Engineering Gas Diffusion Layers for Optimal Energy and Catalytic Reaction of Hydrogen Fuel Cells

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Abstract

Hydrogen fuel cells (HFCs) are energy converter devices which turn the chemical energy of the reactants, oxygen and hydrogen gases, to electricity via electrochemical reactions. We consider the cathode part of a HFC, which consists of a flow channel, gas diffusion layer (GDL), and catalyst layer. When oxygen is delivered through the flow channel, it diffuses through the GDL to reach the catalyst layer to react with the hydrogen protons. The hydrogen protons pass from the cell's anode part though a proton electrolyte membrane (PEM), which functions effectively when it remains hydrated.

Traditionally, HFCs are manufactured with constant porosity GDLs. Literature has shown that a HFC with a constant porosity GDL has a non-uniform oxygen distribution in the GDL due to the gas pressure drop along the flow channel. Non-uniform oxygen distribution would result in the following issues:

1. Cell heat accumulation happens in regions of high reaction rates due to the excess amount of oxygen. The overheating can dehydrate the PEM, which then reduces its efficiency in transporting the protons to the cathode side, and hence reducing the oxygen-hydrogen electrochemical reaction.

2. Cell water accumulation takes place in regions of low reaction rates. In this case, water-drops prevent the oxygen transport and block the catalytic sites, and hence reduce the cell's productivity.

The electricity production and stability of a HFC mainly depend on the fluid distribution of oxygen. The more uniform is the oxygen distribution, the more efficient and stable is catalytic oxygen-hydrogen reaction.

In our research, we show that there exists a correlation between the oxygen distribution and the porosity design of the cathode GDL. The correlation helps us find optimum porosity designs of the GDL so that the oxygen distribution becomes uniform in the GDL. Using optimum porosity designs of the GDL, we show that the oxygen-hydrogen reaction can take place uniformly over the catalyst layer making the cell's operation efficient and stable.
We first introduce a mathematical model involving: the mass and momentum (Darcy) transport equations:

$$\nabla \cdot \left(\rho_g \boldsymbol{u_g}\right) = 0, \tag{1}$$
$$\boldsymbol{u_g} + K(\varepsilon)\nabla p_g = \mathbf{0}, \tag{2}$$

where $\boldsymbol{u_g}$ denotes the gas velocity, $\boldsymbol{p_g}$ pressure, and $\boldsymbol{\rho_g}$ density given by a state equation.
The GDL's permeability $\boldsymbol{K}(\boldsymbol{\varepsilon})$ is function of the GDL's porosity $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\mathbf{x})$, which is considered in our model as a fluid control function of $\boldsymbol{x}$ (the streamline direction).

An optimum design of $\boldsymbol{\varepsilon}$ would lead to a uniform catalytic reaction:

$$2H^+ + \frac{1}{2}O_2 + 2e^- \rightarrow H_2O + Heat \quad (3)$$

The catalytic reaction takes place uniformly when oxygen concentration is uniformly distributed over the catalyst layer, assuming uniform distribution of the hydrogen protons and the electric charges.

The oxygen mass fraction c_o is modeled by the convection-diffusion equation, interpreting the oxygen mass conservation:

$$\nabla \cdot \left(-\varepsilon D_o^{eff} \rho_g \nabla c_o + \varepsilon \rho_g c_o \boldsymbol{u_g}\right) = 0. \quad (4)$$

The set of the above equations is a nonlinear coupled system is incorporated with suitable boundary conditions and solved numerically for every given porosity function $\boldsymbol{\varepsilon}$.

An optimum choice of ε minimizes the total variation of oxygen mass fraction over surface of the catalyst layer (S):

$$\int_S \left(c_o - \frac{1}{|S|}\int_S c_o\right)^2 \quad (5)$$

The above cost functional is minimized subject to the state equations (1), (2) and (4).

We apply optimization and numerical techniques for solving the mathematical model and the optimization problem. We present our findings and illustrate the impact of the GDL's porosity design on the fluid flow.

Keywords: engineering porous mediums; fluid flow control in porous mediums; optimal porosity designs; hydrogen fuel cells