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A MINI-REVIEW ON THE FRACTAL-MONTE CARLO METHOD AND ITS APPLICATIONS IN POROUS MEDIA

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ABSTRACT
Porous media are abundant in nature such as soil, rocks, sandstones, oil/gas//water reservoirs, biological tissue and organics, etc., and in many sciences and engineering applications. Since microstructures of porous media are extremely complicated, this makes very difficult to predict the transport properties such as thermal conductivities and permeabilities of porous media by analytical solutions based on Euclid geometry. Usually, numerical simulations such as control volume method, molecular dynamics and Lattice Boltzmann method are often applied. However, results numerical simulations are often correlated as empiric expressions which usually contain one or more empiric constants. Fortunately, many researchers found that the microstructures of porous media have the fractal characters, and transport properties such as thermal conductivities, permeabilities, and gas diffusion coefficients in porous media could be found by applying the fractal geometry theory and technique. In this review, the fractal geometry theory combined with the Monte Carlo method are summarized, and then the current research progresses in several areas are reviewed, including in the areas of permeabilities, thermal conductivities, thermal conductivities of nanofluids, rough surfaces, gas diffusivities and boiling heat transfer etc. Finally, some comments are made regarding the future possible applications.

Keywords: Fractal, Monte-Carlo Method, Porous media, Transport properties.

INTRODUCTION
Transport properties such as permeability, thermal conductivity, electric conductivity and diffusivity in porous media, both saturated and unsaturated, have received steadily attention in the past decades. Since the microstructures of real porous media are usually disordered and extremely complicated, this makes it very difficult to analytically find the transport properties of porous media. Conventionally, transport properties of porous media were found by experiments [1-4] and numerical simulations such as the lattice gas (LG) [5], Lattice Boltzmann method (LBM) [6-7], finite element method [8-9] and commercial CFD soft wares (such as the fluent flow solver [10], and these simulations were based on Euclid geometry.

However, the results from either experiments or numerical simulations based on Euclid geometry are usually expressed as correlations with one or more empirical constants, and the mechanisms behind these empirical constants are not revealed. Therefore, seeking an analytical solution of transport properties of porous media becomes a challenging task.

Fortunately, it has been shown that natural porous media and some synthetic materials have been proved to be fractal objects [11-15].

In the past three decades, fractal geometry and technique have received considerable attention due to its wide applications in sciences and technologies such as physics, mathematics, geophysics, oil recovery, material science and engineering. In this mini-review, recent advances are summarized in the area of transport properties of fractal porous media by fractal-Monte Carlo theory and technique, including a brief summary of the fractal-Monte Carlo theory and technique, and their applications. A few of comments is made with respect to the theoretical studies in the future. In the next section, the fractal-Monte Carlo theory for porous media is summarized first.

NOMENCLATURE

A	=	Cross-sectional area
b	=	Second Letter in English Alphabet
d	=	The Euclidean dimension
D_f	=	Fractal dimension for pore space
D_T	=	Fractal dimension for tortuosity
G	=	Geometry factor
K	=	Permeability
L	=	Length
N	=	Number of pores/particles

P = Pressure
q = Flow rate through a capillary
Q = Total flow rate through a set of fractal Capillaries
R = Random number

Greek Symbols

λ = Diameter of pore or particle
ϕ = Effective porosity

Subscripts

av = Average
max = Maximum
min = Minimum
p = Pore

1 Theory for Fractal-Monte Carlo method for porous media

The size distribution of pores or particles in porous media exhibits the fractal scaling law as [14,15]

$$N(L \geq \lambda) = (\lambda_{\max} / \lambda)^{D_f} \quad (1)$$

where D_f is the fractal dimension for pores/particles, $1 < D_f < 2$ (or 3) in two (or three) dimensions, and $\lambda_{\max}$ is the maximum pore/particle diameter. Eq. (1) describes that the cumulative number of pores/particles, whose sizes (*L*) are greater than or equal to the diameter λ, follows the scaling law by Eq. (1).

Eq. (1) can be considered as continuous and differentiable function, differentiating equation (1) with respect to λ results in the number of pores/particle whose sizes are within the infinitesimal range λ to $\lambda + d\lambda$, i.e.

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

where $d\lambda > 0$ and $-dN > 0$.

The total number of pores/particles, from the smallest diameter $\lambda_{\min}$ to the largest diameter $\lambda_{\max}$, can be obtained from Eq. (1) as

$$N_t(L \geq \lambda_{\min}) = (\lambda_{\max} / \lambda_{\min})^{D_f} \quad (3)$$

Dividing Eq. (2) by Eq. (3) gives

$$-dN / N = D_f \lambda_{\min}^{D_f} \lambda^{-(D_f+1)} d\lambda = f(\lambda) d\lambda \quad (4)$$

where $f(\lambda) = D_f \lambda_{\min}^{D_f} \lambda^{-(D_f+1)}$ is the probability density function and $f(\lambda) \geq 0$.

Patterned after the probability theory, the probability density function $f(\lambda)$ should satisfy the following normalization relationship, i.e.

$$\int_{\lambda_{\min}}^{\lambda_{\max}} f(\lambda) d\lambda = 1 - (\lambda_{\min} / \lambda_{\max})^{D_f} \equiv 1 \quad (5)$$

Eq. (5) shows that Eq. (5) holds if and only if [16]

$$(\lambda_{\min} / \lambda_{\max})^{D_f} \cong 0 \quad (6)$$

is satisfied. Eq. (6) implies that $\lambda_{\min} << \lambda_{\max}$ must be satisfied for fractal analysis of a porous medium, and Eq. (6) can be considered as a criterion whether a porous medium can be characterized by fractal theory and technique.

The cumulative probability (*R*) in the range of $\lambda_{\min} \sim \lambda$ can be found by

$$R(\lambda) = \int_{\lambda_{\min}}^{\lambda} f(\lambda) d\lambda = 1 - (\lambda_{\min} / \lambda)^{D_f} \quad (7)$$

Eq. (7) indicates that $R = 0$ as $\lambda \to \lambda_{\min}$ and $R \approx 1$ as $\lambda \to \lambda_{\max}$. Since the pore size λ in a porous medium is randomly distributed in the range of $\lambda_{\min} \sim \lambda_{\max}$, *R* in Eq. (7) is in the range of 0~1. This corresponds to a set of random numbers of 0~1.

From Eq. (7), we can obtain

$$1 - R = (\lambda_{min} / \lambda)^{D_f} \quad (8)$$

From Eq. (8), the diameter λ of a pore/particle can be rewritten as

$$\lambda = \frac{\lambda_{min}}{(1-R)^{1/D_f}} \quad (9)$$

where $\lambda_{\min} \leq \lambda \leq \lambda_{\max}$. Eq. (9) is a probability model for pore/particle size in simulations. For the i^{th} pore or capillary/particle chosen randomly, Eq. (9) can be written as [17]

$$\lambda_i = \frac{\lambda_{\min}}{(1-R_i)^{1/D_f}} = \left(\frac{\lambda_{\min}}{\lambda_{\max}}\right) \frac{\lambda_{\max}}{(1-R_i)^{1/D_f}} \quad (10)$$

where *i = 1 ,2, 3, ..., J*, and *J* is the total number of Monte Carlo simulations in one run for a given porosity. Eq. (9) or (10) presents an explicit model for pore size distribution in porous media. Eq. (10) denotes that since R_i is a random number of 0~1 produced by computer, thus, the pore size λ_i is determined randomly, and this also simulates the randomness and fractal distribution of pore/particle sizes in porous media. Because Eq. (10) is based on Eq. (1), the pore/particle sizes are not only randomly distributed but also follow the fractal scaling law Eq. (1).

In Eq. (10) the fractal dimension D_f for saturated porous media is given by [16]

$$D_f = d - \frac{\ln \phi}{\ln(\lambda_{min} / \lambda_{max})} \quad (11)$$

where ϕ is the effective porosity of porous media, *d* is the Euclidean dimension, and *d = 2* and *3* refer to the two- and three-dimensional spaces, respectively.

Eqs. (1)-(11) form the theoretical base of the Fractal-Monte Carlo method for simulations of transport properties in porous media, and this will be reviewed in the next section.

2 Applications of the Fractal-Monte Carlo method

2.1 Applications in permeabilites in fractal porous media

The permeability is usually determined by Darcy's law:

$$Q = A\frac{K}{\mu}\frac{\Delta P}{L} \tag{12}$$

where *Q*, *A*, K, ΔP, *L* and μ represent the fluid flow rate, cross sectional area, permeability, pressure drop, distance and fluid viscosity, respectively.

The fluid flow rate through a tortuous capillary is described by modifying the well known Hagen-Poiseulle equation [18] as

$$q(\lambda) = G\frac{\Delta P}{L_t(\lambda)}\frac{\lambda^4}{\mu} \tag{13}$$

where *G* is the geometry factor for flow through a capillary, and $L_t(\lambda)$ is the tortuous length along of a capillary and can be given by [14,15]

$$L_t(\lambda) = \lambda^{1-D_T} L_0^{D_T} \tag{14}$$

where D_T is the tortuosity fractal dimension with $1 < D_T < 2$ (or 3) in two (or three) dimensions and L_0 is the straight distance along the flow direction.

The total flow rate *Q* for flow through a unit cell with total cross-sectional area *A* can be obtained by adding the individual flow rates, $q(\lambda_i)$. Based on Eqs. (10) and (13), the total flow rate *Q* can be obtained as

$$\begin{aligned} Q &= \sum_{i=1}^{J} q(\lambda_i) = \sum_{i=1}^{J} G\left(\frac{\Delta P}{L_0}\frac{A}{\mu}\right)\frac{L_0^{1-D_T}}{A}\lambda_i^{3+D_T} \\ &= G\left(\frac{\Delta P}{L_0}\frac{A}{\mu}\right)\frac{L_0^{1-D_T}}{A}\sum_{i=1}^{J}\lambda_i^{3+D_T} \end{aligned} \tag{15}$$

where L_0 is the representative length of a unit cell and approximated by

$$L_0 = \sqrt{A} \tag{16}$$

Eq. (16) implies that a cubic sample is assumed.

Comparing to Darcy's law, we obtain the permeability expression as follows:

$$K = G\frac{L_0^{1-D_T}}{A}\sum_{i=1}^{J}\lambda_i^{3+D_T} \tag{17}$$

Due to Eqs. (10) and (16), Eq. (17) can be rewritten as

$$K = GA^{-(1+D_T)/2}\left(\frac{\lambda_{\min}}{\lambda_{\max}}\right)^{3+D_T}\lambda_{\max}^{3+D_T}\sum_{i=1}^{J}\frac{1}{(1-R_i)^{(3+D_T)/D_f}} \tag{18}$$

Eq. (18) is the probability model for the effective permeability. Eq. (18) indicates that the permeability is a function of parameters *A*, $\lambda_{\min}$, $\lambda_{\max}$, D_T, D_f and random number R_i. Once the parameters *A*, $\lambda_{\min}$, $\lambda_{\max}$, D_T and D_f are determined, the permeability *K* can be calculated by Monte Carlo simulation through choosing a set of random numbers, R_i, *i = 1, 2, 3, ... J.*

The total cross sectional area *A* (in Eq. (18)) of a unit cell is related to porosity by

$$A = A_p / \phi \tag{19}$$

where A_p is the total pore area in a unit cell and determined by

$$A_p = \sum_{i=1}^{J} a_i = \sum_{i=1}^{J} \pi\lambda_i^2 / 4 \tag{20}$$

where a_i is the area of cross section of the i^{th} capillary chosen by Monte Carlo simulation through Eq. (10). It can be seen that the total cross sectional area *A* in this model can be determined by Eqs. (19) and (20) by the Monte-Carlo method if porosity ϕ is given.

The fractal dimension D_T for tortuous capillaries is usually determined by the box-counting method [19] or by [20]

$$D_T = 1 + \frac{\ln\{[\tau_{av}(D_f + D_T - 1)]/D_f\}}{ln(L_0/\lambda_{\min})} \tag{21}$$

where τ_{av} is the average tortuosity for tortuous flow paths, which can be determined by [21]

$$\tau_{av} = \frac{1}{2}[1 + \frac{1}{2}\sqrt{1-\phi} + \sqrt{1-\phi}\cdot\frac{\sqrt{(\frac{1}{\sqrt{1-\phi}}-1)^2 + \frac{1}{4}}}{1-\sqrt{1-\phi}}] \tag{22}$$

The fractal dimension D_T for tortuous streamlines/capillaries can be also determined by [22]

$$D_T = 1 + \frac{\ln \tau_{av}}{\ln(L_0/\lambda_{av})} \tag{23}$$

where λ_{av} is the average diameter of capillaries and can be found from [36].

$$\lambda_{av} = \int_{\lambda_{\min}}^{\lambda_{\max}} \lambda f(\lambda) d\lambda = \frac{D_f}{D_f - 1}\lambda_{\min}\left[1 - \left(\frac{\lambda_{\min}}{\lambda_{\max}}\right)^{D_f - 1}\right] \tag{24}$$

The above Eqs. (13)-(24) form the probability model for the effective permeability of porous media.

2.2 The Algorithm for the effective permeability

The algorithm for determination of the permeability of a porous medium is summarized as follows:

1. Given a porosity ϕ, determine D_f from Eq. (11) if $\lambda_{\min}/\lambda_{\max}$ is determined; or determine $\lambda_{\min}/\lambda_{\max}$ if D_f is determined.
2. After $\lambda_{\min}/\lambda_{\max}$ is found, find $\lambda_{\max}$ if $\lambda_{\min}$ is known.
3. Produce a random number R_i of 0~1 by the Monte-Carlo method.
4. Calculate λ_i by Eq. (10) and find A_p from Eq. (20).
5. If $\lambda_i > \lambda_{\max}$, return to procedure 4, otherwise continue to the next step.

6. Find A from Eq. (19).
7. Find L_0 from Eq. (16).
8. Find λ_{av} from Eq. (24) and find τ_{av} from Eq. (22), then find D_T from Eq. (23).
9. Calculate the permeability K from Eq. (18).

Steps 4~9 are repeated for calculation of permeability until a converged value is obtained at a given porosity. Step 5 means that the randomly produced pore size λ_i in Monte Carlo simulation is not allowed to exceed the maximum pore size $\lambda_{\max}$ in order to coincide with physical situation.

The convergence criterion is that when the following condition is satisfied,

$$A_J = A_p / \phi > A \tag{25}$$

stop the simulation and record the final/convergent permeability and the total simulated number (J) in one run for a given porosity. In Eq. (25), A_J is the total area calculated after the J^{th} computation in one run and A is given by Eq. (19). If the converged permeability is obtained in one run, set the permeability as K_n (n =1, 2, 3,….N). Then the averaged permeability for a given porosity can be calculated by

$$< K >= \frac{1}{N} \sum_{n=1}^{N} K_n \tag{26}$$

where N is the total number of runs at a given porosity.

Figure 1 shows the simulated permeabilities by the Monte Carlo method in 1000 runs at porosity 0.60 for a bi-dispersed porous medium [17]. It is seen that the pores are randomly chosen, and the rough fluctuations of the permeabilities are observed. The converged permeabilities can be obtained as long as the enough number of runs of simulations is performed.

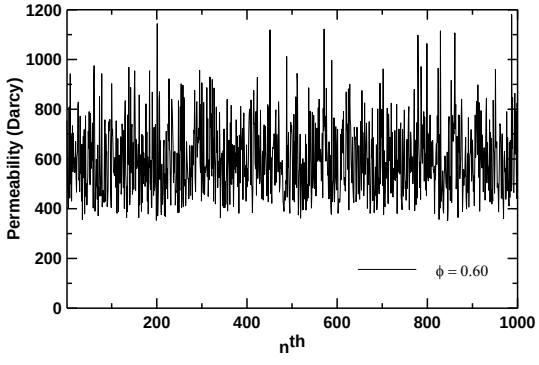

Figure 1: The simulated permeabilities by the Monte Carlo method in 1000 runs at porosity 0.60.

In this Monte Carlo simulation, there is no empirical constant involved and every parameter in the simulation has clear physical meaning.

2.3 Other applications

Xiao et al. [23] applied the fractal-Monte Carlo method to predict the relative permeability of unsaturated porous media by considering the effect of capillary pressure, saturation, and tortuosity of capillaries.

Xu et al. [24] simulated the plane-radial seepage flow toward a well in fractured reservoir engineering. Vadapalli et al. [25] also applied the fractal-Monte Carlo method to estimate the permeabilities at different zones of sandstone reservoirs in India.

In addition, this method was applied to simulate thermal conductivities of nanofluids [26], electrical properties [27], and modeling of rough surfaces [28].

CONCLUSIONS

In this min-review, the Fractal-Monte Carlo method has been reviewed regarding its theoretical basis and algorithm as well as its applications in simulations of the permeability, thermal conductivities of nanofluids, dielectric constant of porous ultra low-k dielectrics, and roughened surfaces. It is expected that this method may also have the potential in other applications such as thermal conductivity and electric conductivity of saturated and unsaturated fractal porous media, transport properties of fractured media, heat transfer of dropwise condensation on surfaces, boiling heat transfer, radiation heat transfer on fractal surfaces etc.

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