THREE-DIMENSIONAL HAUSDORFF DERIVATIVE DIFFUSION MODEL FOR ISOTROPIC/ANISOTROPIC FRACTAL POROUS MEDIA

by

Wei CAI[a], Wen CHEN[b*], and Fajie WANG[b]

[a] State Key Laboratory of Hydrology-Water Resources and Hydraulic Engineering,
College of Mechanical and Electrical Engineering, Hohai University, Changzhou, China
[b] State Key Laboratory of Hydrology-Water Resources and Hydraulic Engineering,
Institute of Soft Matter Mechanics, College of Mechanics and Materials, Hohai University,
Nanjing, China

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The anomalous diffusion in fractal isotropic/anisotropic porous media is characterized by the Hausdorff derivative diffusion model with the varying fractal orders representing the fractal structures in different directions. This paper presents a comprehensive understanding of the Hausdorff derivative diffusion model on the basis of the physical interpretation, the Hausdorff fractal distance and the fundamental solution. The concept of the Hausdorff fractal distance is introduced, which converges to the classical Euclidean distance with the varying orders tending to 1. The fundamental solution of the 3-D Hausdorff fractal derivative diffusion equation is proposed on the basis of the Hausdorff fractal distance. With the help of the properties of the Hausdorff derivative, the Huasdorff diffusion model is also found to be a kind of time-space dependent convection-diffusion equation underlying the anomalous diffusion behavior.

Key words: *anomalous diffusion, Hausdorff derivative, fundamental solution, Hausdorff fractal distance*

Introduction

In recent years, the anomalous diffusion has been widely observed, such as pollutant and gas transport in porous media [1, 2]. The phenomenon is believed to behave as a non-Markovian process, induced by the heterogeneity of the transmission media. The mean square displacement for anomalous diffusion process exhibits $<x^2>\propto t^\alpha$ with $\alpha \neq 1$, which is beyond the description of the well-known classical diffusion model [3].

Recently, fractional calculus has been recognized as an efficient tool for modeling the observed anomalous diffusion [4, 5]. Various fractional diffusion models have been proposed accompanied by the numerical simulation, such as the time- and space-fractional diffusion model, and the tempered fractional diffusion model [6-8]. However, the fractional calculus operator is non-local, which will bring in large computational costs [9, 10]. In addition, the underlying relationship between the fractional order and the fractal dimensionality of the porous media remains not clear.

The Hausdorff fractal derivative, as an alternative modeling tool, has also been employed to describe the anomalous diffusion [11]. Numerical results revealed that the

* Corresponding author, e-mail: chenwen@hhu.edu.cn

Hausdorff fractal derivative models well describe the anomalous diffusion and save the computational costs due to its local property [3, 11]. It should also be mentioned that the Hausdorff derivative is directly related to the fractal dimension with clear physical meaning [12, 13]. Nowadays, it has been successfully applied to other research fields, such as rheology [14], magnetic resonance imaging [15, 16], and heat conduction [17]. It should be pointed out that the Hausdorff derivative for differentiable functions is formally similar to the definition of conformable derivative, which has been well numerically investigated [18, 19] .

Nevertheless, the existing Hausdorff fractal diffusion is limited in the 1-D case [11], and the exploration on physical modeling of the distance in complex materials is still on the way. This paper will propose the 3-D diffusion model on the basis of the Hausdorff fractal derivative and derive the corresponding fundamental solution.

Physical interpretation of Hausdorff derivative

It has been well known that the mass, m, of a 1-D media can be characterized:

$$m = \int_{x_1}^{x_2} \rho(x)\mathrm{d}x \tag{1}$$

where $\rho(x)$ represents the linear density, and x_1 and x_2 ($x_2 > x_1$) are the locations of two ends of the media. In terms of the fractal media, the mass is directly related to the power function of the length metric l [12, 20]:

$$m \propto l^{\beta} \tag{2}$$

where β is the fractal dimension of the given media. The integral formulation of eq. (2) can be formulated:

$$m = \int_{x_1}^{x_2} \rho(x)\mathrm{d}x^{\beta} \tag{3}$$

The Hausdorff derivative in space has been proposed by Chen [21]:

$$\frac{\mathrm{d}m}{\mathrm{d}x^{\beta}} = \lim_{x \to x'} \frac{m(x) - m(x')}{x^{\beta} - x'^{\beta}} = \frac{1}{\beta x^{\beta-1}} \frac{\mathrm{d}m}{\mathrm{d}x} \tag{4}$$

Similarly, the time Hausdorff derivative is stated:

$$\frac{\mathrm{d}l}{\mathrm{d}t^{\alpha}} = \lim_{x \to x'} \frac{l(t) - l(t')}{t^{\alpha} - t'^{\alpha}} = \frac{1}{\alpha t^{\alpha-1}} \frac{\mathrm{d}l}{\mathrm{d}t} \tag{5}$$

where α is the fractal dimensionality in time and l represents the length. It is obvious that the eq. (3) is the integral form of the space Hausdorff derivative, which in turn validates the ability of Hausdorff derivative to characterize fractal media. Thus, the order of space Hausdorff derivative is directly related to the fractal dimensionality. Moreover, the eq. (4) is formally similar to the definition of fractal derivative proposed by Tarasov [20] without the absolute value sign, which ensures the physical meaning of the order of Hausdorff derivative.

The Hausdorff derivative, *i. e.*, eqs. (4) and (5), are firstly proposed via using the following metric transforms [21]:

$$\begin{cases} \hat{t} = t^{\alpha} \\ \hat{x} = x^{\beta} \end{cases} \tag{6}$$

which is directly due to the fractal invariance and fractal equivalence. It should also be pointed out that the uniform mass of the 3-D fractal media is defined [12]:

$$m = \rho l^{\beta} = \rho l^{\beta_1+\beta_2+\beta_3} = \rho l^{\beta_1} l^{\beta_2} l^{\beta_3} \tag{7}$$

where β_1, β_2, and β_3 represent the fractal dimensionality along three different directions.

Generalized non-Euclidean Hausdorff fractal distance

In the Euclidean space, $\mathbf{R}^n$, the distance between the two points $\mathbf{X}(x_1, x_2, ..., x_n)$ and $\mathbf{Y}(y_1, y_2, ..., y_n)$ is usually named as Euclidean distance. The well-known 2-norm Euclidean distance is defined:

$$r = \sqrt{\sum_{i=1}^{n} |x_i - y_i|^2} \tag{8}$$

where $i \in [1, n]$. However, the fractal media is considered to be discontinuous, thus the traditional distance may be not suitable. Usually, the method of scaling transformation is employed to investigate the fractal media, which is also known as the fractal metric. On the basis of scaling transformation, we consider the following mapping $\mathbf{X}(x_1, x_2, ..., x_n) \rightarrow \mathbf{X}'(x_1^{\beta}, x_2^{\beta}, ..., x_n^{\beta})$. The distance between two points with the new metric in the 3-D case can be found in the following formulation:

$$d\left(\mathbf{X}', \mathbf{Y}'\right) = r^{\beta} = \sqrt{\left(x_1^{\beta} - y_1^{\beta}\right)^2 + \left(x_2^{\beta} - y_2^{\beta}\right)^2 + \left(x_3^{\beta} - y_3^{\beta}\right)} \tag{9}$$

It should be stressed that the points **X** and **Y** are located in the first quadrant via choosing the suitable co-ordinate system. In this way, arbitrary element in the fractal metric $\mathbf{X}'(x_1^{\beta}, x_2^{\beta}, ..., x_n^{\beta})$ is ensured to be real number. Obviously, it is easy to verify that the eq. (9) obeys the three fundamental rules for the definition of distance: $d(\mathbf{X}', \mathbf{Y}') = d(\mathbf{Y}', \mathbf{X}')$, $d(\mathbf{X}', \mathbf{Y}') \geq 0$, and $d(\mathbf{X}', \mathbf{Y}') \leq d(\mathbf{X}', \mathbf{Z}') + d(\mathbf{Z}', \mathbf{Y}')$. Hence, $d(\mathbf{X}', \mathbf{Y}')$ can be strictly defined as the distance in the new metric, named as the Hausdorff fractal distance. It is interesting to find that if $\beta = 1$, the fractal distance goes back to the classical Euclidean distance. Specially, considering 1-D case and setting the point $\mathbf{Y}'$ to be the original point, the definition eq. (9) degenerates to the following formulation:

$$r^{\beta} = x_1^{\beta} \tag{10}$$

It coincides with the original concept of fractal metric proposed in [21], as shown in the second line of eq. (6). It can be found that the Hausdorff fractal distance mentioned in this manuscript is a generalization of the scaling transformation.

It has been widely recognized that the fractal dimensionality varies in different directions [12], which means the value of β is not always a constant. Without the loss of generality, the fractal distance for anisotropic fractal media should be reformulated:

$$d\left(\mathbf{X}', \mathbf{Y}'\right) = r^{\beta} = \sqrt{\left(x_1^{\beta_1} - y_1^{\beta_1}\right)^2 + \left(x_2^{\beta_2} - y_2^{\beta_2}\right)^2 + \left(x_3^{\beta_3} - y_3^{\beta_3}\right)^2} \tag{11}$$

where β_1, β_2, and β_3 are the fractal orders along the three directions. It is clear that the eq. (11) is the generalized non-Euclidean Hausdorff fractal distance for anisotropic fractal media. Figure 1 displays the Hausdorff fractal distance between two test points **A** (1, 1, 1) and **B** (3, 3, 3) with varying β_1 and β_2, and $\beta_3 = 1$. It is clear that the value of Hausdorff fractal distance converges to the Euclidean distance with $\beta_1 \rightarrow 1$ and $\beta_2 \rightarrow 1$.

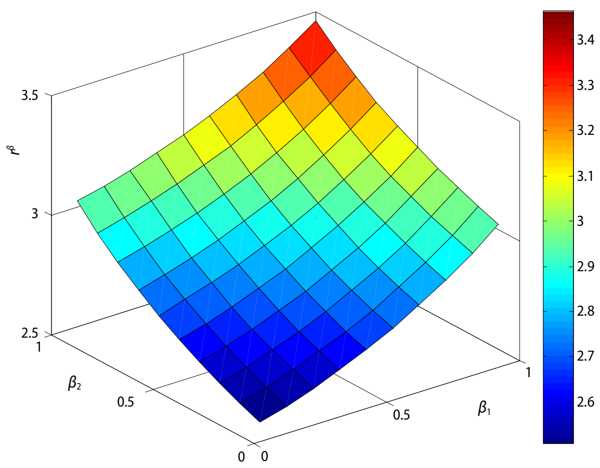

Figure 1. Hausdorff fractal distance between A(1, 1, 1) and B(3, 3, 3) (*for color image see journal web site*)

The Hausdorff derivative diffusion equation and the fundamental solution

The Hausdorff derivative diffusion equation

As mentioned in [3, 21], the laws of physics are invariant regardless of spatial or temporal fractal metric, which will result in the anomalous behaviors. The anomalous diffusion process disobeys the Fick's second law and the mean square displacement is a non-linear function of t. It has reached an agreement that the physical mechanism of anomalous diffusion is due to the fractal structure or fractal distribution of material components.

Recently, the Hausdorff fractal diffusion equation has been proposed to characterize anomalous diffusion behaviors [11], which is formulated:

$$\frac{\partial u(x,t)}{\partial t^{\alpha}} = D\frac{\partial}{\partial x^{\beta}}\left[\frac{\partial u(x,t)}{\partial x^{\beta}}\right] \tag{12}$$

where α and β represent the fractals in time and space, respectively, and D is the diffusion coefficient. The definition of the Hausdorff fractal derivative has been discussed in eqs. (4) and (5). The mean square displacement for eq. (12) follows $<x^2> \propto t^{(3\alpha-\alpha\beta)/2\beta}$. If $\alpha = \beta = 1$, the Hausdorff fractal diffusion model degenerates to classical diffusion equation with $<x^2>\propto t$.

With the help of eqs. (4) and (5), the eq. (12) can be reformulated:

$$\frac{1}{\alpha t^{\alpha}}\frac{\partial u(x,t)}{\partial t} = \frac{D}{\beta^2 x^{\beta-1}}\left[\frac{1-\beta}{x^{\beta}}\frac{\partial u(x,t)}{\partial x} + \frac{1}{x^{\beta-1}}\frac{\partial^2 u(x,t)}{\partial x^2}\right] \tag{13}$$

It is obvious that the eq. (13) is formally to be a kind of convection-diffusion equation with time- and space-dependent characteristics. It makes reasonable that the Hausdorff fractal diffusion equation can characterize the anomalous diffusion behavior.

As previously mentioned, the Hausdorff fractal order is directly related to the fractal properties of the porous media. Without the loss of generality, considering the anisotropic fractal media with three fractal dimensionalities β_1, β_2, and β_3, the 3-D Hausdorff fractal diffusion equation can be generalized:

$$\frac{\partial u}{\partial t^{\alpha}} = D\left[\frac{\partial}{\partial x^{\beta_1}}\left(\frac{\partial u}{\partial x^{\beta_1}}\right) + \frac{\partial}{\partial y^{\beta_2}}\left(\frac{\partial u}{\partial y^{\beta_2}}\right) + \frac{\partial}{\partial z^{\beta_3}}\left(\frac{\partial u}{\partial z^{\beta_3}}\right)\right] \tag{14}$$

The fundamental solution of the Hausdorff derivative diffusion equation

It has been demonstrated that the fundamental solution of the fractal diffusion equation is formulated [11]:

$$u^*\left(x,t\right)=t^{-\alpha/2}\frac{1}{2\sqrt{\pi D}}\exp\left(-\frac{x^{2\beta}}{4Dt^{\alpha}}\right) \tag{15}$$

Considering the fundamental solution underlies the concept the distance, the eq. (15) should be correctly reformulated:

$$u^*(x,y,t,\tau)=\frac{1}{\sqrt{t^{\alpha}-\tau^{\alpha}}}\frac{H(t-\tau)}{\sqrt{4\pi D}}\exp\left[-\frac{(x^{\beta}-y^{\beta})^2}{4D(t^{\alpha}-\tau^{\alpha})}\right] \tag{16}$$

where y and τ, respectively, denote the space and time reference point, and H is the Heaviside function. The eq. (16) goes back to the eq. (15) with the reference point $\tau = 0$ and $y = 0$.

On the other hand, the eq. (15) is only limited for the 1-D case. Considering varying constants β for all directions in eq. (15), the fundamental solution for the 3-D Hausdorff derivative diffusion equation should be generalized:

$$u^*(x,y,t,\tau)=\frac{1}{\sqrt{(t^{\alpha}-\tau^{\alpha})^n}}\frac{H(t-\tau)}{\sqrt{(4\pi D)^n}}\exp\left[-\frac{r^{2\beta}}{4D(t^{\alpha}-\tau^{\alpha})}\right] \tag{17}$$

where n represents the number of dimensions, and r^{β} is defined in eq. (9). It should also be mentioned that the eq. (17) is the fundamental solution of the anisotropic Hausdorff fractal diffusion eq. (14) with the distance r^{β} defined as eq. (11). It is obvious that the two-norm space-fractal distance and one-norm time-fractal distance are inherent in the fundamental solution.

It is noted that the fundamental solution eq. (17) underlies the stretched Gaussian distribution from the viewpoint of space, and the Kohlrausch-Williams-Watts stretched exponential relaxation function in terms of time.

Conclusions

This paper proposed 3-D Hausdorff derivative diffusion model for the anisotropic porous media with different fractal dimensionalities. The fundamental solution of the proposed model was subsequently derived. The underlying distance in the fundamental solution was generalized from the classical Euclidean distance. Moreover, the generalized Hausdorff distance is directly related to the fundamental solution of the Hausdorff diffusion equation for anisotropic media.

The Hausdorff fractal diffusion equation is found to be the time-space dependent convection-diffusion equation underlying the anomalous diffusion in porous media. It is also interesting to find that the definition of the non-Euclidean Hausdorff fractal distance degenerates to the scaling transformations in the 1-D case without considering the reference point. Numerical result reveals that the Hausdorff distance converges to the Euclidean distance with the parameters approaching 1.

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