VARIATIONAL APPROACH TO FRACTAL REACTION-DIFFUSION EQUATIONS WITH FRACTAL DERIVATIVES

by

Yue WU *

College of Economics and Management, Shanghai University of Political Science and Law, Qingpu Area, Shanghai, China

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A fractal modification of the reaction-diffusion process is proposed with fractal derivatives, and a fractal variational principle is established in a fractal space. The concentration of the substrate can be determined according to the minimal value of the variational formulation. The solution process is illustrated step by step for ease applications in engineering, and the effect of fractal dimensions on solution morphology is elucidated graphically.

Key words: *fractal calculus, reaction potential, Michalis-Menten kinetics, least action, ancient Chinese mathematics*

Introduction

Reaction-diffusion processes happen always on an unsmooth boundary, the boundary morphology has a great effect on the process. Recently Mahalakshmi *et al.* [1] studied a non-linear reaction-diffusion equation arising in biomedicine, and an accurate solution was obtained. The dimensionless material balance of substrate inside the support in a solid of planar or spherical shape can be written [1-4]:

$$\frac{1}{x^{\sigma}}\frac{\mathrm{d}}{\mathrm{d}x}\left(x^{\sigma}\frac{\mathrm{d}u}{\mathrm{d}x}\right)-\frac{au}{b+u}=0,\ u(0)=u_0,\ u(1)=u_1 \tag{1}$$

where u is the concentration, $au/(b+u)$ is Michalis-Menten potential, $\sigma = 0$ or 2 presents, respectively, the slab and sphere cases, a and b are constants.

Equation (1) can be solved by various effective methods, for example, the variational iteration method (VIM) [5, 6], the Taylor series method [7-9], the homotopy perturbation method (HPM) [10-12], the reproducing kernel method [13, 14], and the wavelet-based optimization algorithm [1].

Equation (1) cannot model the unsmooth boundary effect on the process, a fractal modification of eq. (1) is given:

$$\frac{1}{X^{\sigma}}\frac{\mathrm{d}}{\mathrm{d}X^{\alpha}}\left(X^{\sigma}\frac{\mathrm{d}u}{dX^{\alpha}}\right)-\frac{au}{b+u}=0,\ u(0^{\alpha})=u_0,\ u(1^{\alpha})=u_1 \tag{2}$$

where the fractal derivative is defined [15-24]:

$$\frac{\mathrm{d}u}{\mathrm{d}X^{\alpha}}(X_0)=\Gamma(1+\alpha)\lim_{X-X_0\to\Delta X}\frac{u(X)-u(X_0)}{(X-X_0)^{\alpha}} \tag{3}$$

where ΔX is the smallest porous size and α – the two-scale fractal dimension.

* Author's e-mail: needlewu@sina.com

The two-scale fractal dimension is defined:

$$\alpha = \frac{V}{V_0} \times \alpha_0 \tag{4}$$

where V and V_0 are the volumes of the studied space in a large-scale and in a small scale, respectively, α_0 is the dimension on a large-scale.

This paper will establish a variational formulation by the semi-inverse method [25], and then use the Ritz method to find an approximate solution of eq. (2).

Variational principle

In the definition of eq. (4), V is measured in a large-scale of x and it is considered as a continuum, V_0 considers the same volume as a porous medium in a small scale of X. The two scales have the relationship:

$$x = X^\alpha \tag{5}$$

By the aforementioned two-scale transform, eq. (2) can be converted to eq. (1). Now by the semi-inverse method [14-19], we can establish easily a variational formulation for eq. (1), which reads:

$$J(u) = \int_0^1 \left\{ -\frac{1}{2}\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2 - a\left[u - b\ln(b+u)\right] \right\} x^\sigma \mathrm{d}x \tag{6}$$

Proof. The stationary condition of eq. (2):

$$\frac{\partial L}{\partial u} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial L}{\partial u_x}\right) = 0 \tag{7}$$

where L is the Lagrange function defined

$$L(u) = \left\{ -\frac{1}{2}\left(\frac{du}{dx}\right)^2 - a\left[u - b\ln(b+u)\right] \right\} x^\sigma \tag{8}$$

So the stationary condition:

$$-ax^\sigma \left[1 - \frac{b}{b+u}\right] + \frac{\mathrm{d}}{\mathrm{d}x}\left[x^\sigma \left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)\right] = 0 \tag{9}$$

is obvious that eq. (9) is exactly eq. (1).

The fractal variational principle for eq. (2):

$$J(u) = \int_{0^\alpha}^{1^\alpha} \left\{ -\frac{1}{2}\left(\frac{\mathrm{d}u}{\mathrm{d}X^\alpha}\right)^2 - a\left[u - b\ln(b+u)\right] \right\} X^\sigma \mathrm{d}X^\alpha \tag{10}$$

We assume that the solution can be expressed:

$$u(x) = \sum_{n=0}^{N} c_n x^n \tag{11}$$

where c_n ($n = 0 \sim N$) are constants to be determined later. In view of the boundary conditions:

$$u(0) = c_0 = u_1 \tag{12}$$

$$u(1) = \sum_{n=0}^{N} c_n = u_1 \tag{13}$$

Substituting eq. (11) into eq. (6) results:

$$J(c_0,c_1,c_2,\cdots,c_N)=\int_0^1\left\{-\frac{1}{2}\left(\sum_{n=1}^{N}nc_nx^{n-1}\right)^2-a\left[\sum_{n=0}^{N}c_nx^n-b\ln\left(b+\sum_{n=0}^{N}c_nx^n\right)\right]\right\}x^{\sigma}\mathrm{d}x \tag{14}$$

The stationary condition of eq. (6) can be approximately obtained:

$$\frac{\partial}{\partial c_n}J(c_0,c_1,c_2,\cdots,c_N)=0, n=2\sim N \tag{15}$$

Solving eqs. (12), (13), and (15) simultaneously, we can identify $c_n(n = 0 \sim \mathrm{N})$.

An example

We consider following fractal reaction-diffusion equation:

$$\frac{\mathrm{d}^2u}{\mathrm{d}X^{2\alpha}}-\frac{0.02u}{1+u}=0,\ \frac{\mathrm{d}u}{\mathrm{d}X^{\alpha}}(0^{\alpha})=0,\ \frac{\mathrm{d}u}{\mathrm{d}x^{\alpha}}(1^{\alpha})=1^{\alpha}-u(1^{\alpha}) \tag{16}$$

Its fractal variational principle:

$$J(u)=\int_{0^{\alpha}}^{1^{\alpha}}\left\{-\frac{1}{2}\left(\frac{\mathrm{d}u}{\mathrm{d}X^{\alpha}}\right)^2-0.02\left[u-\ln(1+u)\right]\right\}\mathrm{d}X^{\alpha} \tag{17}$$

By the two-scale transform given in eq. (5), we can convert eq. (16) into:

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2}-\frac{0.02u}{1+u}=0,\ u'(0)=0,\ u'(1)=1-u(1) \tag{18}$$

This equation was studied in [1].

The variational formulation:

$$J(u)=\int_0^1\left\{-\frac{1}{2}\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2-0.02\left[u-\ln(1+u)\right]\right\}\mathrm{d}x \tag{19}$$

According to the boundary conditions, we assume that its solution can be expressed:

$$u(x)=(1-3c)+cx^2 \tag{20}$$

where c is an unknown constant. It is obvious that eq. (20) satisfies the boundary conditions.

Substituting eq. (20) into eq. (19) leads:

$$J(c)=\int_0^1\left\{-2c^2x^2-0.02\left[1-3c+cx^2-\ln(2-3c+cx^2)\right]\right\}\mathrm{d}x \tag{21}$$

Its stationary condition requires:

$$\frac{\mathrm{d}}{\mathrm{d}c}J(c)=\int_0^1\left\{-4cx^2-0.02\left[-3cx^2-\frac{-3+x^2}{2-3c+cx^2}\right]\right\}\mathrm{d}x=0 \tag{22}$$

We can solve c from eq. (15) by some a mathematical software. For audience who are not familiar with mathematical software, we suggest an approximate solution process according to an ancient Chinese algorithm called Ying-buzu algorithm [26-28].

The Ying-buzu algorithm is to solve the equation by two trial solutions:

$$f(c)=\int_0^1\left\{-4cx^2-0.02\left[-3cx^2-\frac{-3+x^2}{2-3c+cx^2}\right]\right\}\mathrm{d}x=0 \tag{23}$$

We assume the two trial solutions are c_1 and c_2, which lead to the residuals of $f(c_1)$ and $f(c_2)$, respectively, the approximate solution can be calculated:

$$c=\frac{c_2 f(c_1)-c_1 f(c_2)}{f(c_1)-f(c_2)} \tag{24}$$

We choose two trial values for c, for example, $c_1 = 0.005$ and $c_2 = 0.00495$, then we obtain easily the residuals by eq. (22), which are, respectively:

$$f(0.005)=\int\left\{-4\times 0.005x^2-0.02\left[-3\times 0.005x^2-\frac{-\ \ +}{2-3\times 0.005+0.005}\right]\right\}\mathrm{d}x$$
$$=-0.03341 \tag{25}$$

$$f(0.00495)=\int_0^1\left\{-4\times 0.00495x^2-0.02\left[-3\times 0.00495x^2-\frac{-3+x^2}{2-3\times 0.00495+0.00495x^2}\right]\right\}\mathrm{d}x$$
$$=-0.07338 \tag{26}$$

According to the Ying-buzu algorithm [20-22], we have:

$$c=\frac{c_2 f(c_1)-c_1 f(c_2)}{f(c_1)-f(c_2)}=\frac{-0.7338\times 0.00495+0.03341\times 0.005}{-0.7338+0.03341}=0.00489 \tag{27}$$

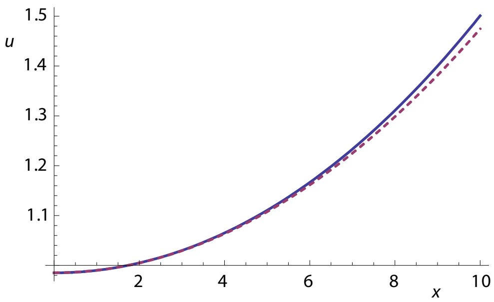

Figure 1. Comparison of the approximate solution of eq. (28) with the exact one

Therefore, we obtain the following approximate solution, fig. 1:

$$u(x)=0.98533+0.00489x^2 \tag{28}$$

This approximate solution is closed to that by Mahalakshmi *et al.* [1]:

$$u(x)=0.98743+0.00496x^2 \tag{29}$$

The accuracy can be improved if more terms are included in the trial solution.

Solution morphology

The approximate solution of eq. (16):

$$u(X)=0.98533+0.00489\mathrm{X}^{2\alpha} \tag{30}$$

It is obvious that:

$$\frac{\mathrm{d}}{\mathrm{d}X}u(X)=0.00978\alpha X^{2\alpha-1} \tag{31}$$

When $X = 0^\alpha$, we have the properties:

$$\frac{\mathrm{d}}{\mathrm{d}X}u(0)=\begin{cases}0,\alpha>0.5\\0.00978,\ \alpha=0.5\\\infty,\alpha<0.5\end{cases} \tag{32}$$

Equation (32) implies that u will change suddenly at $X = 0^\alpha$, as shows in fig. 2. When $\alpha = 0.5$, a linear relationship is obtained, see fig. 3, and when $\alpha > 0.5$, the slope at $X = 0^\alpha$ becomes very small as shown in fig. 4. So the solution properties depend strongly upon the value of α. When $\alpha \to 1$, the solution morphology tends to that of the classical model.

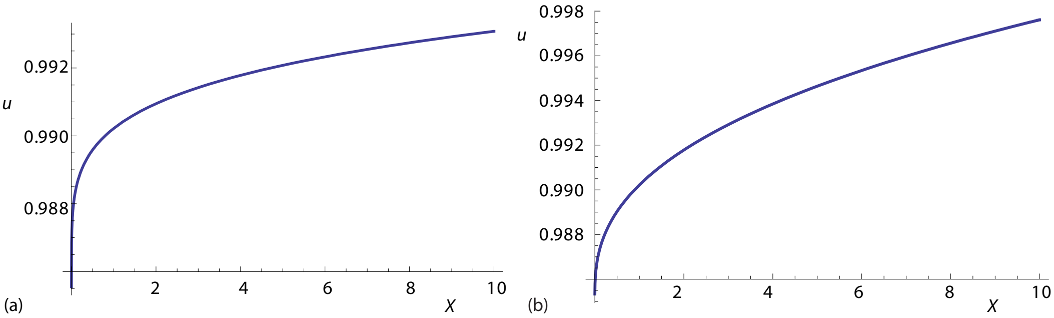

Figure 2. Solution morphology when $\alpha < 0.5$; (a) $\alpha = 0.1$ and (b) $\alpha = 0.2$

Discussion and conclusion

This paper suggests a variational approach to eq. (1) and its fractal modification. As the variational formulation has an energy integral, which can suggest possible solution structure. According to eq. (6), $1/2(\mathrm{d}u/\mathrm{d}x)^2$ can be understood as the kinetic energy of the reaction-diffusion process, while $a[b\ln(b + u) - u]$ is the reaction potential, its derivative with respect to u is the well-known Michalis-Menten potential. As the solution process is simple and straightforward, the variational approach can be extended to more complex non-linear systems, and this paper can be used as a paradigm for practical applications.

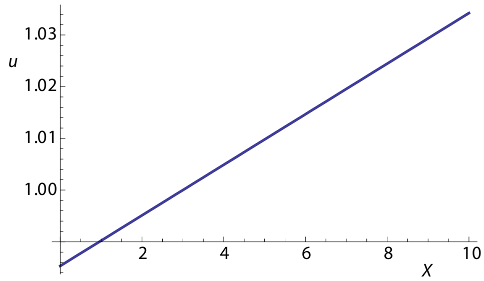

Figure 3. Solution morphology when $\alpha = 0.5$

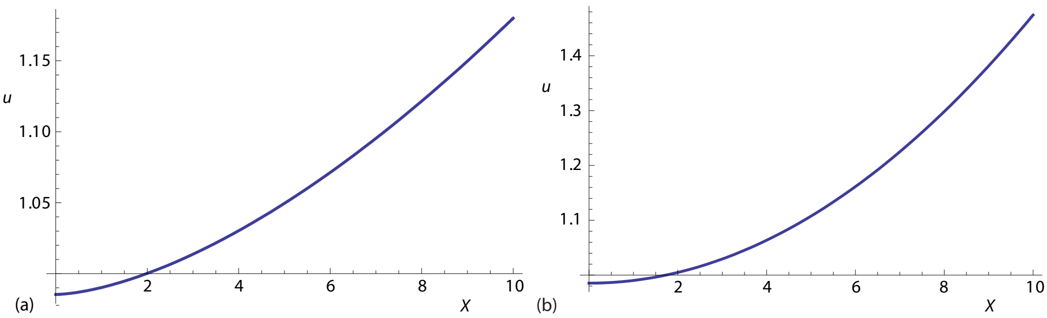

Figure 4. Solution morphology when $\alpha > 0.5$; (a) $\alpha = 0.8$ and (b) $\alpha = 0.1$

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