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# An analytical solution for transport of oxygen in cathode gas diffusion layer of PEMFC

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### Abstract

A two-dimensional theoretical model is developed in this study to simulate the transport phenomena of oxygen in cathode gas diffusion layer (GDL) of proton exchange membrane fuel cell (PEMFC). An analytical solution is then obtained accordingly to characterize the effects of GDL on cell performance. It is found that the concentration flux of oxygen across the GDL is primarily dominated by the thickness and porosity of GDL. For a thicker GDL, the diffusion resistance increases and thus lowers the cell performance especially under high current density condition. On the other hand, an increase of porosity will enhance the transport of oxygen and result in significant improvement of cell performance. The influences of system parameters including the temperature, channel height, inlet velocity, and inlet pressure on the diffusion of oxygen in GDL are also examined systematically. Results provide insights into the characteristics of oxygen diffusion in GDL and benefit the optimal design of PEMFC.

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# 1. Introduction

In the past decade, proton exchange membrane fuel cell (PEMFC) has received much attention due to its widely promising applications in portable power sources, automobile power systems, and stationary power plants. Numerous studies have devoted to develop theoretical models in order to simulate the transport of reactants, electrochemical reactions, and characteristics of membrane in PEMFC [1–22]. Particularly, since it is well known that the performance of PEMFC is cathode limited, most of the research efforts have focused on the cathode side of PEMFC [8–22] to investigate the composition and performance of catalyst layer, transport of reactants in feed channel and porous electrode, and water management problem.

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Recently, many investigations [23–31] have concentrated on the GDL because of its substantial influence on fuel cell performance. The GDL makes the gas reactant transports to the catalyst layer in a diffusive way rather than direct contact in order to avoid the possible breakdown of the membrane caused by the strong impact of reactant on the membrane surface. However, the existence of GDL affects the mass transport of reactant profoundly and results in a loss of cell performance. Thus, it is quite important to understand the characters of GDL for the design work of PEMFC. Jordan et al. [23] performed an experimental study to find the effect of carbon morphology in GDL and proposed a model to explain how the hydrophobicity and porosity of GDL affect water impregnation and gas diffusion through this layer. Park et al. [24] considered the GDL consists of the gas diffusion medium (GDM) and the micro-layer, and investigated the water transportation in GDM with different PTFE contents. A novel design of GDL has been developed by Chen et al. [25] that insert a water management layer between the

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traditional GDL and the catalyst layer. The effects of different fabrication methods and thickness of GDL were also discussed by Lee et al. [26]. Mirzazadeh et al. [27] studied the role of GDL in the cell performance and evaluated the electrode with or without this layer. They found that the effect of GDL is more pronounced at higher current densities. Jeng et al. [28] developed a two-dimensional model for oxygen mass transfer in the GDL of air-breathing PEMFC under the influence of current collector ribs. The resulting equations were discretized and solved by a numerical technique. Their results indicate that the GDL is used only partly in the mass transfer process due to the existence of ribs. Williams et al. [29] examined the limiting factors for the oxygen transport in the cathode GDL with several kinds of commercial GDL. They further studied the influence of convection through the GDL on the cathode limiting current by using three GDLs with different gas permeability [30]. A computational analysis for the effect of GDM permeability on convective transport also has been performed by Pharoah [31].

Although the GDL plays an important role in the optimization of PEMFC, it is still difficult to evaluate the influence of an individual property of GDL on cell performance in experiments or theoretical analyses, because the electrochemical reactions in gas diffusion electrode involve complicated factors and they are strongly coupled in general. Therefore, a simplified model is necessary and helpful to understand the characteristics of GDL. In the present study, we have developed a two-dimensional theoretical model for the GDL along the cathode channel of PEMFC. The system is simplified and thus an analytical solution can be obtained to characterize the transport of oxygen in GDL. Accordingly, the influences of physical factors of the system on the cell performance can be easily examined based on this simple analytical solution.

# 2. Theoretical model and formulation

Consider the two-dimensional model of cathode GDL as shown in Fig. 1. The GDL with thickness *H* is confined between the catalyst layer and the gas channel. The interface between the GDL and the gas channel is located at y = 0. Pure oxygen is fed into the gas channel with inlet velocity  $v_0$ , where the channel height and length are  $h_c$  and *L*, respectively. To study the characteristics of transport and consumption of oxygen in this system, some simplifications are made as list below:

1. The system is isothermal and in a steady state.



Fig. 1. Schematic representation of the two-dimensional model for the gas diffusion layer in cathode side of PEMFC.

- 2. The catalyst layer is very thin and can be treated as a boundary adjacent to the upper surface of GDL. The electrochemical reaction occurs at this layer only.
- 3. The GDL is isotropic and the transport of oxygen in this layer can be described by Darcy's law.
- 4. The generation and transport of water are ignored.
- 5. The oxygen in the system behaves as an ideal gas.

Accordingly, the continuity equation in the GDL can be expressed by

$$\frac{\partial(\rho v_x)}{\partial x} + \frac{\partial(\rho v_y)}{\partial y} = 0,$$
(1)

where  $\rho$  is the density,  $v_x$  and  $v_y$  are respectively the *x* and *y* components of the superficial velocity which is defined as the volume flow rate through an unit cross-sectional area in a porous medium. By utilizing the Darcy's law, the velocity components  $v_x$  and  $v_y$  can be written as

$$v_x = -\frac{\kappa}{\mu} \frac{\partial P}{\partial x}, \qquad v_y = -\frac{\kappa}{\mu} \frac{\partial P}{\partial y},$$
 (2)

where  $\kappa$  is the permeability,  $\mu$  the dynamic viscosity, and *P* is the pressure. According to the ideal gas equation of state, the pressure *P* can be substituted by

$$P = C_{\rm d} RT,\tag{3}$$

where  $C_d$  is the molar concentration, R the universal gas constant, and T is the absolute temperature. Note that  $\rho = C_d M$  in which M is the molecular weight of oxygen. Eqs. (1)–(3) can be combined together in the form:

$$\nabla^2 \left[ \frac{C_d^2(x, y)}{2} \right] = 0, \tag{4}$$

where  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$  is the Laplace operator. Define:

$$\Phi(x, y) = \frac{C_{\rm d}^2(x, y)}{2},$$
(5)

thus, Eq. (4) becomes

$$\nabla^2[\Phi(x, y)] = 0. \tag{6}$$

The above equation characterizes the concentration distribution in the GDL and can be solved simply with appropriate boundary conditions. At the side walls of GDL x=0 and x=L, there is no concentration flux and the boundary conditions are

$$\left. \frac{\partial \Phi}{\partial x} \right|_{x=0} = \left. \frac{\partial \Phi}{\partial x} \right|_{x=L} = 0.$$
(7)

At the interface between the GDL and the gas channel y = 0, the concentration is continuous across the interface and the boundary condition is given by

$$\Phi|_{y=0} = \frac{C_0^2}{2} \exp\left(-\frac{2x}{L_1}\right).$$
(8)

In above equation, the results for the profile of oxygen concentration along the channel given by Dohle et al. [11] are used and the corresponding equation is

$$C_{\rm d}(x,0) = C_0 \exp\left(-\frac{x}{L_1}\right),\tag{9}$$

where  $C_0$  is the inlet concentration and  $L_1$  the characteristic length of oxygen consumption at the reaction order  $\gamma = 1$ . To derive the boundary condition at the interface between the GDL and the catalyst layer y = H, we can define the mass flux of oxygen  $\dot{m}_0$  as a function of local current density i(x) according to the electrochemical reaction at the catalyst layer:

$$O_2 + 4H^+ + 4e^- \to 2H_2O,$$
 (10)

so we have:

$$\dot{m}_0|_{y=H} = \rho v_y = MC_{\rm d} v_y = \frac{iM}{nF},\tag{11}$$

where n = 4 is the number of electrons transferred per mole of oxygen consumed and *F* the Faraday constant. The mass flux  $\dot{m}_0$  also satisfies the relation [9]:

$$\dot{m}_0|_{y=H} = -\varepsilon D_0^e M \left. \frac{\partial C_d}{\partial y} \right|_{y=H} + \varepsilon M v_y C_d \Big|_{y=H}, \tag{12}$$

where the first and second terms on the right hand side are the amounts of oxygen flux caused by diffusion and convective motion, respectively. Here,  $\varepsilon$  is the porosity of GDL and  $D_0^e$ the effective molecular diffusion coefficient of oxygen that is related to the diffusion coefficient in a nonporous domain  $D_0$  by  $D_0^e = D_0 \varepsilon^{1.5}$  [9]. By equating both Eqs. (11) and (12), we may obtain:

$$\left. \frac{\partial C_{\rm d}}{\partial y} \right|_{y=H} = \frac{\varepsilon - 1}{n\varepsilon F D_0^{\rm e}} i(x).$$
(13)

The Tafel equation [9,12] is used to describe the distribution of current density along the boundary of catalyst layer:

$$i(x) = i_0 \left(\frac{C_{\rm d}|_{y=H}}{C_{\rm ref}}\right) \exp\left(\frac{\alpha F}{RT}\eta\right),\tag{14}$$

where  $i_0$  is the exchange current density,  $C_{\text{ref}}$  the reference concentration of oxygen,  $\alpha$  the charge transfer coefficient and  $\eta$  the electrode activation overpotential. Therefore, Eq. (13) becomes

$$\left. \frac{\partial C_{\rm d}}{\partial y} \right|_{y=H} = \frac{(\varepsilon - 1)}{n\varepsilon F D_0^{\rm e}} \frac{i_0}{C_{\rm ref}} \exp\left(\frac{\alpha F}{RT}\eta\right) C_{\rm d}|_{y=H}.$$
(15)

Note that Eq. (9) indicates the concentration of oxygen decays exponentially along the channel. Hence, it is reasonable to assume that the concentration of oxygen in the GDL also behaves in a similar way. Thus, the concentration function  $C_d(x, y)$  can be written by separation of variables:

$$C_{\rm d}(x, y) = C(x)\theta(y), \tag{16}$$

and then Eq. (15) can be solved to get the boundary condition at y = H:

$$\begin{split} \Phi|_{y=H} &= \frac{C^2(x)G^2}{2} \\ &= \frac{C^2(x)}{2} \exp\left(\frac{2(\varepsilon-1)}{n\varepsilon D_0^{\rm e}F} \frac{i_0H}{C_{\rm ref}} \exp\left(\frac{\alpha F}{RT}\eta\right)\right), \quad (17) \end{split}$$

where

$$G = \exp\left(\frac{(\varepsilon - 1)}{n\varepsilon D_0^{\rm e}F}\frac{i_0H}{C_{\rm ref}}\exp\left(\frac{\alpha F}{RT}\eta\right)\right).$$
(18)

Eq. (6) together with the boundary conditions (7), (8), and (17) can be solved to obtain an analytical solution in the form:

$$\Phi(x, y) = \frac{C_0^2 L_1}{4L} \left[ 1 - \exp\left(\frac{2L}{L_1}\right) \right] \left[ \left( 1 + \frac{G^2 - 1}{H} \right) y \right] \\
+ \sum_{n=1}^{\infty} \frac{C_0^2}{L} \frac{\left[ 1 - \exp\left(-\frac{2L}{L_1}\right) \cos(n\pi) \right]}{\frac{L_1}{2} \left(\frac{n\pi}{L}\right)^2 + \frac{2}{L_1}} \\
\times \cos\left(\frac{n\pi}{L}x\right) \left\{ \frac{G^2 \sinh\frac{n\pi}{L}y}{\sinh\frac{n\pi}{L}H} \\
- \frac{\left[ \sinh\left(\frac{n\pi}{L}y\right) - \tanh\left(\frac{n\pi}{L}H\right) \cosh\left(\frac{n\pi}{L}y\right) \right]}{\tanh\left(\frac{n\pi}{L}H\right)} \right\}. (19)$$

This equation gives the concentration of oxygen in the GDL in a simple analytical form.

To determine the voltage–current curves of the PEMFC, we define the average current density  $\overline{i}$  over the channel length L as

$$\dot{i} = \frac{1}{L} \int_0^L \bar{i}(x) \,\mathrm{d}x,\tag{20}$$

and the operating cell voltage is given by

$$V = V_{\text{cell}} - \eta - \eta_{\text{ohm}},\tag{21}$$

where  $V_{\text{cell}}$  is the open circuit voltage,  $\eta$  can be determined from the Tafel Eq. (14), and  $\eta_{\text{ohm}}$  is the ohmic losses. Since in most PEMFCs the electrical resistance is mainly caused by the ion transport through the membrane, the ohmic losses are approximated by a plain expression:

$$\eta_{\rm ohm} = \frac{il_{\rm m}}{\sigma_{\rm m}},\tag{22}$$

where  $l_{\rm m}$  is the membrane thickness and  $\sigma_{\rm m}$  the membrane conductivity. Eqs. (19)–(22) provide a simple technique to estimate the influence of GDL on fuel cell performance.

## 3. Results and discussion

We first examine the influence on cell performance due to the existence of GDL and compare the results with those of Dohle et al. [11] in which they considered the case without GDL. Fig. 2 illustrates the variations of I-V curves for several assigned values of the GDL thickness. Based on the same parameters used in Ref. [11], it is found that the present results



Fig. 2. Voltage-current curves for four assigned values of GDL thickness.

are in agreement with those of Ref. [11] for the case without GDL. The use of GDL apparently lowers the cell performance and the curve falls gradually with increase of GDL thickness. This effect is more pronounced especially at high current density condition, which indicates that a thicker GDL gives rise to a higher resistance for oxidant transport toward the electrode surface. The influence of GDL for different channel length is demonstrated in Fig. 3 for three assigned values of L. It has been proposed by Dohle et al. [11] that a decrease of channel length will improve cell performance in the whole range of current densities because the oxygen concentration is more uniform in shorter L and this effect raises the overall performance per unit area as shown in Fig. 3 for the cases without GDL. When we take the GDL into consideration, it is found that the influence of GDL is quite significant especially in short channel length. For the case L = 400 cm, the limiting current density reduces only 11% approximately. While for the case L = 100 cm it reduces about 29%, which reveals that it is very important to improve the losses caused by the use of GDL particularly in relatively short channel length.

Table 1 gives the values of parameters used in the following analysis for a base operating condition of the fuel cell.

![](_page_3_Figure_5.jpeg)

Fig. 3. Volage–current curves for three assigned values of channel length L with and without GDL.

Table 1				
Values of physical	parameters used	in the	base	case

Cell temperature, $T(K)$	343
Inlet pressure, P (atm)	1
Inlet flow velocity, $v_0$ (cm s <sup>-1</sup> )	145
Inlet concentration, $C_0 \pmod{\mathrm{cm}^{-3}}$	$3.87 \times 10^{-5}$
Reference concentration, $C_{\rm ref} ({\rm mol}{\rm cm}^{-3})$	$3.18 \times 10^{-5}$
Channel length, $L$ (cm)	44
Channel height, $h_c$ (cm)	0.1
Membrane thickness, $l_{\rm m}$ (cm)	0.018
Gas diffusion layer thickness, H (cm)	0.04
Transfer coefficient, α	1
Number of electrons, n	4
Exchange current density, $i_0$ (A cm <sup>-2</sup> )	$5.74 \times 10^{-7}$
Molecular weight, $M$ (kg mol <sup>-1</sup> )	32
Dynamic viscosity, $\mu$ (g cm <sup>-1</sup> s <sup>-1</sup> )	$2.03 \times 10^{-4}$
Permeability, $\kappa$ (cm <sup>2</sup> )	$10^{-8}$
Universal gas constant, $R (\text{J mol}^{-1} \text{ K}^{-1})$	8.314
Faraday constant, $F(C \mod^{-1})$	96487
Porosity, $\varepsilon$	0.4
Diffusion coefficient of oxygen, $D_0$ (cm <sup>2</sup> s <sup>-1</sup> )	0.0991
Ideal open circuit voltage, $V_{cell}$ (V)	1.2
Conductivity, $\sigma_m (1 \ \Omega^{-1} \ cm^{-1})$	0.0868

The variations of the distribution of oxygen concentration in the gas channel and GDL for three assigned values of porosity  $\varepsilon$  under the same output of cell voltage 0.5 V are shown in Fig. 4(a)–(c) and the corresponding *I*–V curves are shown in Fig. 5.The channel height  $h_c$  and the thickness of GDL *H* are respectively 0.1 and 0.04 cm with the interface at Y=0.1 cm indicated by the dashed line. One can see that at  $\varepsilon=0.3$  in

![](_page_3_Figure_10.jpeg)

Fig. 4. Distribution of oxygen concentration in the cathode gas channel and GDL for three assigned values of porosity with the same output of cell voltage 0.5 V; (a)  $\varepsilon = 0.3$ , (b)  $\varepsilon = 0.4$ , (c)  $\varepsilon = 0.5$ .

![](_page_4_Figure_2.jpeg)

Fig. 5. Variation of voltage-current curves with porosity.

Fig. 4(a), the oxygen concentration within the GDL descends rapidly toward the electrode surface and most of oxygen near the catalyst layer is consumed due to the low diffusivity in accord with the low porosity of GDL. Hence, the concentration flux through the GDL is small and fails to supply sufficient oxidant to the catalyst layer for electrochemical reaction. Consequently, the cell voltage falls quickly against the current density as shown in Fig. 5. As the porosity of GDL increases, for example,  $\varepsilon = 0.4$  and 0.5 as shown in Fig. 4(b) and (c), the mass transport through the GDL will be increased and therefore the voltage loss due to the presence of GDL will diminish obviously as indicated in Fig. 5. These results suggest that the porosity of GDL plays an important role in the factors to affect the cell performance and should be as large as possible in practical design of PEMFC.

The operating temperature of fuel cell is also an important factor and its effect on the mass transport of GDL is displayed in Fig. 6(a)–(c) via the velocity profiles in the GDL for three given temperatures. It is noted that actually many parameters in the system are functions of temperature and the influences of temperature variation on cell performance are quite complicated. Here, we simply consider the effect of temperature arising from the ideal gas equation as indicated in Eq. (3) and assume the other parameters are invariant with temperature to simplify the analysis. At lower operating temperature as shown in Fig. 6(a)for T = 323 K, it is found that the x-component of velocity for the gas in GDL is very small and the direction of velocity is almost toward and perpendicular to the catalyst layer. Thus, the diffusive direction of oxygen in GDL is primary dominated by the catalyst layer where the electrochemical reaction occurs. Simultaneously, the magnitude of velocity decays along *x*-axis direction while grows gradually approaching the catalyst layer. Similar results can also be observed in Fig. 6(b) and (c) for T = 343 and 363 K, respectively. Apparently, an increase of temperature enhances the diffusive velocity in the GDL and thus improves the cell performance as shown in Fig. 7. While the concentration is in inverse proportional to the temperature for a constant inlet pressure, the improvement of cell performance by increasing temperature is limited. Moreover, the I-V curve for higher temperature appears to possess smaller limiting cur-

![](_page_4_Figure_6.jpeg)

Fig. 6. Velocity profiles in the GDL for three assigned temperatures; (a) T = 323 K, (b) T = 343 K, (c) T = 363 K.

rent density because the potential loss due to mass transport is more significant at higher temperature that causes the corresponding I-V curve fall faster early than the lower temperature case.

The geometric effect of channel size is a critical factor as well. Here we simply consider the variations of the channel height and the results are demonstrated in Fig. 8 for three assigned values of channel height with the same inlet velocity  $200 \text{ cm s}^{-1}$ . It is found that the limiting current density will be enlarged by an increase of channel height and the cell performance will be raised significantly at high current density. Since the mass flow rate is larger for a higher channel height, the average concentration will increase within the same channel length and results in better cell performance especially at high current density condition.

![](_page_4_Figure_10.jpeg)

Fig. 7. Variation of voltage-current curves with temperature.

![](_page_5_Figure_1.jpeg)

Fig. 8. Variation of voltage-current curves with channel height.

![](_page_5_Figure_3.jpeg)

Fig. 9. Variation of voltage-current curves with inlet pressure.

Similar results also can be obtained for different inlet velocities with a fixed channel height due to the same causes.

Fig. 9 illustrates the variations of I-V curves with three different inlet pressures. From Eq. (3) it is known that the concentration is proportion to the pressure for an isothermal system. Consequently, the cell performance appears to be quite sensitive to the inlet pressure and limiting current density is also approximately proportion to the inlet pressure. This finding suggests that it should be an efficient way to enhance the cell performance by utilizing a high inlet pressure in comparison with the other factors such as temperature and channel height.

#### 4. Conclusions

We have developed a simple two-dimensional model for the mass transport of oxygen within the GDL of PEMFC and accordingly obtained an analytical solution for the distribution of oxygen concentration in GDL. Based on this analytical solution, the influence of GDL on cell performance has been examined and the results indicate that the utilization of GDL indeed produce significant potential losses. Such losses can be improved if one used a thinner GDL or increases the porosity of GDL, and the effect of porosity seems to be more pronounced. The other physical factors including the temperature, channel height, inlet velocity, and inlet pressure are also investigated. It is found that the most efficient way to enhance the cell performance is to increase the inlet pressure since the concentration flux through the GDL to the catalyst layer will greatly increase especially under high current density condition.

Although the system is simplified by some critical assumptions such as to treat the catalyst layer as a thin boundary and neglect the water transport problem, the present model still provides a simple and direct technique to estimate the influence of GDL, and will be helpful for the design work of PEMFC.

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