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Homotopy Method for Parameter Determination of Solute Transport with Fractional Advection-dispersion Equation

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Abstract: The unknown parameters are critical factors in fractional derivative advection-dispersion equation describing the solute transport in soil. For examples, the fractional derivative order is the index of anomalous dispersion, diffusion coefficient represents the dispersion ability of media and average pore-water velocity denotes the main trend of transport, etc. This paper is to develop a homotopy method to determine the unknown parameters of solute transport with spatial fractional derivative advection-dispersion equation in soil. The homotopy method can be easily developed to solve parameter determination problems of fractional derivative equations whose analytical solutions are difficult to obtain. The sigmoid function is involved to adjust the homotopy parameter during the iterative processes. Numerical results show that the presented method is efficient and feasible in several benchmark examples.

Keywords: Homotopy method, Parameter determination, Fractional advection-dispersion equation, Sigmoid function.

1 Introduction

Many studies indicated that the conventional advection-dispersion equation (ADE) can be obtained based on Fick's law, for example, to simulate the contaminant transport in homogenous media. However, most natural porous media (i.e., natural soils or aquifers) are heterogeneous. Hereby the transport processes may no longer follow Fick's second law and should be called anomalous dispersion, due to the heterogeneity of media. The distribution of the contaminant concentration versus

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time is no longer in Gaussian form. The measured concentrations are usually much higher than those estimated by ADE at the early stage of the breakthrough curves, this phenomena was so called as anomalous or non-Fickian transport [Lévy and Berkowitz (2003)]. The classical ADE fails to model the anomalous character of the solute transport in heterogeneous soil and other medium [Fomin et al. (2011)]. To more accurately describe the non-local property of anomalous diffusion (super-diffusion) in soil, fractional derivative has become a promising approach in recent years [Berkowitz and Scher (1997); Cortis and Berkowitz (2004); Fomin et al. (2011); Klafter et al. (1987); Metzler Ralf and Klafter (2000); Metzler R et al. (1994)].

Non-local diffusion processes can be governed by a generalized space-fractional diffusion equation. It is obtained from the standard linear diffusion equation by replacing the second-order space derivative with a suitable fractional derivative operator [Gorenflo and Mainardi (1998)]. Based on Lévy motion theory, Benson et al. [Benson D A (1998); Benson D A et al. (2000); Benson David A et al. (2001)] described the spatial and temporal distribution of contaminant concentration by a fractional advection-dispersion equation (FADE). The one-dimensional FADE for describing non-reactive contaminant transport is given by

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + \frac{1}{2}(1+\gamma)D\frac{\partial^\alpha C}{\partial x^\alpha} + \frac{1}{2}(1-\gamma)D\frac{\partial^\alpha C}{\partial (-x)^\alpha}, \tag{1}$$

where C is the solute concentration, v is the average pore-water velocity, x is the spatial coordinate, t is the time, D is the diffusion coefficient with dimension of $[L^\alpha T^{-1}]$, $\gamma(-1 \leq \gamma \leq 1)$ is the skewness, i.e. the relative weight of solute particle forward versus backward transition probability, and $\alpha(1 < \alpha \leq 2)$ is the order of fractional derivative. The above FADE reduces to ADE when α equals to 2. The definitions of the fractional derivative operator can be [Samko et al. (1993)]

$$\frac{\partial^\alpha C}{\partial x^\alpha} = \frac{1}{\Gamma(m-\alpha)}\left(\frac{\partial^m}{\partial x^m}\right)\int_{-\infty}^{x}\frac{C(\xi,t)}{(x-\xi)^{-m+\alpha+1}}d\xi, \tag{2}$$

$$\frac{\partial^\alpha C}{\partial (-x)^\alpha} = \frac{(-1)^m}{\Gamma(m-\alpha)}\left(\frac{\partial^m}{\partial x^m}\right)\int_{x}^{\infty}\frac{C(\xi,t)}{(\xi-x)^{-m+\alpha+1}}d\xi. \tag{3}$$

The model (1) has been used to simulate the non-Fickian process for conservative solute by Pachepsky [Pachepsky et al. (2000)] and Huang [Huang G et al. (2005)]. For the, the more popularity used FADE model (symmetrical dispersion $\gamma = 0$) can be written as follow [Huang G et al. (2005)]

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^\alpha C}{\partial x^\alpha}. \tag{4}$$

Nowadays, parameter determination has been caught more and more attention with development of the fractional derivative model. Variety of softwares have been developed to estimate the parameters for ADE models, i.e., CXTFIT [Toride et al. (1995)]. But, to the best of our knowledge, very limited literatures on parameter estimation of FADE model can be found.

Huang [Huang G et al. (2005)] developed a software named as FADEMain based on FORTRAN, to estimate the parameters of Eq. (4): the fractional order α, the dispersive coefficient D and the average pore-water velocity v. FADEMain is based on the nonlinear least square fitting algorithm [Press et al. (1992)]. Huang [Guanhua (2003)] employed the analytical solution of Eq. (4) to get the Hesse matrix in their method. However, analytical solutions of fractional derivative models are usually difficult to obtain or too complex to use. Therefore, Huang's method is difficult to be extended to solve other problems. Hereby, based on the homotopy method, we develop a numerical method to determine the unknown parameters of Eq.(4). The presented method does not have to involve the analytical solution of direct problem.

The idea of homotopy, which is a basic concept of algebraic topology [Watson (1979, 1989)], has been widely used to find the approximate solution of nonlinear differential equation. It can be able to eliminate the drawback of the traditional numerical iteration which easily falls into local convergence and broaden the rigorous restrictions on selecting initial guess. The homotopy method has been proved to be efficient and large-scale convergent, and successfully used to solve the nonlinear complementarity problem [Watson (1979)], fractional differential equations [Odibat and Momani (2008)], the optimal projection equations problems [ŽIGIĆ et al. (1992)], multiobjective programming problem [Yao and Song (2013)] and highly-nonlinear (buckling) structural mechanics problem [Elgohary et al. (2014)].

The rest of this paper is organized as below. Section 2 introduces the parameter determination problem and the homotopy method. In section 3, two examples are involved to illustrate the feasibility and efficiency of the homotopy method. Finally, some conclusions are summarized in section 4.

2 Methodology

In this section, the parameter determination problem of FADE is presented. Then the homotopy method is introduced to solve this problem.

2.1 Parameter determination

We consider unabsorbed solute transport in a soil column with symmetrical spatial FADE model in a finite domain

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^{\alpha} C}{\partial x^{\alpha}}, 0 < x < L, 1 < \alpha < 2, \tag{5}$$

subject to the following initial and boundary conditions

$$C(x,0) = 0, 0 \le x \le L, \tag{6}$$

$$\begin{cases} C(0,t) = C_0, t > 0 \\ \left.\frac{\partial C}{\partial x}\right|_{x=L} = 0, t > 0 \end{cases}. \tag{7}$$

If all the parameters of the model (5)-(7) are given, we can solve the concentration distribution with time and space, it is so called the direct problem. For the direct problem, we can employ numerical methods to get the numerical solution, such as finite difference scheme [Lin and Xu (2007); Meerschaert and Tadjeran (2004); Su et al. (2009); Yuste (2006)], finite element method [Deng (2008)]. Actually, not all the parameters of the model can be determined in prior or measured directly. Thus, we need to determine the unknown parameters via mathematical algorithms by adding some additional conditions, which is so-called the inverse problem, namely, parameter determination. From the experiences of parameter inversion of ADE, the measured breakthrough curves of solute in soil column experiments can be considered as additional conditions in this article.

The observed concentration data versus times at a particular observation point, the breakthrough curve, can be denoted as

$$\widetilde{C}_{obs}(t_i), i = 1, 2, \cdots N, \tag{8}$$

Denote the unknown parameters, the fractional derivative order α, diffusion coefficient D and average pore-water velocity v as a parameter vector $\mathbf{p} = (\alpha, D, v)^T$. Construct an objective function as follow

$$F(\mathbf{p}) = \left\| \widetilde{\mathbf{C}}_{\mathbf{p}} - \widetilde{\mathbf{C}}_{obs} \right\|, \tag{9}$$

where $\widetilde{\mathbf{C}}_{obs} = \left(\widetilde{C}_{obs}(t_1), \widetilde{C}_{obs}(t_2), \cdots, \widetilde{C}_{obs}(t_N)\right)^T$ represents the observed data, $\widetilde{\mathbf{C}}_{\mathbf{p}} = \left(\widetilde{C}_{\mathbf{p}}(\mathbf{p}, t_1), \widetilde{C}_{\mathbf{p}}(\mathbf{p}, t_2), \cdots, \widetilde{C}_{\mathbf{p}}(\mathbf{p}, t_N)\right)^T$ represents the computed results under the estimated parameter vector $\mathbf{p} = (\alpha, D, v)^T$, $\|\cdot\|$ represents a norm. To determine the unknown parameters, we can minimize the objective function (9) to get the optimal solution. Thus the parameter determination problem is converted into a nonlinear optimization problem. When we choose l^2-norm, the problem is reduced to a nonlinear least square problem

$$\min_{\mathbf{p}} F(\mathbf{p}) = \left\| \widetilde{\mathbf{C}}_{\mathbf{p}} - \widetilde{\mathbf{C}}_{obs} \right\|^2 . \tag{10}$$

As we known, the solution of the problem (10) nonlinearly depends on the unknown parameters: the fractional derivative order α, the diffusion coefficient D and the average pore-water velocity v. Therefore, the problem (10) is ill-posed in the sense of Hadamard [Tikhonov (1977)]. In this situation, the solution of this problem exists but may not be unique. However, the solution should be unique if the range of the exact solution would be known a prior. Namely, we can obtain the approximate solution in the neighborhood domain of the exact solution by applying appropriate numerical methods, the details of prove can be referred to references [Isakov (1998); Li (2007.12); Ma (2005.5)] .

2.2 Homotopy method

In this section, the homotopy method is introduced to determine the parameters of FADE models of solute transport in soil column.

Consider a nonlinear operator equation

$$F(\mathbf{x}) = 0. \tag{11}$$

Let $F : X_1 \to X_2$ be a Fréchet differentiable operator, mapping a Banach space X_1 to a Banach space X_2, $\mathbf{x}^*$ be a exact solution of the problem (11), $\mathbf{x}^{(0)}$ be a initial approximate value of the iterative process. The thought of the homotopy method is to include a parameter λ and construct a mapping H, such that

1. For $\lambda = 0$, $\mathbf{x}(0)$ is the solution of equation $H(\mathbf{x}, \lambda) = F(\mathbf{x}(0)) = 0$, which corresponds to the initial value $\mathbf{x}^{(0)}$;
2. For $\lambda = 1$, $\mathbf{x}(1)$ is the solution of equation $H(\mathbf{x}, 1) = F(\mathbf{x}(1)) = 0$, which corresponds to the exact solution $\mathbf{x}^*$;
3. For $0 \le \lambda \le 1$, the solution $\mathbf{x}(\lambda)$of the homotopy equation $H(\mathbf{x}, \lambda) = 0$ exists, and is changed from $\mathbf{x}(0)$ to $\mathbf{x}(1)$ as λ changing from 0 to 1.

where $\mathbf{x}(\lambda)$, the solution of the nonlinear equation (11), can be called the homotopy path, which is a function with respect to the homotopy parameter λ. There are two approaches to obtain the optimal solution by tracking the homotopy path. One is starting from the homotopy equation; another one is based on the initial value problem of differential equation. These two approaches are equivalent. In this study, we consider starting from the homotopy equation. For the parameter determination problem (10), differentiating the form (10) with $\mathbf{p}$, and let it equal to 0, we have

$$\left(\frac{\partial \widetilde{\mathbf{C}}_{\mathbf{p}}}{\partial \mathbf{p}}\right)^T \left(\widetilde{\mathbf{C}}_{\mathbf{p}} - \widetilde{\mathbf{C}}_{obs}\right) = 0. \tag{12}$$

Thus the nonlinear inverse problem is converted to finding zero points of equations (12). The problem (12) is equivalent to the nonlinear least square problem (10).

Based on the homotopy method, we construct fixed homotopy equations

$$H(\mathbf{p},\lambda) = \lambda \left(\frac{\partial \widetilde{\mathbf{C}}_{\mathbf{p}}}{\partial \mathbf{p}}\right)^T \left(\widetilde{\mathbf{C}}_{\mathbf{p}} - \widetilde{\mathbf{C}}_{obs}\right) + (1-\lambda)(\mathbf{p} - \mathbf{p}^{(0)}) = 0, \tag{13}$$

where $\mathbf{p}^{(0)}$ is the initial guess value and λ the homotopy parameter. When $\lambda = 1$, the problem (13) is reduced to the problem (12). Based on the homotopy method, we can find a tracking path $\mathbf{p}(\lambda)$, such that, the parameter vector tends to the optimal solution when λ is changed from 0 to1. The convergence of the homotopy method can be referred to the references [Cui (2003); Garcia and Zangwill (1981)]. As we known, the observed data usually contain noisy data. Thus the homotopy parameter is usually a positive constant, which is very close but not equal to 1.

Let $\mathbf{p}^{n+1}$ be the $(n+1)$-th iteration parameter vector, and then expanding $\widetilde{\mathbf{C}}_{\mathbf{p}}(\mathbf{p}^{n+1},t_i)$ in Taylor series near the point $\mathbf{p}^n$, we have

$$\widetilde{\mathbf{C}}_{\mathbf{p}}(\mathbf{p}^{n+1},t_i) \approx \widetilde{\mathbf{C}}_{\mathbf{p}}(\mathbf{p}^{n},t_i) + \left.\frac{\partial \widetilde{\mathbf{C}}_{\mathbf{p}}}{\partial \mathbf{p}}\right|_n \left(\mathbf{p}^{n+1} - \mathbf{p}^n\right). \tag{14}$$

Substituting the relation (14) into (13) and replacing $\mathbf{p}^{(0)}$ by $\mathbf{p}^n$, we have

$$\lambda \left(\left.\frac{\partial \widetilde{\mathbf{C}}_{\mathbf{p}}}{\partial \mathbf{p}}\right|_n\right)^T \left[\left.\frac{\partial \widetilde{\mathbf{C}}_{\mathbf{p}}}{\partial \mathbf{p}}\right|_n (\mathbf{p}^{n+1} - \mathbf{p}^n) + \widetilde{\mathbf{C}}_{\mathbf{p}} - \widetilde{\mathbf{C}}_{obs}\right] + (1-\lambda)\left(\mathbf{p}^{n+1} - \mathbf{p}^n\right) = 0. \tag{15}$$

Denote the gradient matrix as $\mathbf{G} = \left.\frac{\partial \widetilde{\mathbf{C}}_{\mathbf{p}}}{\partial \mathbf{p}}\right|_n$ and the increment $d\mathbf{p} = \mathbf{p}^{n+1} - \mathbf{p}^n$, rewrite the relation (15) as follows

$$\lambda \mathbf{G}^T \mathbf{G} d\mathbf{p} + \mathbf{G}^T \left(\widetilde{\mathbf{C}}_{\mathbf{p}} - \widetilde{\mathbf{C}}_{obs}\right) + (1-\lambda) d\mathbf{p} = 0. \tag{16}$$

Then the increment $d\mathbf{p}$ can be obtained by solving the following equation

$$\left[\lambda \mathbf{G}^T \mathbf{G} + (1-\lambda)\mathbf{I}\right] d\mathbf{p} = -\lambda \mathbf{G}^T \left(\widetilde{\mathbf{C}}_{\mathbf{p}} - \widetilde{\mathbf{C}}_{obs}\right) \tag{17}$$

According to Eq.(17), we can see that $\lambda \mathbf{G}^T\mathbf{G}+(1-\lambda)\mathbf{I}$ is nonsingular when $0<\lambda<1$. Thus, a nonlinear inverse problem is converted to a well-posed problem. The derivatives of the fitted concentration with respect to the parameter p_j ($j=1,2,\cdots,M$) are evaluated by

$$\frac{\partial \widetilde{C}_{\mathbf{p}}(t_i)}{\partial p_j}=\frac{\widetilde{C}_{\mathbf{p}}(p_1,p_2,\cdots,p_j+\tau,\cdots,p_M,t_i)-\widetilde{C}_{\mathbf{p}}(p_1,p_2,\cdots,p_j,\cdots,p_M,t_i)}{\tau}. \quad (18)$$

The current setting for the small interval τ is 0.01 for all parameters, which can be appropriate for most cases [Toride et al. (1995)]. Hence, $\mathbf{G}$ is a $N\times M$ matrix and $G_{ij}=\frac{\partial \widetilde{C}_{\mathbf{p}}(t_i)}{\partial p_j}$. We can obtain the best fitted solution of the original problem by iterative process with Eq. (17).

However, there still exists a key problem-how to choose the homotopy parameter. In this study, we involve a sigmoid function to adjust the homotopy parameter. More details of this method can referred to refs [Cui (2003); Fan and Yu (2008); Han Bo et al. (1991); Han Hua et al. (2004); Watson (1989); ŽIGIĆ et al. (1992)].

A sigmoid function can be expressed as follow

$$\lambda(n)=\frac{1}{1+e^{-\theta n}}, \quad (19)$$

where θ is a inclination coefficient. The sigmoid function has an “S” shape, see Fig. 1, which satisfies the following properties:

1. The sigmoid function is continuous and smooth;
2. The range of the sigmoid function (19) is $(0,1)$, and $\lim_{n\to\infty}\lambda(n)=1$ and $\lim_{n\to-\infty}\lambda(n)=0$ hold.

Based on the above-mentioned two properties of the sigmoid function, we can adjust the homotopy parameter by using the sigmoid function during the iterative process. The modified homotopy parameters can be chosen as follow

$$\lambda^{(k)}=\frac{1}{1+e^{-\beta k}}, \quad (20)$$

where k represents the$k$-th iteration, β is the modified parameter, in general, $0<\beta<1$.

In fact, for practical problems, the measurement data usually contain noise, namely

$$\widetilde{\mathbf{C}}_{obs}=\mathbf{C}^*_{obs}+\sigma \quad , \quad (21)$$

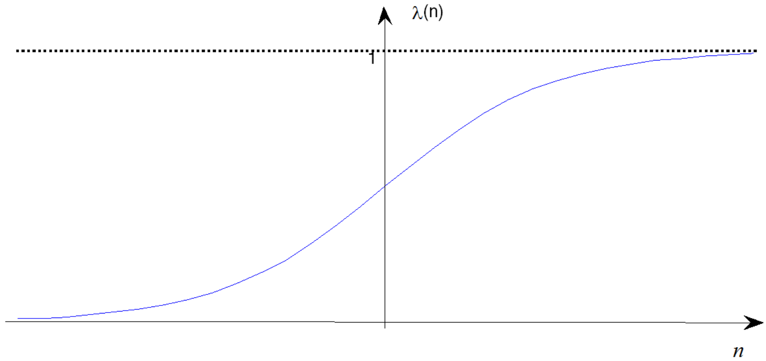

Figure 1: The sigmoid function.

where $\mathbf{C}^*_{obs}$ represents the concentration without noise, and σ denotes the measurement noise. Let $\Delta\mathbf{C} = \widetilde{\mathbf{C}}_{\mathbf{p}} - \mathbf{C}^*_{obs}$, the formula (17) can be rewritten as

$$\left[\lambda\mathbf{G}^T\mathbf{G} + (1-\lambda)\mathbf{I}\right] d\mathbf{p} + \lambda\mathbf{G}^T(\Delta\mathbf{C} - \sigma) = 0 \tag{22}$$

Applying the singular value decomposition, the singular value decomposition of the matrix $\mathbf{G} \in R^{N\times M}$ $(N \geq M)$ is a decomposition of the form

$$\mathbf{G} = \mathbf{U}\Sigma\mathbf{V}^T = \sum_{i=1}^{N} \mathbf{u}_i s_i \mathbf{v}_i^T \tag{23}$$

where $\mathbf{U} = (\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_N)$ and $\mathbf{V} = (\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_N)$ are matrices with orthonormal columns, $\mathbf{U}^T\mathbf{U} = \mathbf{V}^T\mathbf{V} = \mathbf{I}$, and where $\Sigma = diag(s_1, s_2, ..., s_N)$ had non-negative diagonal elements appearing in non-increasing order such that

$$s_1 \geq s_2 \geq ... \geq s_N \geq 0 \tag{24}$$

Then the increment $d\mathbf{p}$ can be obtained as

$$d\mathbf{p} = \sum_{i=1}^{N} \frac{\lambda s_i \mathbf{u}_i^T \Delta\mathbf{C}}{\lambda s_i^2 + (1-\lambda)} \mathbf{v}_i - \sum_{i=1}^{N} \frac{\lambda s_i \mathbf{u}_i^T \sigma}{\lambda s_i^2 + (1-\lambda)} \mathbf{v}_i \tag{25}$$

From the formula (25), we can see that the homotopy parameter should be an appropriate value to be effectively against the effect of the measurement noise. Note that the role of the homotopy parameter is similar to the role of regularization parameter in regularization method.

Now the strategies of the homotopy method to solve the parameter determination problem are given as follow:

1. Given an initial guess parameter vector $\mathbf{p}^{(0)}$, the iteration termination criterion ε(or setting the maximum iterations), the modified parameterβ, and set $k = 0$;

2. Use the implicit finite difference to solve the direct problem, and then obtain the concentration values $C(\mathbf{p}^{(k)}, t_i) i = 1, 2, \cdots, N$; if $\left\| \widetilde{\mathbf{C}}_{\mathbf{p}} - \widetilde{\mathbf{C}}_{obs} \right\| < \varepsilon$, then $\mathbf{p}^{(k)}$ should be the finial regularization solution of the original problem, end; Otherwise, go to the step (3);

3. Select a appropriate homotopy parameter $\lambda^{(k)}$, and calculate $\mathbf{G}^{(k)}$ by the relation (18) and $d\mathbf{p}^{(k)}$ by using the relation(17), and then set $k = k$+1;

4. Let $\mathbf{p}^{(k+1)} = \mathbf{p}^{(k)} + d\mathbf{p}^{(k)}$, then go to the step (2).

The homotopy method is a large-scale convergence method, which have made important contributions in nonlinear problems of real-world applications. One may find more details about this method in the references [Han Bo et al. (1991); Han Hua et al. (2004)].

Note that we employ the implicit finite difference method proposed by Meerschaert [Meerschaert and Tadjeran (2004)] to solve the direct problem in this study. All the programs are run in Matlab 2011b environment, Windows 7, 32 bits, P6000 @1.87GHz, RAM 2.00GB.

3 Examples

To reflect the goodness-of-fit, we employ the coefficient of determination $r^2$and the root mean square error (*RMSE*)

$$r^2 = 1 - \frac{\sum_{i=1}^{N} \left[\widetilde{C}_{\mathbf{p}}(t_i) - \widetilde{C}_{obs}(t_i) \right]^2}{\sum_{i=1}^{N} \left[\widetilde{C}_{obs}(t_i) - \overline{C}_{obs} \right]^2} \tag{26}$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left[\widetilde{C}_{\mathbf{p}}(t_i) - \widetilde{C}_{obs}(t_i) \right]^2} \tag{27}$$

where $\overline{C}_{obs}$ is the average value of the observations $\widetilde{C}_{obs}(t_i), i = 1, 2, \cdots N$, N is the number of observed concentration data at a particular observation point.

Example 1

To examine the convergence of the homotopy method with initial guess value, we test different initial guess values in this example. Firstly, we choose the exact parameter vector as $\mathbf{p} = (\alpha, D, v)^T = (1.78, 0.55, 1.05)^T$, the distance L=100cm, the total time T=270 minutes, calculate the breakthrough curve value at every 5 minutes by using the implicit finite difference method, which can be considered as the measured data. Then we employ the homotopy method under the measured data to determine the unknown parameters α, D, v. In this example, the homotopy parameter is chosen as $\lambda^{(k)} = \frac{1}{1+e^{-0.5k}}$, and the iteration termination $RMSE = 10^{-12}$. Tab. 1 shows the results under different initial guess values. From Tab. 1, the parameters can be obtained very well under five initial guess values expect the last one. From the results of the first five groups, *RMSE* reaches 10^{-13} under appropriate initial guess value and the determination coefficient tends to 1. But the last one may be a local optimal solution of this problem. Thus, choosing an appropriate initial guess value is very necessary for the present method. The homotopy method is a wide-ranged convergence method, but sometime it converges to a local optimal solution. In our study, we test variety of initial guess values to insure the results correct.

Fig. 2 shows the iterative process when we choose the first initial guess value in Tab. 1: the fractional derivative order α, the diffusion coefficient D, the average pore velocity v and the *RMSE* changes with the iteration step (the maximum iterations is 60 steps). From Fig. 2, we can see that the iterative process is stable and fast-convergent. Fig. 3 shows the inversion result compares to the measured data, which shows that the fitted curve is well-fitted with the measured data.

Table 1: The inversion results under different initial guess values.

No.	Initial guess value			Iterations	Inverse results			*RMSE*	r^2
	α	D	v		α	D	v		
1	1.500	1.010	1.000	21	1.780	0.550	1.050	7.9794e-014	1.000
2	1.500	0.010	0.300	21	1.780	0.550	1.050	3.1874e-013	1.000
3	1.500	5.010	4.300	22	1.780	0.550	1.050	4.1221e-014	1.000
4	1.800	9.010	10.300	22	1.780	0.550	1.050	7.5221e-013	1.000
5	1.800	20.000	1.000	24	1.780	0.550	1.050	3.3619e-014	1.000
6	1.800	1.100	10.500	300	1.065	0.470	1.408	0.0014	1.000

Example 2

We consider a laboratory experiment conducted through 1250cm long, horizontally placed column packed with heterogeneity sandy soil [Huang K et al. (1995)]. NaCl was used as the tracer, the concentrations of Cl^- were measured with electrical conductivity at 100cm intervals in the column. We consider the second experiment, i.e., a tracer injection (transport) experiment in the heterogeneous sandy soil

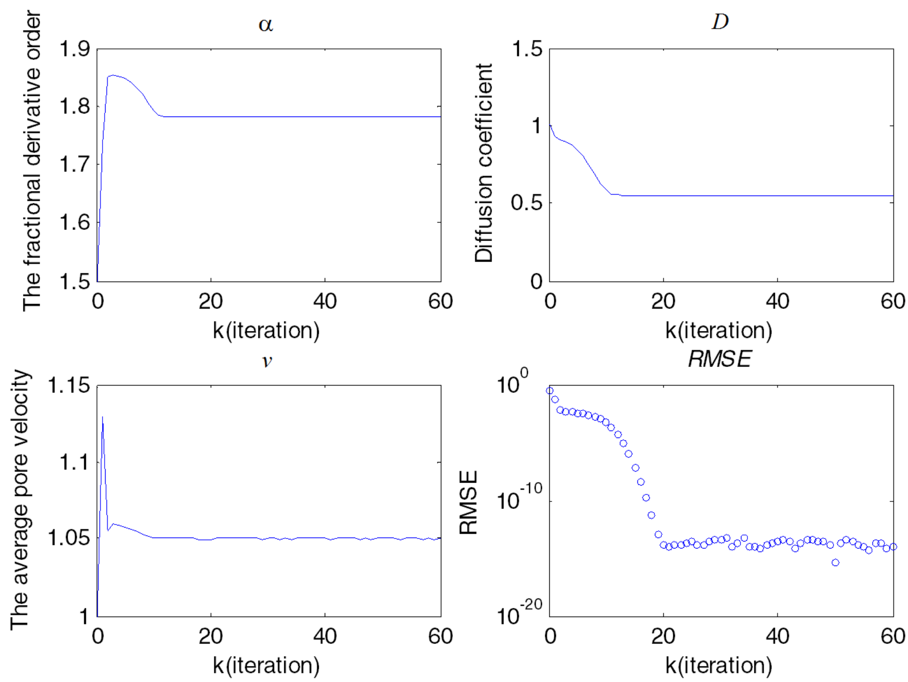

Figure 2: The fractional derivative order α, the diffusion coefficient D, the average pore velocity v and the $RMSE$ changes with the iteration step (the maximum iterations is 60 steps) under the initial guess value $\mathbf{p}^{(0)} = (\alpha, D, v)^T = (1.500, 1.010, 1.000)^T$.

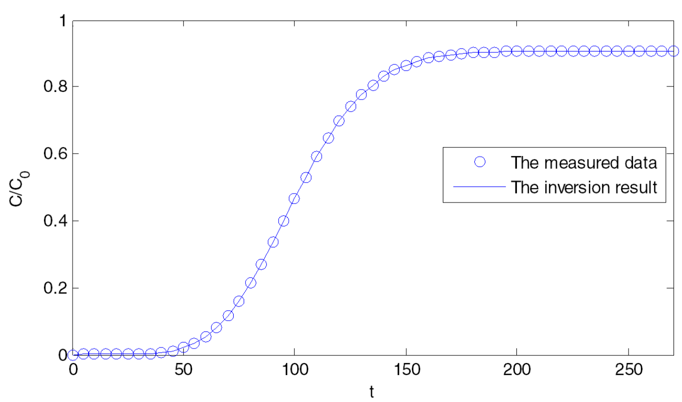

Figure 3: The inversion result compares to the measured data under the initial guess value $\mathbf{p}^{(0)} = (\alpha, D, v)^T = (1.500, 1.010, 1.000)^T$.

column by replacing inflowing tap water with a NaCl solution of concentration C_0 = 6 g/L at the coarse end. The details of this experiment can be referred to [Huang K et al. (1995)]. In term of the analysis by Gao [Garcia and Zangwill (1981)] and Pachepsky [Pachepsky et al. (2000)], the solute transport in the soil column can be modeled by a symmetrical spatial fractional advection-dispersion equation as follows

$$\begin{cases} \frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^\alpha C}{\partial x^\alpha}, 0 < x < L, 1 < \alpha < 2 \\ C(0,t) = 0 \\ C(0,t) = C_0 \\ \left.\frac{\partial C}{\partial x}\right|_{x=L} = 0 \end{cases} \tag{28}$$

We employ the homotopy method to determine the fractional derivative order α, the diffusion coefficient D and the average pore-water vecolcity v in different distances by using the measured breakthrough curves (BTCs). In this example, set the spatial step $dx = 10cm$ and the time step $dt = 10$ mins for the finite difference method. Set the maximum iteration as 200 steps for the termination condition.

Tabl. 2 shows the inversion results under different initial guess values at different distances L=600, 800, 1000cm. The optimal solutions under different initial guess values are obtained by several iterations at a fixed distance. It's seen that the iterative process fast converges to a stable value. The *RMSE* is less than 5% and the determination coefficient reaches 0.97.

Fig. 4 shows the fractional derivative order α, the diffusion coefficient D, the average-water pore velocity v and the *RMSE* changes with the iteration step under the initial guess value $\mathbf{p}^{(0)} = (\alpha, D, v)^T = (1.400, 5.500, 1.500)^T$ at the distance L=600cm. Fig. 6 shows the fractional derivative order α, the diffusion coefficient D, the average pore-water velocity v and the *RMSE* changes with the iteration step under the initial guess value $\mathbf{p}^{(0)} = (\alpha, D, v)^T = (1.500, 60.680, 0.220)^T$ at the distance L=800cm. Fig. 7 shows the fitted BTC and the measured BTC at the distance L=800cm. Fig. 8 shows the fractional derivative order α, the diffusion coefficient D, the average pore-water velocity v and the *RMSE* changes with the iteration step under the initial guess value $\mathbf{p}^{(0)} = (\alpha, D, v)^T = (1.400, 0.500, 0.500)^T$ at the distance L=1000cm. Fig. 9 shows the fitted BTC and the measured data at the distance L=1000cm.

From these results, we can see that the homotopy method is feasible and stable for this parameter determination problem.

Table 2: The inversion results under different initial values at the distances L=600,800,1000cm.

L(cm)	Initial guess value $\mathbf{p}^{(0)} = (\alpha, D, v)^T$			Inversion result $\mathbf{p} = (\alpha, D, v)^T$			r^2	*RMSE*
600	1.400	5.500	1.500	1.760	5.781	1.226	0.977	0.037
	1.500	15.500	1.500					
	1.800	1.500	0.300					
800	1.630	1.680	1.220	1.931	49.110	1.151	0.972	0.048
	1.630	4.680	1.220					
	1.500	60.680	0.220					
1000	1.500	60.680	0.220	1.865	15.489	0.967	0.980	0.030
	1.500	6.000	1.000					
	1.500	0.500	0.500					

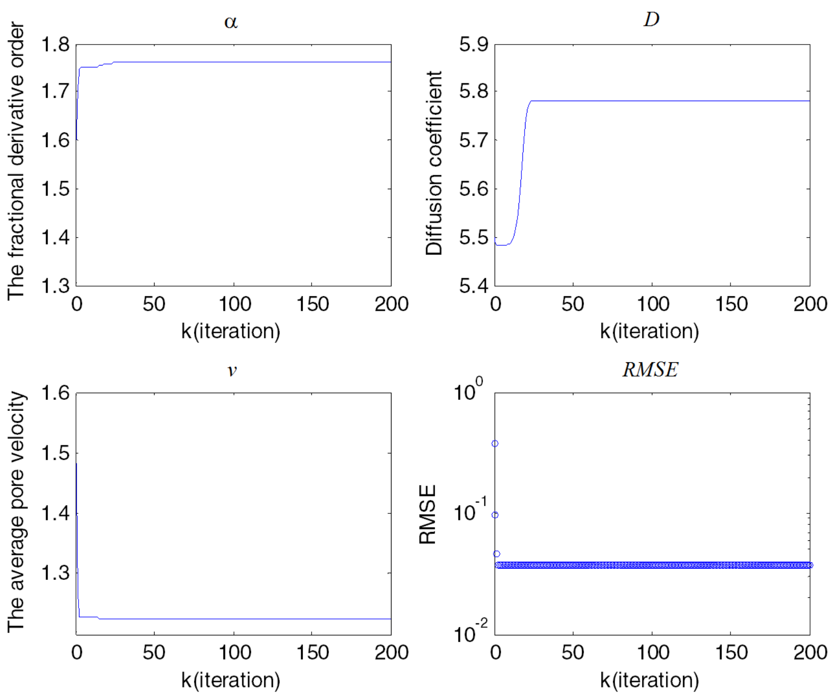

Figure 4: The fractional derivative order α, the diffusion coefficient D, the average pore-water velocity v and the *RMSE* changes with the iteration step under the initial guess value $\mathbf{p}^{(0)} = (\alpha, D, v)^T = (1.400, 5.500, 1.500)^T$ at the distance L=600cm, the maximum iterations equals to 200 steps.

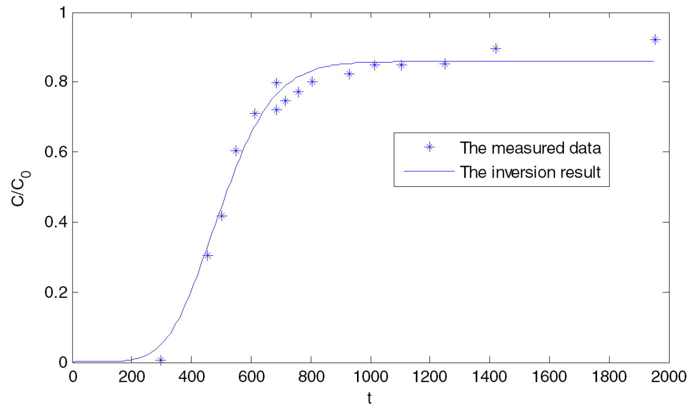

Figure 5: The fitted BTC compares to the measured BTC at L=600cm.

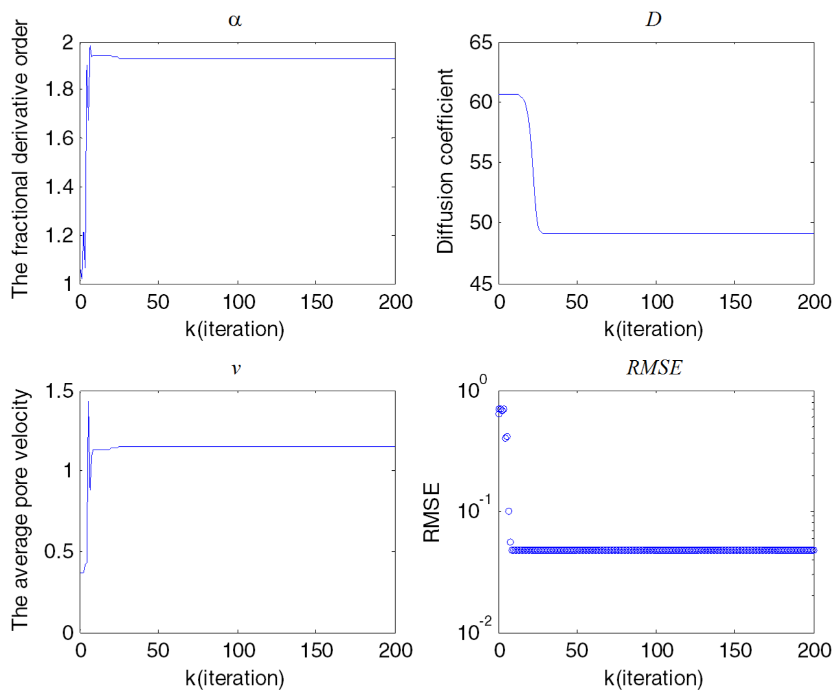

Figure 6: The fractional derivative order α, the diffusion coefficient D, the average pore-water velocity v and the $RMSE$ changes with the iteration step, under the initial guess value $\mathbf{p}^{(0)} = (\alpha, D, v)^T = (1.500, 60.680, 0.220)^T$ at the distance L=800cm, the maximum iterations equals to 200 steps.

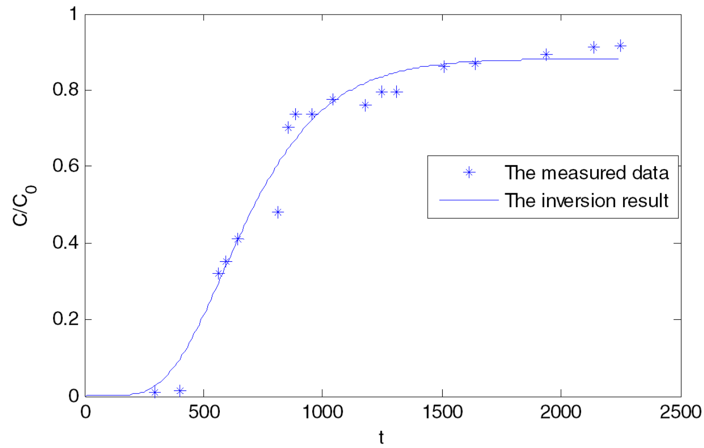

Figure 7: The fitted BTC compares to the measured BTC at L=800cm.

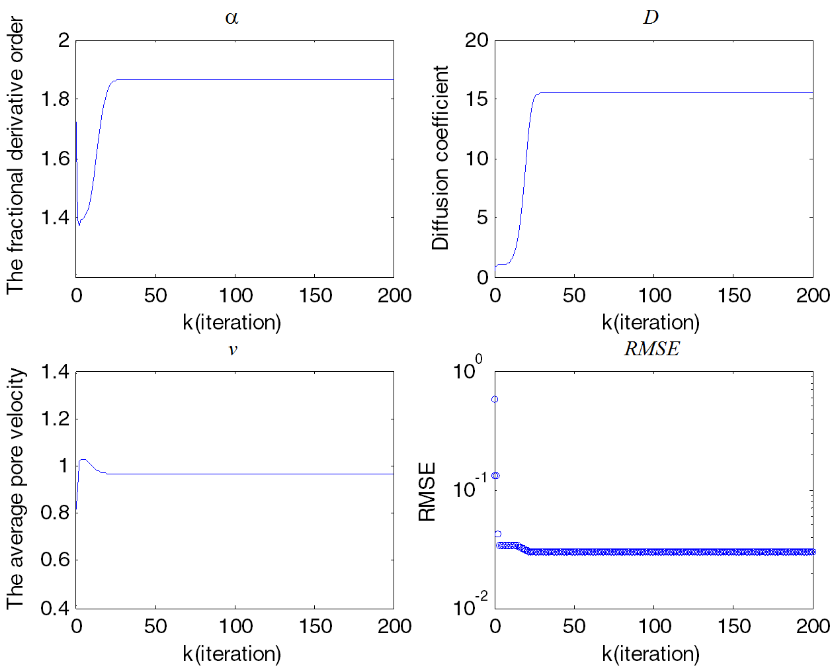

Figure 8: The fractional derivative order α, the diffusion coefficient D, the average pore-water velocity v and the *RMSE* changes with the iteration step under the initial guess value $\mathbf{p}^{(0)} = (\alpha, D, v)^T = (1.400, 0.500, 0.500)^T$ at the distance L=1000cm, the maximum iterations equals to200 steps.

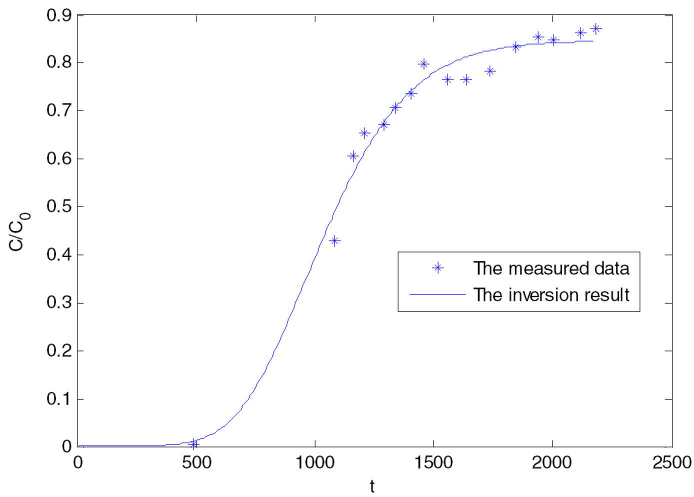

Figure 9: The fitted BTC compares to the measured BTC at L=1000cm.

4 Some remarks

As we known, the homotopy method is a large-scale convergence method for solving nonlinear inverse problems. We employ the method to determine the unknown parameters of the spatial fractional derivative advection-dispersion equation for solute transport in soil column. From the analysis of this study, it is confirmed that the homotopy method is a fast-convergent and efficient method for this kind of parameter inversion problems. In particular, it can be easily developed to solve the problems without analytical solutions.

For the homotopy method, the iteration should be convergent and the unknown parameters can be obtained well under an appropriate initial guess value. Otherwise, the iterative process may trap into local optimum or evenly diverge. It shows that the method is still sensitive for the initial guess value and should be further improved.

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