VARIATIONAL PRINCIPLE OF THE 2-D STEADY-STATE CONVECTION-DIFFUSION EQUATION WITH FRACTAL DERIVATIVES

by

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The convection-diffusion equation describes a convection and diffusion process, which is the cornerstone of electrochemistry. The process always takes place in a porous medium or on an uneven boundary, and an abnormal diffusion occurs, which will lead to deviations in prediction of the convection-diffusion process. To overcome the problem, a fractal modification is suggested to deal with the "abnormal" problem, and a 2-D steady-state convection-diffusion equation with fractal derivatives in the fractal space is established. Furthermore, its fractal variational principle is obtained by the semi-inverse method. The fractal variational formula can not only provide the conservation law in the fractal space in the form of energy, but also give the possible solution structure of the equation.

Key words: *the convection-diffusion equation, He's fractal derivatives, two-scale transform, fractal variational formulation*

Introduction

The convection-diffusion process arises in many natural phenomena, and has a wide range of applications in practical problems, such as chemical reaction process [1], miscible displacement in soils [2], the contaminant transport [3], migration of heavy metals in soil [4], liquid droplet's ignition process [5], electron's propagation in a semiconductor [6], sediment transport [7, 8], and electrochemical reaction in electrodes [9, 10].

The convection-diffusion equation can be written:

$$\frac{\partial C}{\partial T} = \nabla(D\nabla C - uC) \tag{1}$$

where C is the concentration of the solute, D – the hydrodynamic dispersion coefficient, and u – the penetration rate of solution. When the solution is in the uniform seepage field of saturated porous media, D and u are real constants. After some time, the concentration will not change with the time $(\partial C/\partial T = 0)$, and it is called the steady-state convection-diffusion process. Considering the 2-D case, the equation can be expressed:

$$D_1 \frac{\partial^2 C}{\partial X^2} + D_2 \frac{\partial^2 C}{\partial Y^2} - u_1 \frac{\partial C}{\partial X} - u_2 \frac{\partial C}{\partial Y} = 0 \tag{2}$$

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in which D_1 and D_2 are the hydrodynamic dispersion coefficient in the *X*- and *Y*-directions, u_1 and u_2 – the penetration rate of solution in the *X*- and *Y*-directions. Equation (2) was widely studied in various methods, for example, Stynes discussed a series of steady-state convection-diffusion processes [11, 12]. Kennedy and O'Connor used transmission line modeling method to analyze steady-state convection-diffusion equations [13]. In general, 2-D and 3-D solutions can be obtained by numerical methods, but analytical solutions are more popular in practical applications. In 2011, analytical solutions for some special conditions were appeared, for examples, Chen *et al.* [14] obtained analytical solution for a spherical coordinate system. Yadav *et al.* [15] used the variable coordinate transformation to find an analytical solution of the 2-D convection-diffusion equation.

The convection-diffusion process takes place in an uneven boundary or in a porous medium, which causes abnormal diffusion. In the previous literature, homogenization and pseudo-homogenization had to be assumed for a porous medium, but it can not deal with the abnormal diffusion.

In recent years, much literature showed that such abnormal diffusion can be effectively modeled by the fractal calculus [16-18]. Its key point is to use fractional derivatives instead of integer derivatives. Therefore, smooth space (*X*, *Y*) should be transformed into fractal space (X^α, Y^β), where α and β are the fractal dimensions. Under the fractal space, the 2-D steady-state convection-diffusion equations can be modified:

$$D_1 \frac{\partial^2 C}{\partial X^{2\alpha}} + D_2 \frac{\partial^2 C}{\partial Y^{2\beta}} - u_1 \frac{\partial C}{\partial X^{\alpha}} - u_2 \frac{\partial C}{\partial Y^{\beta}} = 0 \tag{3}$$

where $\partial c/\partial X^{\alpha}$ and $\partial c/\partial Y^{\beta}$ are the fractal derivative defined [19, 20]:

$$\frac{\partial C}{\partial X^{\alpha}}(X_0, Y) = \Gamma(1+\alpha) \lim_{\substack{X - X_0 \to \Delta X \\ \Delta X \neq 0}} \frac{C(X,Y) - C(X_0,Y)}{(X - X_0)^{\alpha}} \tag{4}$$

$$\frac{\partial C}{\partial Y^{\beta}}(X, Y_0) = \Gamma(1+\alpha) \lim_{\substack{Y - Y_0 \to \Delta Y \\ \Delta Y \neq 0}} \frac{C(X,Y) - C(X,Y_0)}{(Y - Y_0)^{\beta}} \tag{5}$$

We have:

$$\frac{\partial^2}{\partial X^{2\alpha}} = \frac{\partial}{\partial X^{\alpha}} \frac{\partial}{\partial X^{\alpha}}, \quad \frac{\partial^2}{\partial Y^{2\beta}} = \frac{\partial}{\partial Y^{\beta}} \frac{\partial}{\partial Y^{\beta}} \tag{6}$$

where ΔX and ΔY are the smallest spatial scale for discontinuous boundaries scales for observing the concentration. When the spatial scale of the two directions is larger than ΔX and ΔY, the problem studied at this time becomes the traditional smooth homogeneous solute transport problem.

The fractal differential models have become useful tools for various discontinuous problems, for examples, porous concrete [21, 22], composites [23], fractal Toda oscillator [24], fractal MEMS oscillator [25], fractal vibration systems [26-29], and fractal solitary waves [30-34].

Variation principle

The variational principle is an energy method for describing motion, which has a wide range of applications and can solve non-linear problems well [35-37]. Wang *et al.* [38] established the variational principle of traveling waves in fractal space by using the semi-inversion method, and now various fractal variational principles were appeared, for examples, fractal variational principle for solitary waves [39-44], fractal optimization [45], fractal Evans variational principle [46], and variational-based approximate methods are effective for complex problems [47-52].

Based on the basic properties of fractal derivatives, we give the following two-scale transformation [19, 20]. Let:

$$x = X^{\alpha} \tag{7}$$

$$y = Y^{\beta} \tag{8}$$

Equation (3) can be written:

$$D_1 \frac{\partial^2 C}{\partial x^2} + D_2 \frac{\partial^2 C}{\partial y^2} - u_1 \frac{\partial C}{\partial x} - u_2 \frac{\partial C}{\partial y} = 0 \tag{9}$$

Then, we write eq. (9) in the following conservative form, which is more convenient to apply the semi-inverse method [36] to establish the variational formula of the equation:

$$(D_1 C_x - u_1 C)_x + (D_2 C_y - u_2 C)_y = 0 \tag{10}$$

According to eq. (10), we define an auxiliary function ϕ that satisfies:

$$\varphi_x = -(D_2 C_y - u_2 C) \tag{11}$$

$$\varphi_y = D_1 C_x - u_1 C \tag{12}$$

Through the semi-inverse method [36], we establish the following variational formula:

$$J(C,\varphi) = \iint L(C, C_x, C_y, C_{xx}, C_{yy}, C_{xy}, \varphi, \varphi_x, \varphi_y, \varphi_{xx}, \varphi_{yy}, \varphi_{xy}) \mathrm{d}x\mathrm{d}y \tag{13}$$

where L is the trial-Lagrange function. Then, we set the trial-Lagrange function to the following form:

$$L = (D_1 C_x - u_1 C)\varphi_x + (D_2 C_y - u_2 C)\varphi_y + F \tag{14}$$

where F is an unknown undetermined function of C and/or φ and/or their derivatives. When F is independent of φ and its derivatives, eq. (10) is the stationary condition that φ must satisfy.

The stationary condition about C can be expressed:

$$-u_1 \varphi_x - u_2 \varphi_y - D_1 \varphi_{xx} - D_2 \varphi_{yy} + \frac{\delta F}{\delta C} = 0 \tag{15}$$

in which $\delta F / \delta C$ is called He's variational derivative defined [36]:

$$\frac{\delta F}{\delta C} = \frac{\partial F}{\partial C} - \frac{\partial}{\partial t}\left(\frac{\partial F}{\partial C_t}\right) - \frac{\partial}{\partial x}\left(\frac{\partial F}{\partial C_x}\right) + \frac{\partial^2}{\partial t^2}\left(\frac{\partial F}{\partial C_{tt}}\right) + \frac{\partial^2}{\partial t \partial x}\left(\frac{\partial F}{\partial C_{tx}}\right) + \frac{\partial^2}{\partial x^2}\left(\frac{\partial F}{\partial C_{xx}}\right) - \cdots \tag{16}$$

Under eqs. (11) and (12), we have:

$$\frac{\delta F}{\delta C} = u_1\varphi_x + u_2\varphi_y + D_1\varphi_{xx} + D_2\varphi_{yy} = -u_1(D_2C_y - u_2C) + u_2(D_1C_x - u_1C) -$$

$$-D_1(D_2C_y - u_2C)_x + D_2(D_1C_x - u_1C)_y = 2u_2D_1c_x - 2u_1D_2c_y \tag{17}$$

From eq. (17), it is difficult to find F. Therefore, we need to make the following modifications to the trial-Lagrange function [36]:

$$L = A(D_1C_x - u_1C)\varphi_x + B\varphi_x\varphi_y + (D_2C_y - u_2C)\varphi_y + F \tag{18}$$

In eq. (8), A and B are unknown constants. The stationary conditions are given by:

$$-Au_1\varphi_x - u_2\varphi_y - AD_1\varphi_{xx} - D_2\varphi_{yy} + \frac{\delta F}{\delta C} = 0 \tag{19}$$

$$-A(D_1C_x - u_1C)_x - 2B\varphi_{xy} - (D_2C_y - u_2C)_y + \frac{\delta F}{\delta\varphi} = 0 \tag{20}$$

From eqs. (19) and (20), we have:

$$\frac{\delta F}{\delta C} = Au_1\varphi_x + u_2\varphi_y + AD_1\varphi_{xx} + D_2\varphi_{yy} =$$

$$-Au_1(D_2C_y - u_2C) + u_2(D_1C_x - u_1C) - AD_1(D_2C_y - u_2C)_x + D_2(D_1C_x - u_1C)_y =$$

$$= (A-1)u_1u_2C + (1+A)(u_2D_1C_x - u_1D_2C_y) + (1-A)D_1D_2C_{xy} \tag{21}$$

$$\frac{\delta F}{\delta\varphi} = A(D_1C_x - u_1C)_x + 2B\varphi_{xy} + (D_2C_y - u_2C)_y =$$

$$= A(D_1C_x - u_1C)_x + (1-2B)(D_2C_y - u_2C)_y \tag{22}$$

Let:

$$\frac{\delta F}{\delta\varphi} = 0 \tag{23}$$

we have:

$$A + 2B = 1 \tag{24}$$

In order to get the undetermined function F, we need let the coefficient of C_x and C_y in eq. (21) be equal to zero. We know $A = -1$, then $B = 1$. So, we have:

$$\frac{\delta F}{\delta C} = -2u_1u_2C + 2D_1D_2C_{xy} \tag{25}$$

From eq. (25), we can determine that F is uniquely identified:

$$F = -u_1u_2C^2 - D_1D_2C_xC_y \tag{26}$$

Therefore, we have successfully obtained the variational formula of eq. (18):

$$J(C,\varphi)=\iint\{-(D_1C_x-u_1C)\varphi_x+\varphi_x\varphi_y+(D_2C_y-u_2C)\varphi_y-u_1u_2C^2-D_1D_2C_xC_y\}\mathrm{d}x\mathrm{d}y \tag{27}$$

Proof. According to the mentioned variational principle, the Euler-Lagrange equation of eq. (27) can be given in the following form:

$$u_1\varphi_x-u_2\varphi_y+D_1\varphi_{xx}-D_2\varphi_{yy}-2u_1u_2C+2D_1D_2C_{xy}=0 \tag{28}$$

$$(D_1C_x-u_1C)_x+(D_2C_y-u_2C)_y=0 \tag{29}$$

Compared with the previous constraints, it is obvious that eqs. (28) and (29) are equivalent to eqs. (10) and (19), respectively.

In the fractal space (X^α, Y^α), the variational formulation can be expressed in the following form:

$$J(C,\varphi)=\iint\left\{-\left(D_1\frac{\partial C}{\partial X^\alpha}-u_1C\right)\frac{\partial\varphi}{\partial X^\alpha}+\frac{\partial\varphi}{\partial X^\alpha}\frac{\partial\varphi}{\partial Y^\beta}+\left(D_2\frac{\partial C}{\partial Y^\beta}-u_2C\right)\frac{\partial\varphi}{\partial Y^\beta}-\right.$$

$$\left.-u_1u_2C^2-D_1D_2\frac{\partial C}{\partial X^\alpha}\frac{\partial C}{\partial Y^\beta}\right\}\mathrm{d}X^\alpha\mathrm{d}Y^\beta \tag{30}$$

Conclusion

In the problem of discontinuous media, fractal derivatives have a wide range of applications. In this paper, we establish a variational formulation for 2-D steady-state convection-diffusion equation in the fractal space (X^α, Y^β) by the semi-inverse method. The variational principle can not only be used to construct the conservation law and solutions structure, but also provide a theoretical basis for the analysis and numerical methods.

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