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Fractal model for prediction of effective thermal conductivity of gas diffusion layer in proton exchange membrane fuel cell

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ABSTRACT

The process of heat transfer within porous media is usually considered as a transport through large numbers of straight channels with uniform pore sizes. For the prediction of effective thermal conductivity of gas diffusion layer (GDL), morphological properties such as the tortuosity of channels and pore-size distribution of this porous layer should be considered. Thus in this article, novel parallel and series-parallel prediction models of effective thermal conductivity for the GDL in proton exchange membrane fuel cell (PEMFC) have been derived by fractal theoretical characterization of the real microstructure of GDL. The prediction of fractal parallel model for carbon paper, a basal material of the GDL, is in good agreement with the reference value supplied by Toray Inc. The prediction results from the proposed models are also reasonable because they are distributed between the upper and lower bounds. Parametric effect has been investigated by using the presented models in dimensionless formalism. It can be concluded that dimensionless effective thermal conductivity (k'_{eff}) has a positive correlation with effective porosity (ε) or the pore-area fractal dimension (D_p) when $k_s/k_g < 1$; whereas it has a negative correlation with ε or D_p when $k_s/k_g > 1$ and with tortuous fractal dimension (D_t) whether $k_s/k_g < 1$ or not. Furthermore, these fractal models have been modified by considering the effect of polytetrafluoroethylene (PTFE) incorporated into the pore spaces of carbon paper, and the corresponding model prediction shows that there is an increase in the effective thermal conductivity due to the filling of PTFE that has high thermal conductivity.

1. Introduction

Thermal conductivity is generally considered as a significant material parameter in the heat transfer within a gas diffusion layer (GDL), which is modeled as a uniform porous medium, and is inevitably used in the thermal simulation of a proton exchange membrane fuel cell (PEMFC). In this article, the process of heat transfer within porous GDL has been investigated and suitable prediction models of effective thermal conductivity have been suggested by fractal theoretical characterization of the real microstructure of GDL.

The complexity of heat transfer in inhomogeneous porous media is due to both solid and fluid phases and random pore morphology. The process of heat transfer follows different patterns for varied pore structures. In general, heat transfer is controlled by the mechanisms of convection, radiation, and conduction.

Convective heat transfer occurs when fluid flows within pores. Generally, the effect of convection is more apparent in the case of large pore sizes, whereas it can be neglected for small pore sizes (<100 μm) at lower temperatures (<373 K) [1] because of lack of intensive fluid-circulation within the pores.

Radiative heat transfer occurs through the adsorptive or radiative heat emission of pore walls. From a study on coal chars, it has been found that the mechanism of radiation has a significant effect on heat transfer through large pore sizes (>10 μm) at high temperatures (>1000 K) [2], whereas for most carbonaceous materials, the effect of radiative heat transfer can be neglected for temperatures below 1000 K.

For the GDL of PEMFCs, because the working temperature is lower than 373 K and because the pore sizes of GDL are smaller than 100 μm [3], neither convection nor radiation is significantly involved. Thus, heat transfer within GDL is controlled only by the mechanism of conduction. Although the process comprises only

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heat conduction, it is still complex because it involves the following three processes:

(1) Heat transport within carbon fiber;
(2) Heat transport within fluid in pores;
(3) Heat transport between connected carbon fibers.

The dominant mode of transfer is determined by the contribution of the solid and fluid phases to thermal conductivity. If the thermal conductivity of the fluid is greater than that of the carbon fibers, the heat transfer through fluid becomes dominant. The complexity of the heat-transfer process is attributed to various factors, such as material properties of the solid phase; shape, size, and size-distribution of pores; and type of component, state, and properties of fluids. In addition, pressure and temperature also have significant effects on heat transfer. Therefore, the exact determination of the effective thermal conductivity is highly difficult.

2. Prediction methods for effective thermal conductivity of porous media

In general, thermal conductivity can be predicted by empirical formulas, numerical simulations, or theoretical models. Table 1 shows some specific values of thermal conductivity, which are derived from experimental measurements [4].

2.1. Empirical formulas

Most of the pure empirical or semiempirical formulas with several empirical constants are derived by polynomial fitting methods [2,5,6]. Generally, these empirical constants do not indicate any specific physical meanings, and their values derived from different researches lack uniformity.

2.2. Numerical simulations

Numerical simulations can be used for the research of heterogeneous media with discrete hierarchies. For the study of a porous medium, it is necessary to build a geometrical model of the porous medium and specify one of the numerical methods, such as finite element method [7], finite difference method [8], or boundary element method [9]. Subsequently, through simulation, thermal conductivity can be predicted and parametric effect can be studied. However, because the geometrical model varies with the microstructure of porous media, it always needs rebuilding for different research objects; moreover, numerical simulation is time-consuming, and this prediction method is unsuitable for fast and convenient prediction of thermal conductivity.

2.3. Theoretical models

Theoretical model prediction of thermal conductivity is carried out by using theoretical expressions. For the theoretical researches on porous media with idealized structures, there are two types of theoretical models, effective medium model and layer model.

Table 1
Various specific values of thermal conductivity

Material	Thermal conductivity ($W m^{-1} K^{-1}$)	Material	Thermal conductivity ($W m^{-1} K^{-1}$)
Silver	4.186×10^2	Hydrogen	0.167
Aluminum	2.093×10^2	Oxygen	0.025
Quartz	8.392	Air	0.026
Sandstone	3.767	Benzene	0.159
Clay	0.837–1.256	Petroleum	0.147
Water	0.461	Glass	0.502–1.088

2.3.1. Effective medium model

Typical effective medium models are sphere, ellipsoid, cube, and tube models.

Hashin and Shtrikman [10] have applied the sphere model, along with the variation principle, to find the upper and lower bounds of the effective magnetic conductivity for a multiphase mixture on the basis of uniform and isotropic assumptions. These bounds are also applicable to the thermal conductivity. Furthermore, the lower bound k_{low} and upper bound k_{upper} can be determined by the following equations:

$$k_{low} = k_1 + \frac{\varepsilon_2}{1/(k_2 - k_1) + \varepsilon_1/3k_1} \quad (1)$$

$$k_{upper} = k_2 + \frac{\varepsilon_1}{1/(k_1 - k_2) + \varepsilon_2/3k_2} \quad (2)$$

where $k_2 > k_1$, they are the widely accepted bounds for uniform and isotropic materials and are dependent only on the volumetric fraction.

Grant and West [11] have adopted a three-dimensional tube unit to emulate a two-phase system and have obtained the effective thermal conductivity k_{eff} as

$$k_{eff} = \frac{1}{3} X_m k_m + (1 - X_m) k_s \quad (3)$$

where k_m and X_m are the thermal conductivity and the volumetric fraction of tubular inclusions, respectively, and k_s is the thermal conductivity of the second phase.

Hsu et al. [12] have used a three-dimensional lumped-parameter model for the derivation of the effective thermal conductivity of spatially periodic porous media and have obtained the following result:

$$\frac{k_{eff}}{k_f} = 1 - \gamma_a^2 - 2\gamma_a\gamma_c + 2\gamma_a^2\gamma_c + \frac{\gamma_a^2\gamma_c^2}{\lambda} + \frac{\gamma_a^2 - \gamma_a^2\gamma_c^2}{1 - \gamma_a + \gamma_a\lambda} + \frac{2(\gamma_a\gamma_c - \gamma_a^2\gamma_c)}{1 - \gamma_a\gamma_c + \gamma_a\gamma_c\lambda} \quad (4)$$

where k_f is thermal conductivity of the fluid phase, $\gamma_a = a/l$, $\gamma_c = c/a$, l and a are the geometrical lengths, c is the contact length, λ represents fluid/solid thermal conductivity ratio.

Every parameter in these effective medium models has a clear physical meaning, but it is difficult to obtain some of the model parameters; moreover, the above models, not the general ones, can be only applied to specific porous media.

2.3.2. Layer model

The parallel or series layer models are widely used for prediction of the effective thermal conductivity of a two-phase system. The effective thermal conductivity k_p can be calculated by the parallel model using the following equation:

$$k_p = k_1\varepsilon_1 + k_2\varepsilon_2 \quad (5)$$

where ε_1 and ε_2 are the volumetric fractions, respectively; and k_1 and k_2 are the effective thermal conductivities of the two phases, respectively.

Using the series model, effective thermal conductivity k_s can be obtained as

$$\frac{1}{k_s} = \frac{\varepsilon_1}{k_1} + \frac{\varepsilon_2}{k_2} \quad (6)$$

Both parallel and series models are usually used for the determination of the upper and lower bounds of the effective thermal conductivity.

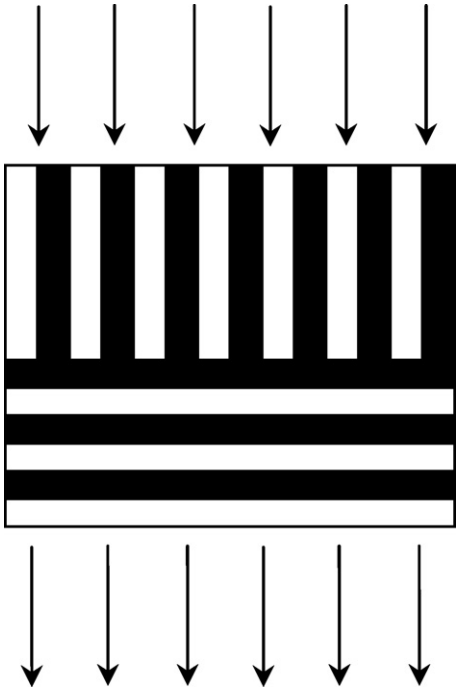

Fig. 1. Porous medium composed of pores in two directions.

For porous media, numerous capillary channels both parallel and perpendicular to the flow direction (Fig. 1) exist; therefore, the effective thermal conductivity can be determined by the series-parallel model:

$$k_{\text{eff}} = \frac{1}{((1-\xi)/k_{\text{p}}) + (\xi/k_{\text{s}})} \tag{7}$$

where ξ is the ratio of the number of perpendicular channels to the total number of channels.

Usually, ideal geometrical models are used for inferential reasoning formulas. Among these models, the straight capillary model with uniform pore sizes is widely used. Because these geometrical models are regularly arranged, they are inapplicable to real porous media with disordered microstructural characteristic.

Thompson et al. [13] have found that real porous media have a fractal characteristic. Several studies have focused on the application of the fractal method to the prediction of effective thermal conductivity [14–19]. It can be accomplished by two methods. One method is the application of fractal geometrical models such as random Sierpinski carpets in the simulation of thermal equations [14,15]. In contrast with the normal volume-average models, the fractal models are more realistic because they consider the disordered characteristic, but the numerical simulation needed in this method is time-consuming. The second method is the application of fractal theoretical models, along with the effective medium and layer-analog methods [15–19]. This method is suitable for both analytical solution and fast prediction. Therefore, this method has been adopted here.

A previous study by the authors has shown that microstructures and pore-size distribution of the GDL in PEMFC have a fractal characteristic [3]. In the following section, the analytical solution model of the effective thermal conductivity is derived on the basis of the fractal description of GDL. Subsequently, the effects of microstructural parameters on effective thermal conductivity are investigated.

3. Fractal model of effective thermal conductivity of GDL in PEMFC

3.1. Fractal parallel model

Experimental investigations on permeation in porous media have shown that the channels through which liquids permeate have fractal characteristics. Similarly, the heat-transfer routes within porous media may also have fractal characteristics and can be represented as random Koch curves. Porous carbon paper, made from graphite fibers, is used for the preparation of the GDL in PEMFC. The heat transfer within GDL is assumed to be similar to that within the tortuous fractal parallel channels with different pore sizes and is depicted in Fig. 2.

The length $L(\lambda)$ of the capillary pathway is related to the capillary size λ (i.e. the pore diameter) by the following fractal relationship [20]:

$$\frac{L(\lambda)}{L_0} = \left(\frac{L_0}{\lambda}\right)^{D_{\text{t}}-1} \tag{8}$$

where L_0 is the representative or linear length of these capillary pathways towards the flowing direction, and D_{t} is the tortuous fractal dimension.

The tortuosity of the capillary pathway τ can be obtained by

$$\tau = \left(\frac{L(\lambda)}{L_0}\right)^2 = \left(\frac{L_0}{\lambda}\right)^{2D_{\text{t}}-2} \tag{9}$$

Another characteristic of porous media is that the cumulative pore population N in a unit cross-section may be mathematically expressed as follows [20]:

$$N(L \geq \lambda) = \left(\frac{\lambda_{\max}}{\lambda}\right)^{D_{\text{p}}} \tag{10}$$

where D_{p} is the pore-area fractal dimension, and λ and $\lambda_{\max}$ are the pore size and the maximum pore size of porous media, respectively. The first derivative of Eq. (10) with respect to λ is

$$-\text{d}N = D_{\text{p}}\lambda_{\max}^{D_{\text{p}}}\lambda^{-(D_{\text{p}}+1)}\,\text{d}\lambda \tag{11}$$

The total area of the unit cell A can be described as follows [21]:

$$A = \frac{\pi D_{\text{p}}\lambda_{\max}^2}{4\varepsilon(2-D_{\text{p}})}\left[1-\left(\frac{\lambda_{\min}}{\lambda_{\max}}\right)^{2-D_{\text{p}}}\right] \tag{12}$$

On the basis of the above fractal descriptions of the GDL, the heat transfer through parallel channels is studied, and than the proposed model is modified by the series-parallel method. A schematic representation of a porous medium with parallel channels is shown in Fig. 3, where ε is the porosity and A is the cross-sectional area perpendicular to the direction of heat flow; then, the effective area of heat transfer for the solid phase is εA. The heat transfer within a porous GDL can be simplified as a transport through parallel channels of the solid and gas phases as shown in Fig. 3, where the parallel gas channels have fractal structure, and R_{g} and R_{s} are the thermal resistances of the gas and solid phase, respectively, k_{g} and k_{s}

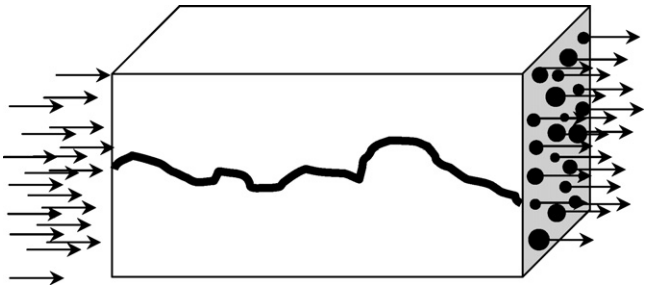

Fig. 2. Effective fractal path of heat transfer.

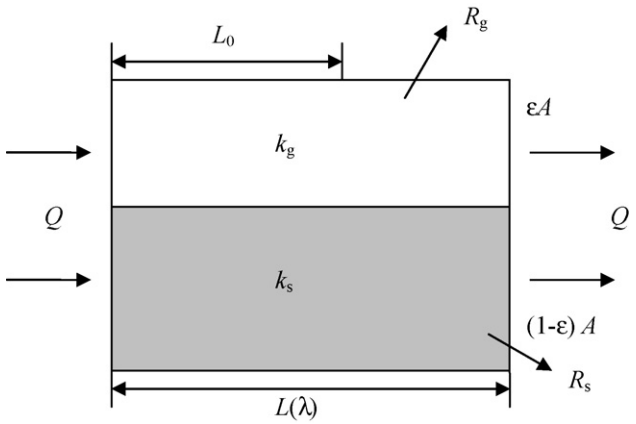

Fig. 3. Parallel paths for the conduction of heat within the gas and solid phases of the GDL.

are their respective thermal conductivities, L_0 indicates the linear lengths of the channels for the transfer of heat flux Q, and $L(\lambda)$ denotes the actual length of the tortuous channel.

First, a fractal parallel model of effective thermal conductivity for the GDL is deduced as follows.

The thermal resistance of a single channel, $R(\lambda)$, can be expressed as

$$R(\lambda) = \frac{L(\lambda)}{A(\lambda)k_g} = \frac{L(\lambda)}{(\pi\lambda^2/4)k_g} = \frac{4L(\lambda)}{\pi\lambda^2 k_g} \tag{13}$$

Furthermore, the number of channels with pore size λ is $-dN$; their parallel thermal resistance $R_N(\lambda)$ can thus be expressed as

$$R_N(\lambda) = \frac{R(\lambda)}{-dN} = \frac{4L(\lambda)}{\pi\lambda^2 k_g D_p \lambda_{max}^{D_p} \lambda^{-(D_p+1)}\, d\lambda} \tag{14}$$

Substituting the definition formula of $L(\lambda)$ into Eq. (14), the following relation is obtained:

$$R_N(\lambda) = \frac{4L_0^{D_t}\lambda^{1-D_t}}{\pi k_g D_p \lambda_{max}^{D_p}\lambda^{1-D_p}\, d\lambda} = \frac{4L_0^{D_t}}{\pi k_g D_p \lambda_{max}^{D_p}\lambda^{D_t-D_p}\, d\lambda} \tag{15}$$

According to the parallel principle of electric resistance, the thermal resistance of the gas phase, R_g, can be calculated by the expression

$$\begin{aligned} R_g &= \frac{1}{\int_{\lambda_{min}}^{\lambda_{max}} 1/R_N(\lambda)} = \frac{1}{\int_{\lambda_{min}}^{\lambda_{max}} (\pi k_g D_p \lambda_{max}^{D_p}\lambda^{D_t-D_p}/4L_0^{D_t})\, d\lambda} \\ &= \frac{4L_0^{D_t}(D_t - D_p + 1)}{\pi k_g D_p \lambda_{max}^{D_t+1}[1-(\lambda_{min}/\lambda_{max})^{D_t-D_p+1}]} \end{aligned} \tag{16}$$

The thermal resistance of the solid phase, R_s, is as follows:

$$R_s = \frac{L_0}{(1-\varepsilon)Ak_s} \tag{17}$$

Thus, the total resistance of the porous medium, R, can be obtained as follows:

$$R = \frac{1}{(1/R_g)+(1/R_s)} = \frac{L_0}{Ak_{eff,p}} \tag{18}$$

where $k_{eff,p}$ is the parallel effective thermal conductivity of the porous GDL, and from Eq. (18), the following expression is derived:

$$\begin{aligned} k_{eff,p} &= \frac{L_0}{A}\left(\frac{1}{R_g}+\frac{1}{R_s}\right) \\ &= \frac{\pi k_g D_p \lambda_{max}^{D_t+1}[1-(\lambda_{min}/\lambda_{max})^{D_t-D_p+1}]}{4AL_0^{D_t-1}(D_t-D_p+1)} + (1-\varepsilon)k_s \end{aligned} \tag{19}$$

Substituting Eq. (12) into Eq. (19), $k_{eff,p}$ is obtained:

$$\begin{aligned} k_{eff,p} &= \frac{\pi k_g D_f \lambda_{max}^{D_t+1}[1-(\lambda_{min}/\lambda_{max})^{D_t-D_p+1}]}{4L_0^{D_t-1}(D_t-D_p+1)} \\ &\quad\times \frac{4(2-D_p)\varepsilon}{\pi D_p \lambda_{max}^2[1-(\lambda_{min}/\lambda_{max})^{2-D_p}]} + (1-\varepsilon)k_s \\ &= \frac{k_g(2-D_p)\varepsilon\lambda_{max}^{D_t-1}[1-(\lambda_{min}/\lambda_{max})^{D_t-D_p+1}]}{L_0^{D_t-1}(D_t-D_p+1)[1-(\lambda_{min}/\lambda_{max})^{2-D_p}]} + (1-\varepsilon)k_s \end{aligned} \tag{20}$$

This is the fractal model of effective thermal conductivity for the GDL based on parallel theory.

When the channels are straight, i.e. $D_t = 1$, substituting this value into Eq. (20), the following relation is obtained:

$$k_{eff,p} = k_g\varepsilon + (1-\varepsilon)k_s \tag{21}$$

It is the general formula for the calculation of effective thermal conductivity for a two-phase parallel system.

The comparison of Eq. (20) with Eq. (21) indicates that their second terms are the same, whereas the first ones are not. Eq. (20) shows that the microstructural parameters affect only the thermal conduction of the gas phase because the fractal characteristics of the pores that have an effect only on gas phase are considered.

From Eq. (20), it also can be observed that the parameters have clear physical meanings and there are no empirical constants. This general theoretical model can be used both for prediction of effective thermal conductivity of two-phase porous systems and for the study of the effect of porosity and other microstructural parameters (such as tortuous fractal dimension D_t and pore-area fractal dimension D_p). From the viewpoint of characterization of microstructure, this fractal model is closer to reality than the common models based on volume average.

3.2. Modification of the fractal parallel model

Because there are channels both parallel and perpendicular to the direction of heat flow within GDL in PEMFCs, both their effects should be considered. For the ultrathin GDL with a thickness of 1.9×10^{-4} m, there may be a few channels perpendicular to the direction of heat transfer. The series theory can be applied to modify the fractal parallel model proposed above and to obtain the effective thermal conductivity of the gas and solid phases in series:

$$k_{eff,s} = \frac{1}{\varepsilon/k_g + (1-\varepsilon)/k_s} \tag{22}$$

Using the series-parallel model, the effective thermal conductivity of the GDL can be expressed as

$$k_{eff} = \frac{1}{((1-\xi)/k_{eff,p}) + (\xi/k_{eff,s})} \tag{23}$$

where ξ is the ratio of the number of perpendicular channels to the total number of channels, with values ranging from 0 to 1.

Eqs. (20), (22), and (23) can be rewritten in terms of dimensionless variables, by dividing both sides of these equations by k_g:

$$\begin{aligned} k'_{eff,p} = \frac{k_{eff,p}}{k_g} &= \frac{(2-D_p)\varepsilon\lambda_{max}^{D_t-1}[1-(\lambda_{min}/\lambda_{max})^{D_t-D_p+1}]}{L_0^{D_t-1}(D_t-D_p+1)[1-(\lambda_{min}/\lambda_{max})^{2-D_p}]} \\ &\quad + (1-\varepsilon)\frac{k_s}{k_g} \end{aligned} \tag{24}$$

$$k'_{eff,s} = \frac{k_{eff,s}}{k_g} = \frac{1}{\varepsilon + (1-\varepsilon)/(k_s/k_g)} \tag{25}$$

$$k'_{eff} = \frac{k_{eff}}{k_g} = \frac{1}{((1-\xi)/k'_{eff,p}) + (\xi/k'_{eff,s})} \tag{26}$$

In the above derivations, the GDL is considered as a two-phase system and a general fractal model has been deduced. Because carbon paper, a basal material of GDL, is always treated with polytetrafluoroethylene (PTFE) before being applied to PEMFC, the effect of the PTFE incorporated into the pore spaces of carbon paper should be considered as follows:

$$k_{\mathrm{eff,p}} = \frac{k_{\mathrm{g}}(2-D_{\mathrm{p}})\varepsilon\lambda_{\max}^{D_{\mathrm{t}}-1}[1-(\lambda_{\min}/\lambda_{\max})^{D_{\mathrm{t}}-D_{\mathrm{p}}+1}]}{L_0^{D_{\mathrm{t}}-1}(D_{\mathrm{t}}-D_{\mathrm{p}}+1)[1-(\lambda_{\min}/\lambda_{\max})^{2-D_{\mathrm{p}}}]} + 0.22k_{\mathrm{s1}} + (0.78-\varepsilon)k_{\mathrm{s2}} \quad (27)$$

$$k_{\mathrm{eff,s}} = \frac{1}{\varepsilon/k_{\mathrm{g}} + 0.22/k_{\mathrm{s1}} + (0.78-\varepsilon)/k_{\mathrm{s2}}} \quad (28)$$

$$k_{\mathrm{eff}} = \frac{1}{((1-\xi)/k_{\mathrm{eff,p}}) + (\xi/k_{\mathrm{eff,s}})} \quad (29)$$

where k_{s1} and k_{s2} are the thermal conductivities of the carbon fiber and PTFE, respectively. The modified equations are suitable for the prediction of the effective thermal conductivity of a GDL.

Eqs. (23), (26), and (29) are all functions of the fractal dimensions D_p, D_t, and other microstructural parameters, among which there is only one empirical constant with a clear physical meaning.

4. Results and discussion

4.1. Fractal prediction of effective thermal conductivities

The effective thermal conductivities k_{eff} can be predicted by Eq. (23) or (29) when air is passed through the samples (two samples are used: sample 'a' is the TGP-H-060 carbon paper; sample 'b' is the TGP-H-060 carbon paper treated with PTFE). Subsequently, a comparison is made between different theoretical models. The parameters of GDL used in the study are listed in Table 2; the values of fractal dimension are derived from scanning electron microscopic micrographs of the two samples.

The fractal parallel model (Eq. (20)) can be used to predict the upper bound of k_{eff} of sample 'a'; the result obtained, $k_{eff} = 1.771\ \mathrm{W\,m^{-1}\,K^{-1}}$, is in good agreement with the reference value supplied by Toray Inc. ($1.7\ \mathrm{W\,m^{-1}\,K^{-1}}$). With this reference value, ξ can be calculated as 0.0008 using Eq. (23), which indicates that the number of perpendicular channels in the GDL is very small. If the effect of the perpendicular channels is ignored, k_{eff} can be predicted by the fractal parallel model, and an error of 4.2% is found between the two models for sample 'a'.

Table 2
Microstructure and material parameters of the samples 'a' and 'b'

Parameter	Sample 'a'	Sample 'b'	Description
λ_{max}	8×10^{-5} m	7×10^{-5} m	Maximum pore diameter
λ_{min}	3.079×10^{-8} m	1.487×10^{-8} m	Minimum pore diameter
Φ	0.78	0.55	Porosity
L_0	1.9×10^{-4} m	1.9×10^{-4} m	Thickness of the gas diffusion layer
k_{s1}	$8\ \mathrm{W\,m^{-1}\,K^{-1}}$	$8\ \mathrm{W\,m^{-1}\,K^{-1}}$	Thermal conductivity of carbon fiber
k_g	$0.02624\ \mathrm{W\,m^{-1}\,K^{-1}}$	$0.02624\ \mathrm{W\,m^{-1}\,K^{-1}}$	Thermal conductivity of gas
k_{s2}	$0.25\ \mathrm{W\,m^{-1}\,K^{-1}}$	$0.25\ \mathrm{W\,m^{-1}\,K^{-1}}$	Thermal conductivity of PTFE
D_p	1.9669	1.9276	Pore area dimension
D_t	1.1447	1.1447	Tortuous dimension

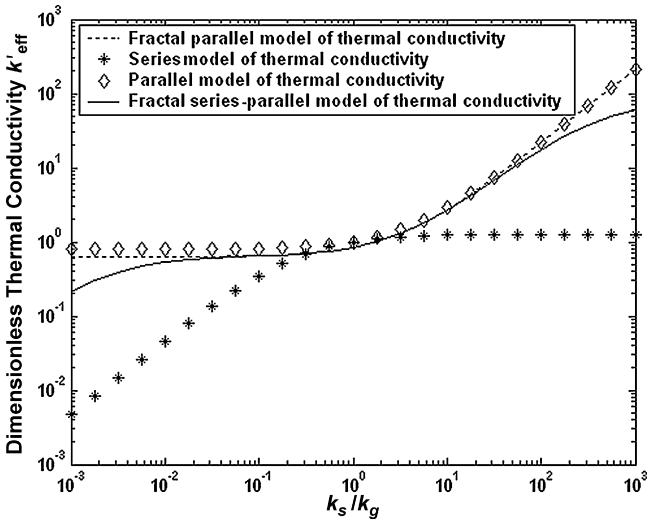

Fig. 4. A comparison of the effective thermal conductivities between the proposed fractal models and the series-parallel layer models.

k_{eff} and its upper bound of sample 'b' are $1.7694\ \mathrm{W\,m^{-1}\,K^{-1}}$ and $1.8251\ \mathrm{W\,m^{-1}\,K^{-1}}$ calculated using Eq. (29) with the value of ξ substituted, and Eq. (27), respectively. If the effect of the perpendicular channels is ignored, k_{eff} can be predicted by the fractal parallel model (Eq. (27)), and there is an error of 3.2% between the two models.

The comparison between the results of the two samples shows that the k_{eff} value of sample 'b' is greater than that of sample 'a'. The increase in k_{eff} is attributed to the filling of PTFE, which has a high thermal conductivity, in the pore space of carbon paper.

Fig. 4 shows the prediction results of the fractal models (Eqs. (24) and (26)) and the series-parallel layer models (Eqs. (5) and (6)), with $\xi = 0.05$. It can be observed that the fractal model prediction results are distributed between upper and lower bounds, indicating the rationality of these models.

4.2. Microstructure parametric effects on effective thermal conductivity

The effect of the microstructural parameters, the pore-area dimension D_p, the tortuous dimension D_t, and porosity ε on k'_{eff} is studied using Eq. (26) with the data of sample 'a'.

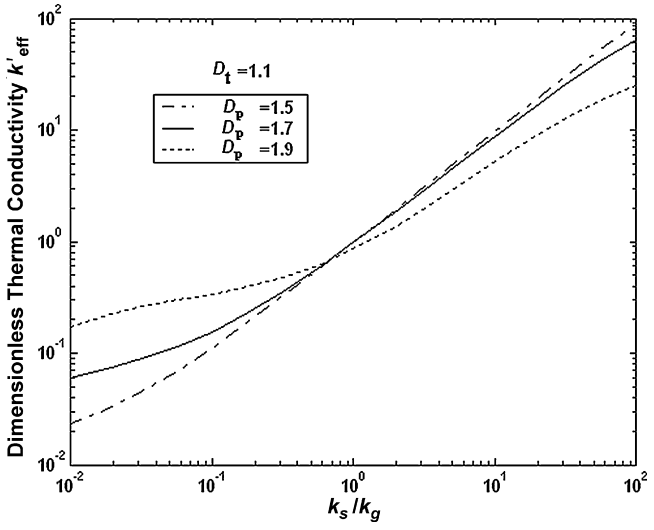

Fig. 5. Effect of D_p on the effective thermal conductivity of carbon paper.

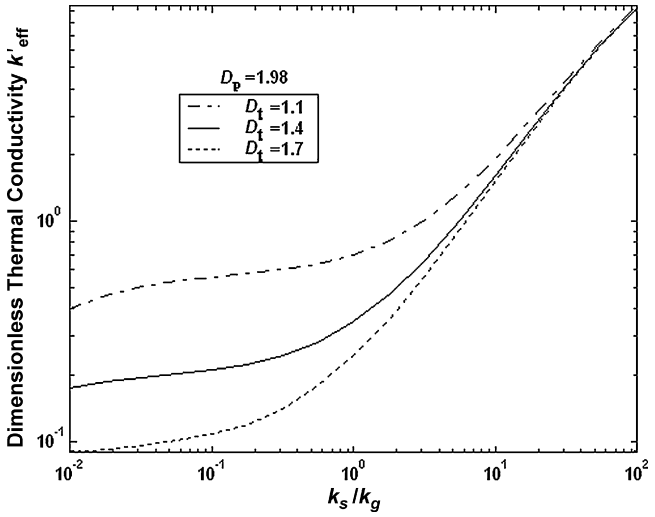

Fig. 6. Effect of D_t on the effective thermal conductivity of carbon paper.

Fig. 5 shows the variation of k'_{eff} with D_p at a fixed value of D_t = 1.1. There are two trends in the variations: k'_{eff} decreases with increase in D_p when $k_s/k_g > 1$, whereas it increases with increase in D_p when $k_s/k_g < 1$. It also can be observed that the effect of D_p on k'_{eff} becomes more significant when $k_s/k_g < 1$ than when $k_s/k_g > 1$. On one hand, the increase in D_p corresponds to the increase of pore area of a representative carbon-paper unit, which leads to an increase in the proportion of the gas phase. On the other hand, the relationship of $k_s/k_g > 1$ indicates that the solid phase has a higher capacity of heat transmission than the gas phase. With the synthesis of the effects of both D_p and k_s/k_g, an important role is detected for the solid phase in heat transfer when $k_s/k_g > 1$, and the decrease in the proportion of the solid phase with the increase in D_p results in the decrease in k'_{eff}; whereas the gas phase plays an important role in heat transfer when $k_s/k_g < 1$ and the increase in proportion of the gas phase with the increase in D_p results in the increase in k'_{eff}.

The variation of k'_{eff} with D_t is plotted in Fig. 6 at a fixed pore-area fractal dimension of D_p = 1.98. It can be observed that k'_{eff} decreases as D_t increases. The decrease in k'_{eff} with increase in D_t is due to the increase in thermal resistance caused by the longer distance of heat transport through more tortuous channels. Furthermore, the effect of D_t on k'_{eff} becomes more significant when $k_s/k_g < 1$ than when $k_s/k_g > 1$. The reason is that D_t has a significant effect on the heat transfer of the gas phase, which plays the leading role when $k_s/k_g < 1$, whereas it becomes insignificant when $k_s/k_g > 1$.

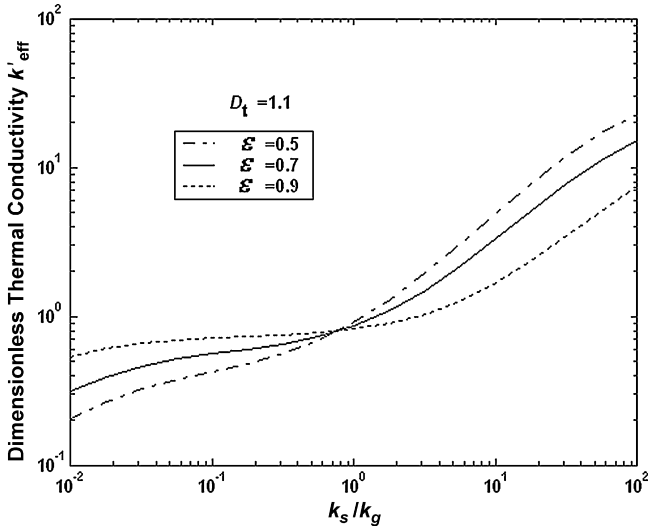

Fig. 7. Effect of porosity on the effective thermal conductivity of carbon paper.

Fig. 7 shows the effect of the porosity ε on k'_{eff}, which is similar to the effect of D_p. There are two trends of variations in this case also: k'_{eff} decreases with increase in ε when $k_s/k_g > 1$, whereas it increases with increase in ε when $k_s/k_g < 1$.

5. Conclusions

A novel fractal prediction model for the effective thermal conductivity of the GDL in a PEMFC was presented by considering the real microstructures with the fractal theory. The prediction of the fractal parallel model for carbon paper, a basal material of GDL, is in good agreement with the reference value supplied by Toray Inc. The prediction results from the proposed models are also reasonable because they are distributed between the upper and lower bounds. By using the fractal series-parallel model, the ratio of the number of perpendicular channels to the total number of channels was obtained as 0.0008, which indicates that few perpendicular channels exist in the GDL; therefore, the fractal parallel model can be used for the prediction of k_{eff} with a low level of error. Moreover, the comparison between the k_{eff} values of two samples showed that there is an increase in the k_{eff} of GDL due to the filling of PTFE, which has a high thermal conductivity.

Finally, the microstructural parametric effect on k'_{eff} was studied using the herein-presented model in dimensionless formalism. It could be concluded that k'_{eff} has a positive correlation with the effective porosity (ε) or pore-area fractal dimension (D_p) when $k_s/k_g < 1$, whereas it has a negative correlation with ε or D_p when $k_s/k_g > 1$ and with tortuous fractal dimension (D_t) whether $k_s/k_g < 1$ or not.

The above fractal models have the following merits: (1) The equations deduced above, except Eqs. (27)–(29), are generally applicable for the prediction of the effective thermal conductivity of two-phase systems. (2) Every parameter in the model has a clear physical meaning. (3) Due to the consideration of the effect of pore-size distribution, this fractal model is more realistic in comparison with empirical formulas and other fractal models. (4) By using this model, it is possible to quantitatively analyze the relationship between the microstructure and the macroscopical material parameters of the GDL.

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References

[1] R. Olives, S. Mauran, Transport Porous Media 43 (2001) 377–394.
[2] L. Onyebueke, M. Feidt, High Temp.-High Press. 24 (1992) 409–414.
[3] Y. Shi, J.S. Xiao, M. Pan, R.Z. Yuan, J. Wuhan Univ. Technol.: Mater. Sci. Ed. 21 (1) (2006) 22–25.
[4] J. Bell, J.S. Li, C.X. Chen, Hydrokinetics of Porous Media, first ed., China Architecture & Building Press, Beijing, 1983, pp. 511–523.
[5] N.H. Abu-Hamdeh, A.I. Khdair, R.C. Reeder, Int. J. Heat Mass Transfer 44 (2001) 1073–1078.
[6] F.B. Nimick, J.R. Leith, J. Heat Transfer 114 (1992) 505–508.
[7] J.K. Carson, S.J. Lovatt, D.J. Tanner, A.C. Cleland, Int. J. Refrigeration 26 (2003) 873–880.

[8] L.J. Davies, P.J. Fryer, Proceedings of the 8th International Congress on Engineering and Food, vol. 5, 2000, pp. 9–13.
[9] B.A. Baltz, M.S. Ingber, Eng. Anal. Bound. Elem. 19 (1997) 3–11.
[10] Z. Hashin, S. Shtrikman, J. Appl. Phys. 33 (1962) 3125–3131.
[11] F.S. Grant, G.F. West, Interpretation Theory in Applied Geophysics, McGraw-Hill Book Company, New York, 1965.
[12] C.T. Hsu, P. Cheng, K.W. Wong, ASME J. Heat Transfer 117 (2) (1995) 264–269.
[13] A.H. Thompson, A.J. Katz, C.E. Krohn, Adv. Phys. 36 (5) (1987) 625–694.
[14] X.L. Huai, W.W. Wang, Z.G. Li, Appl. Therm. Eng. 27 (2007) 2815–2821.
[15] R. Pitchumani, J. Heat Transfer 121 (1999) 163–166.
[16] L.W. Fan, Y.C. Hu, T. Tian, Z.T. Yu, Int. J. Heat Mass Transfer 49 (2006) 4116–4123.
[17] P. Lehmann, M. Stahli, A. Papritz, A. Gygi, H. Fluhler, Transport Porous Media 52 (2003) 313–332.
[18] B.X. Wang, L.P. Zhou, X.F. Peng, Int. J. Heat Mass Transfer 46 (2003) 2665–2672.
[19] Y.P. Cheng, M.H. Shi, J. Therm. Sci. 8 (2) (1999) 102–107.
[20] R. Pitchumani, B. Ramakrishnan, Int. J. Heat Mass Transfer 42 (1999) 2219–2232.
[21] Y. Shi, J.S. Xiao, M. Pan, R.Z. Yuan, J. Power Sources 160 (2006) 277–283.