)

Electrons produced by this reaction migrate across the cell through the following elements: carbon support particles embedded in the anode catalyst layer, fibers of GDLs, current collector, external circuit, cathode catalyst layer. On the other hand, protons follow a shorter path, across the membrane from the anode towards the cathode catalyst layer. Here, we assume that water molecules are not involved in the proton transport. The adopted model incorporates the effect of the water content at the cell inlet by a proper setting of the ionic conductivity from experimental data.

We can infer that a dry input of H₂ and O₂ gases would produce a decrease in the PBI membrane conductivity. Moreover, the local current density for the hydrogen oxidation reaction is expressed by a linearized concentration dependent Butler-Volmer expression

\[ i_a = i_{0a}^{ref} \left( \frac{C_{H_2}}{C_{H_2}^{ref}} \right)^{0.5} \left( \frac{\alpha}{RT} \right) F \eta \]

where \( i_{0a}^{ref}, C_{H_2}^{ref}, C_{H_2}^{ref} \) are the exchange current density, the local hydrogen and a hydrogen reference concentrations, respectively, with \( \alpha \) being a reaction coefficient, \( T \) the temperature, \( F \) the Faraday, \( R \) the ideal gas constants and \( \eta \) a local over-potential. The effective surface area, \( a_v \), is defined as the ratio of the total active catalyst surface area to the total CL volume. The cathode channel is fed by air. At the cathode, oxygen reacts with protons to form water as follows:

\[ \frac{1}{2}\text{O}_2 + 4\text{H}^+ + 4\text{e}^- \rightarrow 2\text{H}_2\text{O} \]

A simplified Butler-Volmer expression can be considered, where the anodic term has been omitted, and a Tafel-equation (thus introducing a dependency on concentrations) can be used as a current density expression for the oxygen reduction reaction

\[ i_a = -i_{0a}^{ref} \left( \frac{C_{O_2}}{C_{O_2}^{ref}} \right) \exp\left( \frac{\alpha}{RT} F \eta \right) \]

where \( i_{0a}^{ref}, C_{O_2}, C_{O_2}^{ref} \) are the exchange current density, the local hydrogen concentration and an oxygen reference concentrations.

The mass transport process in PEMFCs takes place in three different media: the gas channels, gas diffusion layer, and catalyst layer. The electrolyte membrane is considered to be impermeable to all gasses.

The following incompressible Navier-Stokes equations can be used to describe the fluid continuity and momentum transport of the laminar gas flow within channels at both
cathode and anode sides:
\[
\rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \left[ -p I + \mu \nabla \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \right] + \rho \nabla \cdot \mathbf{u} = 0;
\]
\( \rho \) - density; \( \mathbf{u} \) - vector velocity; \( p \) - pressure; \( \mu \) - dynamic viscosity

To describe the flow within GDL and CL porous media Brinkman equations can be utilized:
\[
\frac{\rho}{\varepsilon} \left( \mathbf{u} \cdot \nabla \mathbf{u} \right) = \nabla \left[ -p I + \frac{\mu}{\varepsilon} \nabla \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \right] - \frac{2\mu}{3\varepsilon} \left( \nabla \mathbf{u} \right) - \left( \frac{\mu}{k} + \beta_\epsilon \right) \left| \mathbf{u} \right| S_\mu \mathbf{u}
\]

where, \( k, \varepsilon \) characterize porous medium, namely porosity and permeability.

The mass source can be explicitly written as:
\[
S_m = \begin{cases} 
-M H_2 i_a \frac{i_a}{2F} & \text{at the anode CL} \\
M O_2 i_a - M H_2 O i_c \frac{i_c}{2F} & \text{at the cathode CL}
\end{cases}
\]

The equation for the conservation of the chemical species in channels is written using the Stefan-Maxwell equations accounting for diffusion of hydrogen (\( H_2 \)) and water (\( H_2 O \)) at the anode side, as well as oxygen (\( O_2 \)), water (\( H_2 O \)) and nitrogen (\( N_2 \)) at the cathode side
\[
\rho \mathbf{u} \cdot \nabla \omega_i = \nabla \left[ \rho c p \sum D_{i\epsilon} \frac{M_i}{M_k} \nabla \omega_i + \frac{\omega_i}{p} \frac{M_i}{M_k} - 1 \right] \nabla p \right] + S_\mu
\]

where, \( \omega_i \) is a mass fraction for \( i \)-th species, \( M \) is molar mass, \( D_{i\epsilon} \) is the binary diffusion coefficient with \( M_{\text{total}} \) being:
\[
M_{\text{total}} = \left( \sum \frac{\omega_i}{M_i} \right)^{-1}
\]

The source terms for all species in the last equation are:
\[
S_m = \begin{cases} 
i_a \frac{i_a}{2F} & \text{for } H_2 \text{ at anode CL} \\
i_a \frac{i_a}{4F} & \text{for } O_2 \text{ at cathode CL} \\
i_c \frac{i_c}{2F} & \text{for } H_2 O \text{ at cathode CL}
\end{cases}
\]

The Stefan-Maxwell (SM) model for diffusion is the most general approach for describing multicomponent mass transport. As opposed to Fick’s model, it allows to reproduce typical diffusive effects of ternary mixtures, which are not present in binary diffusion mixtures such as counter diffusion. In the limit of binary mixtures, the Stefan-Maxwell model reduces to Fick’s model. In addition, SM model has a more solid thermodynamic basis compared to the phenomenological formulation of Fick’s equation and it can be formulated for taking into account the effect of both external body forces and non-equilibrium behaviors of fluids such as rarefaction.

The transport of charges (electron and proton) may occur through the solid (i.e., a network of carbon support of catalyst and carbon fibers based gas diffusion layer) and the electrolyte (polymer ionomer linkage in catalyst layer and membrane) phases. Poisson equations are used to describe the transport of electrons within the solid-phase (subscript \( s \)) of GDL and CL, as well as in the electrolyte-phase (subscript \( e \)) within CL and membrane accounting for ion transport. This yields:
\[
\nabla \cdot \mathbf{j}_s = S_s, \quad \mathbf{j}_s = -\nabla \phi_s, \\
\nabla \cdot \mathbf{j}_e = -S_e, \quad \mathbf{j}_e = -\delta_e \nabla \phi_e.
\]

Both equations are coupled through their current source terms:
\[
S_s = \begin{cases} 
i_a & \text{at anode CL} \\
i_c & \text{at cathode CL}
\end{cases}
\]

**Shortage of Fuel Cell System**

Our focus has been on PEMFCs because it is one of the more well studied and mature technologies that shows important potential for both high energy and long life applications. However, degradation of PEM fuel cells is a challenge. Fuel cell degradation is an important factor in the design of the fuel cell power supply and these are impacted by operating conditions, such as voltage, temperature, humidity, and voltage oscillations.

Our main purpose is to improve the life and efficiency of power supplies. In the figure there is described the factors which can cause degradation processes of power supplies’ components. As a result of these challenges we lose the durability and effectiveness of fuel cells.
Practically, we know that PEM fuel cells have several major components that are all subject to degradation. In this section we focus our research to the shortage of fuel cells which must be taken into account when design them. Fuel cell degradation is an important factor in the design of the fuel cell power supply and these are impacted by operating conditions, such as:

a) Voltage  
b) Load cycling  
c) Temperature  
d) Humidity

Using the catalyst degradation model, we determine the effect of operating conditions on fuel cell catalyst life. The rate of change in the surface area on the catalyst particles is used to estimate the catalyst life of the fuel cell. Fig. 3 shows that fuel cell catalyst life exponentially increases for lower voltages as shown. To achieve 3 years of life, the fuel cells would have to operate at 0.8 V or less. Increased voltages as had been determined from the model accelerates dissolution of the platinum catalyst, thus reducing its electrochemically active surface area. However, operating at high voltages increases the fuel cell conversion efficiency, but also results in less power output. These conflicting factors need to be considered to determine a suitable operating voltage.

Typically, all but the simplest of electrical devices have varying electrical loads. The work analyzed the effect of voltage fluctuations on fuel cell catalyst life. The results show a linear reduction in catalyst life for a linear increase in voltage oscillation amplitude. To understand the full impact of voltage oscillations, the percentage reduction in life value needs to be multiplied to the expected life in Fig.4 to obtain an absolute effect on catalyst life.
fuel cell power supply consists of several important components: a hydrogen generator, fuel cells, humidity and temperature controller, air management system, and power management controller. All these parameters will be analyzed.

![Figure 5. Proposed fuel cell power supply](image)

A control system is implemented on a micro-controller, an Arduino Mega (Fig. 6). The voltage of each cell is held at between 0.73 and 0.78 V. This is a trade-off to maximize life, power output and fuel cell efficiency.

![Figure 6. Proposed fuel cell power supply with optimal controls](image)

**Conclusion**

We have constructed optimal controls for main parts of PEMFC which occurs degradation process. We first analyzed how to design a fuel cell to achieve long-life by minimizing the effects of catalyst degradation, while maximizing operating efficiency and performance. Using these techniques, we identified operating conditions that will enable fuel cells to achieve more than 5 years of life, by performing temperature, humidity, operating voltage control and by using a hybrid system that maintains the fuel cells at constant voltage.

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