

Optimal and Robust Design of the PEM Fuel Cell Cathode Gas Diffusion Layer

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ABSTRACT

The cathode gas diffusion layer (GDL) is an important component of polymer electrolyte membrane (PEM) fuel cell. Its design parameters, including thickness, porosity and permeability, significantly affect the reactant transport and water management, thus impacting the fuel cell performance. This paper presents an optimization study of the GDL design parameters with the objective of maximizing the current density under a given voltage. A two-dimensional single-phase PEM fuel cell model is used. A multivariable optimization problem is formed to maximize the current density at the cathode under a given electrode voltage with respect to the GDL parameters. In order to reduce the computational effort and find the global optimum among the potential multiple optima, a global metamodel of the actual CFD-based fuel cell simulation, is adaptively generated using radial basis function approximations. For each level of the metamodel in the schematically reduced design space, a gradient-free, multi-island genetic algorithm is used to determine the optimum values of the cathode GDL design parameters for a global maximum current density on the cathode side. It is found that both the reactant and the current density tend to distribute more uniformly under the optimized conditions. Furthermore, as indicated by the polarization curve, the fuel cell with an optimized cathode GDL has a better performance.

NOMENCLATURE

$D_{i,eff}$	Effective diffusion coefficient of species, m^2/s
F	Faraday constant, 96487 C/mol
h	Mixture enthalpy, J/kg
$\mathbf{i}$	Current density vector, A/m^2
j_T	Transfer current due to electrochemical reaction, A/m^2
j_0	Reference current density, A/m^2
$\mathbf{J}_i$	Diffusion flux of species, $kg/m^2 \cdot s$
M	Mixture molecular weight, kg/kmol
N	Number of species
N_w	Net water flux inside membrane, $mol/m^2 \cdot s$
n_d	Electro-osmotic drag coefficient
p	Pressure, Pa
q''	Heat flux, W/m^2



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R Universal gas constant, 8314 J/kmol·K

S Surface area, m²

T Temperature, K

U Velocity vector, m/s

V Volume, m³

Y_i Mass fraction of species

Greek letters

α Tafel constant

δ Average pore size, m

ε Porosity

η Overpotential, V

κ Permeability, m²

$[\Lambda_k]$ Average interfacial molar concentration of species, kmol/m³

λ Thermal conductivity, W/m·K or membrane water content, mol H₂O/mol SO₃

μ Viscosity, kg/m·s

ρ Density, kg/m³

σ Electrical conductivity, 1/Ωm

τ Tortuosity of pores

Φ Phase electric potential, V

$\dot{\omega}_i$ Production rate of species due to electrochemical reactions, kg/m³·s

Subscripts

a Anode

c Cathode

e Electrolyte phase

eff Effective value

i Species

in Inlet

ref Reference value

s Solid phase

1. INTRODUCTION

A fuel cell is an electrochemical device which produces power directly from the electrochemical reaction of hydrogen and oxygen. Among the different types of fuel cells, the polymer electrolyte membrane (PEM) fuel cell is receiving a lot of attention for automotive and small stationary applications due to its low operating temperature, high power density, short start-up time, and very low pollution emissions.

The conventional PEM fuel cell produces electricity directly using hydrogen as a fuel and oxygen or air as an oxidant. The reactants are introduced to the cell through the channels on the bipolar plate. They transport through the gas diffusion layer (GDL) and reach the catalyst layer, where the electrochemical reaction occurs. The GDL is usually made of porous carbon cloth or carbon paper, and is positioned between the bipolar plates (flow plates) and the catalyst layer. Therefore, the GDL prevents the flow plates from a direct contact with the catalyst layer, removes the effects of irregular flow channel surfaces, and ensures a homogeneous and efficient mass transport over the whole active area of the cell [1].

The electrochemical behavior of the porous GDL in PEM fuel cells is influenced by several factors such as porosity, permeability, conductivity and the thickness of the GDL. It is difficult to evaluate how a single parameter influences the fuel cell performance, while other parameters are kept constant. For example, the change of GDL permeability and the gas flow rate may affect the channel pressure drop [2]. The effect of these gas diffusion layer parameters on the fuel cell performance has been studied extensively. Lee et al. [3] investigated the effects of the gas diffusion layer thickness using numerical simulations and concluded that an intermediate thickness enhances the electrodes' performance. Senn and Poulikakos [4] used a two-phase model to investigate the optimum diffusion layer thickness and channel width. Chu [5] investigated the effects of the gas diffusion layer porosity on the cell performance using a half-cell model. Jeng [6] presented a simple two-dimensional model to describe the oxygen mass transfer in the gas diffusion layer and investigated the influence of current collector ribs. Jordan [7] also presented a model to explain the influence of the diffusion layer morphology on water impregnation and gas diffusion. Roshandel [8] investigated the effects of the porosity variation in the gas diffusion layer on the cell performance.

Previous research has clearly showed that the gas diffusion layer design parameters affect the fuel cell performance considerably. However, to the best of our knowledge, the optimal GDL design parameters have not been obtained yet, despite their importance in fuel cell design. Some recent efforts have focused on optimizing the operating parameters [9, 10], the cathode electrodes geometry and flow channels geometry [11-13]. All these studies however, use a gradient-based optimizer which is hardly to obtain a global optimum.

This paper presents an optimization study of the cathode gas diffusion layer using the porosity, permeability and thickness of cathode gas diffusion layer as design variables. The optimized results are applicable to the anode gas diffusion layer since the same material of gas diffusion layer is usually adopted in a fuel cell design in both anode and cathode sides. A Multi-Island Genetic Algorithm (MIGA) is employed to search for the global maximum current density under a given voltage. A two-dimensional, single-phase, steady-state electrochemical mathematical model of a single cell is first presented in section 2 including a validation of the developed model. A multivariable optimization problem is formulated in section 3 using a genetic optimization algorithm in conjunction with an adaptively generated global metamodel using radial basis function (RBF) approximation. This global metamodel is not only a computationally efficient surrogate of the actual fuel cell mathematical model, but also has the ability to represent the potential multiple peaks of the original model. Section 4 presents the optimization results, and the main conclusions are summarized in Section 5.

2. A TWO-DIMENSIONAL PEMFC MODEL

This section describes a two-dimensional, single-phase, steady-state electrochemical mathematical model of a single cell, based on a three-dimensional model the authors has developed [13]. A two-dimensional model is used in order to reduce the computational effort, especially when the model is used in conjunction with a genetic optimization algorithm. Additionally, a two-dimensional model itself is sufficient in studying the transport features of gas diffusion layer since it considers the transport in both in-the-plane-and-through-the-plane directions. The two-dimensional model is based on the following assumptions:

- The fuel cell operates under the steady-state conditions.
- The reactants are ideal gases.
- An isotropic porous media exists in the gas diffusion layers, catalyst layers and the membrane. The gas diffusion layers are composed of carbon fibers and void space. The catalyst layers are formed of a mixture of carbon supported platinum electrolyte (Nafion) phase and void space.

- The gas within the electrodes is of a continuous phase so that Darcy's law applies.
- The transport of protons and electrons takes place only through the electrolyte phase and substrate solid (carbon) phase, respectively.
- Water stays in its vapor phase and no liquid is formed.
- The electrical conductivity of gas diffusion layer is assumed to be constant since the major ohmic loss in a fuel cell is due to the membrane resistance.

Figure 1 shows the computational domain of the unit cell in a rectangular coordinate. It consists of five different regions: cathode gas diffusion layer, cathode catalyst layer, polymer electrolyte membrane, anode catalyst layer and anode gas diffusion layer. The anode and cathode flow fields are in a co-flow orientation and the reactants consist of humidified hydrogen and dry air.

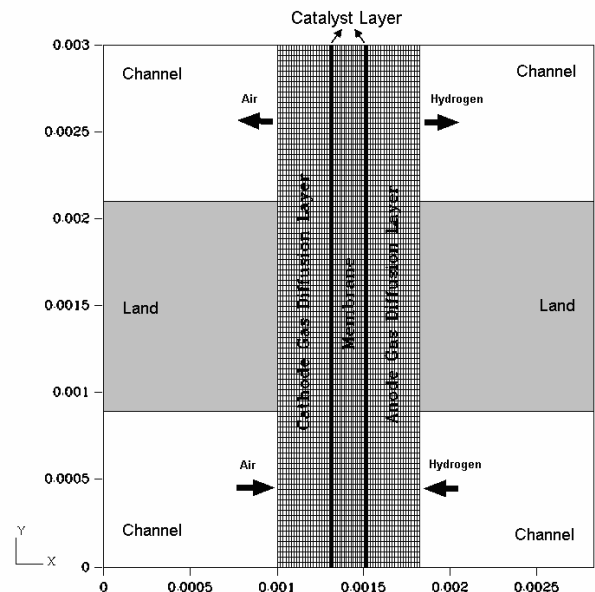


Figure 1. Computational domain and grid

2.1 Model equations

Based on the described assumptions, the transport and electrochemical phenomena inside a fuel cell can be modeled using the conservation equations of mass, momentum, energy, species, and electric current in different components of fuel cells.

2.1.1 Transport phenomena modeling in the gas diffusion layers

The mass and momentum conservation equations in the porous gas diffusion layers are [14]:

$$\nabla \cdot (\varepsilon \rho \mathbf{U}) = 0 \quad (1)$$

and

$$\nabla \cdot (\varepsilon \rho \mathbf{U} \mathbf{U}) = -\varepsilon \nabla p + \nabla \cdot (\varepsilon \mu \nabla \mathbf{U}) - \frac{\varepsilon^2 \mu \mathbf{U}}{\kappa} \quad (2)$$

where ρ is the fluid density, P is the pressure, μ is the fluid dynamic viscosity, $\mathbf{U}$ is the fluid velocity vector. Respectively, where the porosity ε of the medium represents the ratio of the volume occupied by the pores to the total volume of the porous medium and the permeability κ is a quantity representing the square of the effective volume to surface area ratio of the porous matrix. The last term in Eq. 2 represents the Darcy's drag force imposed by the pore walls on the fluid within the pores, which usually results in a significant pressure drop across the porous medium. In general, the Darcy's drag term can be anisotropic, resulting in different pressure drops in different directions due to a directional permeability [15].

The energy conservation equation is

$$\nabla \cdot (\varepsilon \rho \mathbf{U} h) = \nabla \cdot \mathbf{q}'' + \frac{|\mathbf{i} \cdot \mathbf{i}|}{\sigma} \quad (3)$$

where the heat flux $\mathbf{q}''$ is comprised of contributions from thermal conduction and species diffusion. It is given by

$$\mathbf{q}'' = \lambda_{eff} \nabla T + \sum_i \mathbf{J}_i h_i \quad (4)$$

where h_i is the enthalpy of gas phase species, $\mathbf{J}_i$ is the diffusion flux of gas phase species, and T is the bulk temperature. The thermal conductivity, λ_{eff} , of the porous medium is an effective thermal conductivity of the pores and solid regions. It is equal to

$$\lambda_{eff} = -2\lambda_s + \frac{1}{\frac{\varepsilon}{2\lambda_s + \lambda_e} + \frac{1-\varepsilon}{3\lambda_s}} \quad (5)$$

where λ_s and λ_e are the thermal conductivities of the solid (matrix) and fluid regions (pores), respectively. The last term in Eq. 3 represents the Joule heating.

The mass conservation equation for each individual gas phase species is

$$\nabla \cdot (\varepsilon \rho \mathbf{U} Y_i) = \nabla \cdot \mathbf{J}_i \quad (6)$$

where Y_i is the mass fraction of the i -th species. The species diffusion flux $\mathbf{J}_i$ can be written as [16]:

$$\mathbf{J}_i = \rho D_{i,eff} \nabla Y_i + \frac{\rho Y_i}{M} D_{i,eff} \nabla M - \rho Y_i \sum_j D_{j,eff} \nabla Y_j - \rho Y_i \frac{\Delta M}{M} \sum_j D_{j,eff} Y_j \quad (7)$$

where M is the mixture molecular weight. The first term in Eq. 7 represents Fick diffusion due to concentration gradients. The last three terms are correction terms necessary to satisfy the Stefan-Maxwell equations for multicomponent species. In this case, $D_{i,eff}$ is the effective mass diffusion coefficient of species i within the porous medium, and depends on the porosity and tortuosity, τ , of the medium. Therefore, $D_{i,eff}$ can be

described by

$$D_{i,eff} = D_i \varepsilon^\tau \quad (8)$$

where D_i is the free stream diffusion coefficient of the i -th species. It is common practice to use a tortuosity value of 1.5 in Eq. 8, resulting in the so-called Bruggeman model.

2.1.2 Modeling of electrochemical reactions and transport phenomena in the catalyst layers

The continuity of current within any material under electroneutral conditions results in

$$\nabla \cdot \mathbf{i} = 0 \quad (9)$$

where $\mathbf{i}$ is the current density vector. In porous electrodes, the current is split into two parts; one flowing through the polymer electrolyte phase and the other flowing through the solid parts of the porous matrix, which are denoted by $\mathbf{i}_e$ and $\mathbf{i}_s$, respectively. Eq. 9 can be therefore, rewritten as

$$\nabla \cdot \mathbf{i}_e + \nabla \cdot \mathbf{i}_s = 0 \quad (10)$$

During the electrochemical reactions within a porous medium, electrons are either transferred (expressed by the transfer current) from the electrolyte phase to the solid phase or vice versa due to their own electric potential. This results in a source in one phase and a sink in the other phase. Thus, applying Ohm's law to Eq. 10 yields

$$\nabla \cdot (\sigma_e \nabla \Phi_e) = -\nabla \cdot (\sigma_s \nabla \Phi_s) = j_T \left(\frac{S}{V} \right)_{eff} \quad (11)$$

where Φ_e and Φ_s are the electric potentials of the electrolyte and solid phases, respectively. The $(S/V)_{eff}$ in