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# Mathematical Model for Effective Gas Diffusion Coefficient in Multi-scale Fractal Porous Media

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**Abstract.** Based on the capillary hypothesis and fractal theory, a mathematical model for calculating the effective gas diffusion coefficient in porous media is established . By using fractal geometry theory, pore area fractal dimension, tortuosity fractal dimension and pore connectivity are introduced to quantitatively characterize the real internal structure in the porous media . An effective gas diffusion coefficient model for the fractal porous media is derived, and the influence of multi-scale porous media microstructure parameters on the effective gas diffusion coefficient is discussed . The results show that effective gas diffusion coefficient approximates to linearly increase with the increase of porosity, the pore area fractal dimension and the effective gas diffusion coefficient is positive correlation, but the tortuosity fractal dimension is negatively related to it . In the case of different porosities, the gas effective diffusion coefficient varies with the change of the pore diameter ratio, the effective gas diffusion coefficient increases with the increase of pore connectivity .

## 1 Introduction

Gas diffusion in porous media is a fundamental problem in many disciplines and engineering fields. The effective diffusion coefficient is very important for the heat and mass transfer process in porous media. Gas effective diffusion coefficient models usually contain empirical and fitting constants, but few models provide detailed structural information of porous media [1]. The diffusion process of gas in the pores of porous media is mainly affected by the morphological characteristics of its internal pores. The complexity of pore morphology leads to the diffusion process under different transport mechanisms. In the process of mass transfer in the same porous medium, gas diffusion mainly includes volume diffusion, Knudsen diffusion and transition zone diffusion [2]. Therefore, when studying the mass diffusion of gas in porous media, it is necessary to take full account of its morphological characteristics. Most random and disordered porous media have fractal characteristics, and these media are usually called fractal porous media.

Due to the heterogeneity and randomness of the internal structure of porous media, this article is based on the characteristics of microscopic pore structure of porous media. Using fractal theory, a fractal model of the multi-scale pore structure of porous media is constructed. The gas diffusion process under different scale pores in porous media is studied, and the effective gas diffusion coefficient model of fractal porous media is derived. Finally, the influence of porous media microstructure parameters on the effective gas diffusion coefficient is analyzed.

## 2 Pore structure characteristics of porous media

### 2.1 Fractal characteristics of pore size distribution

It is assumed that the porous medium consists of a bundle of curved and parallel capillaries with some connectivity. The cross-sectional area of circular capillary smoothly transitions along the gas diffusion direction, as shown in Fig. 1. In the same cross section, the pore distribution in porous media has fractal characteristics [3]. In porous media, all capillaries and pores have their inlets and outlets in the same plane.

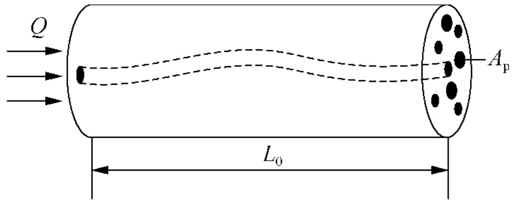


**Fig. 1.** Schematic diagram of porous media structure

The size distribution of capillaries and pores in porous media follows the law of fractal scale. The cumulative number of pores $N$ and the pore diameter $\lambda$ obey the following scaling relationship [4]. Where, $\lambda_{max}$

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is the maximum pore diameter. $D_f$ is the integral dimension of pore surface.

$$N(\lambda)=(\frac{\lambda_{\max}}{\lambda})D_f \tag{1}$$

The number of pores dN with pore diameters in the range of ($\lambda$, $\lambda + d\lambda$) can be expressed as follows. In the equation, $-dN>0$ means that the number of pores increases as pore diameter decreases.

$$-dN=D_f\lambda_{\max}^{D_f}\lambda^{-(D_f+1)}d\lambda \tag{2}$$

Since the pores on the cross-section can be regarded as circles with different diameters $\lambda$, the total pore area $A_p$ on the cross-section of the porous medium can be obtained by using the micro-element method by equation (2). Where, $\lambda$ min is the minimum pore diameter.

$$A_p=-\int_{\lambda_{\min}}^{\lambda_{\max}}\frac{1}{4}\pi\lambda^2dN=\int_{\lambda_{\min}}^{\lambda_{\max}}\frac{1}{4}\pi\lambda^2D_f\lambda_{\max}^{D_f}\lambda^{-(D_f+1)}d\lambda$$
$$=\frac{\pi D_f\lambda_{\max}^2}{4(2-D_f)}[1-(\frac{\lambda_{\min}}{\lambda_{\max}})^{2-D_f}] \tag{3}$$

At the same time, the formula for the total area of cross section of porous media $A$ can be obtained. Where, $\varepsilon$ is plane porosity.

$$A=\frac{A_p}{\varepsilon}=\frac{\pi D_f\lambda_{\max}^2}{4\varepsilon(2-D_f)}[1-(\frac{\lambda_{\min}}{\lambda_{\max}})^{2-D_f}] \tag{4}$$

### 2.2 Pore connectivity

In porous media, different pores are connected with each other. Pore connectivity is an important morphological feature of pore space morphology in porous media. The mass transfer process in porous media is greatly affected by the connectivity of pores. Porous media with the same porosity and the same pore distribution may have very different diffusion coefficients. The better the connectivity of porous media, the greater the diffusion coefficient. In this paper, the pore connectivity distribution is assumed to follow Gaussian normal distribution [5], and the pore connectivity probability density formula is as follows.

$$f(c)=\frac{\partial_c}{\sqrt{2\pi}\sigma_c}e^{-\frac{1}{2}(\frac{c-cm}{\sigma_c})^2} \tag{5}$$

Where, $\partial_c$ is the relative proportionality constant of the distribution; $c$ is the number of connected channels, defined as the number of connected channels with other channels on the same channel, $c > 2$; $C_m$ is the average connectivity number of pores; $\sigma_c$ is the standard deviation of connected number. The change of connectivity number will cause the change of pore connectivity, and then affect the diffusion of components, as shown in Fig. 2.

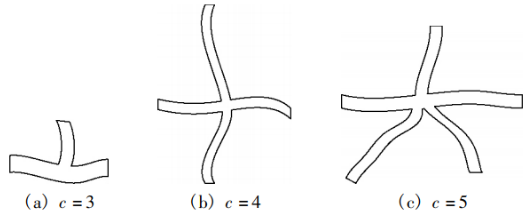


**Fig. 2.** Schematic of different pore connectivity number

### 2.3 Fractal characteristics of tunnel tortuosity

In fractal porous media, curved capillary tubes with smooth cross-sectional area are used to simulate gas channels. The length $L(\lambda)$ and diameter $\lambda$ of the curved capillary tube obey the following fractal relationship.

$$L(\lambda)=\lambda^{1-D_t}L_0^{D_t} \tag{6}$$

In the formula, $L_0$ is the characteristic length of the capillary along the diffusion direction; $D_t$ is the fractal dimension of the pore tortuosity. The tortuosity of pore channel is defined as $\tau = L(\lambda)/L_0$. Substituting it into formula (6), the tortuosity of pore channel can be written as follows. The tortuosity describes the degree of curvature of the flow path in the porous medium.

$$\tau=(\frac{L_0}{\lambda})^{D_t-1} \tag{7}$$

## 3 Mathematical model of effective gas diffusion coefficient

Most of the current research on gas diffusion in porous media involves only one type of diffusion. For the problem of gas diffusion in fractal porous media, the complex pore structure inside the porous media should be the focus. According to the different scales of pore structure, gas diffusion mechanism is classified and studied. There are three kinds of gas diffusion in porous media: volumetric diffusion, Knudsen diffusion and transition diffusion. $K_n$ is defined as the ratio between the characteristic length of space and the free path of gas molecules.

$$K_n=\frac{l}{\lambda} \tag{8}$$

In the formula, $l$ is the free path of gas molecules, $l=k_BT/(\sqrt{2}\pi pd^2)$. Among them, $k_B$ is Boltzmann's constant, $k_B = 1.3806\times10^{-23}$J/K. $T$ is temperature. $p$ is pressure. $d$ is the diameter of gas molecules.

When $Kn<0.1$, that is, pore diameter $\lambda$ is greater than free travel of gas molecules $L$, gas diffusion is completely caused by random movement of molecules independent of wall action. The collision between gas molecules is the main process, so viscous flow predominates. Under this diffusion mechanism, gas diffusion belongs to volumetric diffusion. The flow rate $q_p$ through a single hole can be expressed as the following formula by Hagen-Poiseulle formula.

$$q_p=\frac{\pi\Delta p}{128\mu}\frac{\lambda^4}{L(\lambda)} \tag{9}$$

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When $Kn$>10, the pore diameter $\lambda$ is smaller than the free path $l$ of gas molecules. The collision between gas molecules and pore wall is the main process, so Knudsen diffusion is dominant mechanism. The gas flow rate qk in a single hole can be expressed as the following formula.

$$q_k = \frac{\pi\lambda^3}{12p_m}\sqrt{\frac{8RT}{\pi M}}\frac{\Delta p}{L(\lambda)} \tag{10}$$

When 0.1 <$Kn$<10, the pore diameter of porous medium is closer to free path of gas molecules. The diffusion mechanism of gas is complex and is no longer dominated by a single diffusion mechanism. The gas flow rate $q_{pk}$ passing through a single hole can be expressed as the following equation.

$$q_{pk} = q_p + q_k = \frac{\pi\Delta p}{128\mu}\frac{\lambda^4}{L(\lambda)} + \frac{\pi\lambda^3}{12p_m}\sqrt{\frac{8RT}{\pi M}}\frac{\Delta p}{L(\lambda)} \tag{11}$$

From the analysis of the porous media morphological characteristics, it can be seen that the pores of various sizes exist in the fractal porous media, so the above three kinds of diffusion will occur at the same time. The total flow $Q$ of gas through the cross section of porous medium in the form of diffusion is shown in the following equation.

$$Q = -\int_{\lambda_{\min}}^{\lambda_k} q_k f(c)dN - \int_{\lambda_k}^{\lambda_p} q_{pk} f(c)dN - \int_{\lambda_p}^{\lambda_{\max}} q_p f(c)dN \tag{12}$$

From equations (9) to (12), the following equation can be obtained.

$$Q = C_1\Big[\frac{1}{12p_m(2-D_f+D_t)}\sqrt{\frac{8RT}{\pi M}}\Big(\Big(\frac{10k_BT}{\sqrt{2}\pi pd^2}\Big)^{2-D_f+D_t} - \lambda_{\min}^{2-D_f+D_t}\Big) + \frac{1}{128\mu(3-D_f+D_t)}\Big(\lambda_{\max}^{3-D_f+D_t} - \Big(\frac{0.1k_BT}{\sqrt{2}\pi pd^2}\Big)^{3-D_f+D_t}\Big)\Big]$$

$$C_1 = \frac{\pi\Delta p D_f \lambda_{\max}^{D_f}}{L_0^{D_t}}\frac{\partial_c}{\sqrt{2\pi}\sigma_c}e^{-\frac{1}{2}(\frac{c-cm}{\sigma_c})^2} \tag{13}$$

According to Fick's law, total flow of gas through porous media is shown in the following equation.

$$Q = \frac{AD_{eff}\Delta C}{L_0} \tag{14}$$

In the equation, $D_{eff}$ is the effective diffusion coefficient. $\Delta C$ is the concentration difference between the two ends of the channel, $\Delta C = \Delta p/(RT)$.

From equations (13) and (14), the effective gas diffusion coefficient $D_{eff}$ in fractal porous media is the following equation.

$$D_{eff} = C\Big[\frac{1}{12p_m(2-D_f+D_t)}\sqrt{\frac{8RT}{\pi M}}\Big(\Big(\frac{10k_BT}{\sqrt{2}\pi pd^2}\Big)^{2-D_f+D_t} - \lambda_{\min}^{2-D_f+D_t}\Big) + \frac{1}{128\mu(3-D_f+D_t)}\Big(\lambda_{\max}^{3-D_f+D_t} - \Big(\frac{0.1k_BT}{\sqrt{2}\pi pd^2}\Big)^{3-D_f+D_t}\Big)\Big]$$

$$C = \frac{4RT_\varepsilon(2-D_f)\lambda_{\max}^{D_f-2}}{L_0^{D_t-1}\Big[1-\Big(\frac{\lambda_{\min}}{\lambda_{\max}}\Big)^{2-D_f}\Big]}\frac{\partial_c}{\sqrt{2\pi}\sigma_c}e^{-\frac{1}{2}(\frac{c-cm}{\sigma_c})^2} \tag{15}$$

Equation (15) is the calculation model of the effective gas diffusion coefficient in the range of different Knudsen numbers.

# 4 Results and analysis

## 4.1 Model validation

The predicted value of the proposed multi-scale fractal porous media gas effective diffusivity model is compared with the existing experimental data of different porous media samples [6]. Sample parameters are shown in Table 1.

**Table 1.** Sample parameters

| Parameters | Value |
|---|---|
| $\Lambda_{max}/\mu m$ | 90 |
| $\mu/\mu Pa\cdot s$ | $8.8\times10^{-6}$ |
| $p/kPa$ | 101.325 |
| $T/K$ | 293 |
| $d/nm$ | 0.274 |

Substituting the sample parameters in Table 1 into equations (15) ~ (17), the effective gas diffusion coefficient Deff can be calculated. Figure 3 shows the comparison between the predicted value of gas effective diffusion coefficient model established in this paper and the experimental data of Currie [6]. It can be seen from the figure that predicted value is in good agreement with experimental data. It is also found that effective diffusion coefficient increases linearly with the increase of plane porosity.

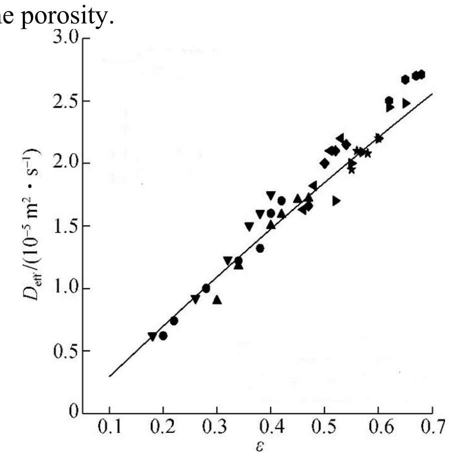


**Fig. 3.** Comparison of model predictions with experimental data

### 4.2 Analysis of influencing factors

This section mainly analyzes the influence of microscopic pore structure characteristic parameters on gas effective diffusion coefficient model established. Figure 4 shows the variation curve of effective gas diffusion coefficient $D_{eff}$ with pore area fractal dimension $D_f$ when porosity is 0.4. It can be found that the effective gas diffusion coefficient $D_{eff}$ increases with the increase of pore area fractal dimension $D_f$. It can also be seen from Figure 4 that the larger the fractal dimension of pores tortuosity, the smaller the effective gas diffusion coefficient, which is consistent with actual situation.

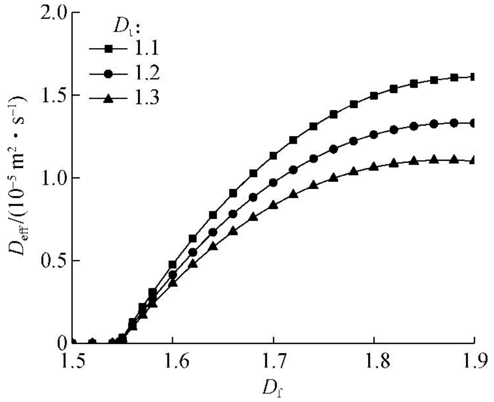


**Fig. 4.** Effect of fractal dimension of pore area $D_f$ on the effective gas diffusion coefficient $D_{eff}$

Fig. 5 shows the variation of effective diffusion coefficient $D_{eff}$ with the fractal dimension of tunnel tortuosity $D_t$. It can be seen from figure that $D_{eff}$ decreases monotonously as $D_t$ increases.

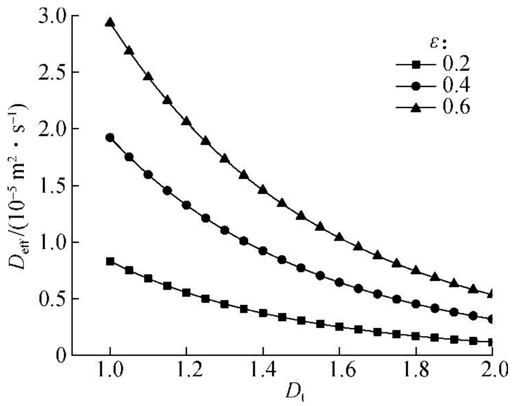


**Fig. 5.** Effect of the tortuosity fractal dimension $D_t$ on the effective gas diffusion coefficient $D_{eff}$

Fig. 6 shows the variation of effective gas diffusion coefficient DEFF with the minimum and maximum pore diameter ratio under different porosity conditions (Dt value is 1.1).

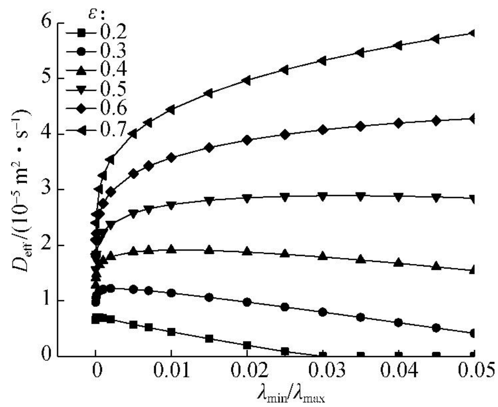


**Fig. 6.** Effect of pore minimum/maximum diameter ratio $\lambda_{min}/\lambda_{max}$ on the effective gas diffusion coefficient $D_{eff}$

It can be seen from the above analysis that, based on the capillary hypothesis, the effective diffusion coefficient model of gas in multi-scale fractal porous media established in this paper can better reveal the mechanism of gas diffusion than the traditional model.

## 5 Conclusion

The effective gas diffusion coefficient $D_{eff}$ increases approximately linearly with the increase of the plane porosity $\varepsilon$. The effective gas diffusion coefficient $D_{eff}$ increases with the increase of pore area fractal dimension $D_f$, and decreases with the increase of pore tortuosity fractal dimension $D_t$.

In the case of different porosity $\varepsilon$, the variation trend of $D_{eff}$ is different with minimum/maximum pore diameter ratio.

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