Numerical Inversion of Space-Time-Dependent Sources in the Integer-Fractional Two-Region Solute Transport System

Chengyuan Yu, Wenyi Liu and Gongsheng Li

Abstract—**This article deals with an inverse problem of determining two space-time-dependent sources in an integer-fractional mobile-immobile two-region solute transport system by additional Dirichlet-Neumann data. The unique existence of a solution to the forward problem is obtained by the method of Laplace transform, and a dynamical system connecting the known data with the unknown sources is established by variational method and boundary homogenization. The dynamical system is discretized to a linear system at a given time in a homogenous polynomial space, and the sources are reconstructed by alternative iterations and Tikhonov regularization. Numerical examples are presented to illustrate the validity of the inversion algorithm.**

Index Terms—**Two-region solute transport, integer-fractional system, inverse source problem, dynamical system, boundary homogenization, numerical inversion.**

I. Introduction

SOIL and groundwater pollution has become a serious threat to sustainable development worldwide. It is essential to characterize migration and diffusion behaviors in mathematics for solute transportation in the soil and groundwater. A typical mathematical model for solute transport in porous media is advection-dispersion equation:

$$u_t - \nabla \cdot (D\nabla u) + q \cdot \nabla u + s(x, t; u) = 0, \tag{1.1}$$

where $u = u(x, t)$ is the state variable at time t and space point x, and D is dispersion/diffusion coefficient tensor, and q is average flow velocity, $s(x, t; u)$ is source term.

Generally speaking, Eq.(1.1) is suitable for equilibrium solute transport, where all porous pores in the media are full of mobile water and chemical reactions of the solute ions possibly occur in a very short period of time. However, some pores in the media could have immobile water, or almost immobile water due to heterogeneity of the media such that the media is divided into mobile and immobile regions. Further assume that there is the first-order kinetic mass transfer between the two regions, and there are no adsorption and degeneration in the process, then there holds (see [11], [12] for instance):

$$\begin{cases} \theta_m \frac{\partial c_m}{\partial t} + \theta_{im} \frac{\partial c_{im}}{\partial t} = \mathcal{L}(x) c_m, \\ \theta_{im} \frac{\partial c_{im}}{\partial t} = \omega (c_m - c_{im}), \end{cases} \tag{1.2}$$

where c_m, c_{im} are solute concentrations in the mobile and immobile regions respectively; θ_m and θ_{im} are volumetric water contents of the mobile and immobile regions respectively, and $\theta_m + \theta_{im} = \theta$ where θ denotes the volumetric water content of the media; $\mathcal{L}(x)$ denotes an elliptic operator describing hydrologic convection and dispersion in space, and ω is the first-order mass transfer rate between the mobile and immobile regions.

The system (1.2) is called the mobile-immobile two-region solute transport model in the case of no sources in heterogeneous porous media. If considering linear adsorption, first-order degeneration and zero-production reaction in the media, and denoting $\beta = \theta_m/\theta$ as a partition parameter, a two-region solute transport model with sources is given as (see [19], [20], [27], [32], for instance)

$$\begin{cases} \beta R \frac{\partial c_m}{\partial t} + (1-\beta) R \frac{\partial c_{im}}{\partial t} = \mathcal{L}(x) c_m - \mu_1 c_m + \gamma_1(x), \\ (1-\beta) R \frac{\partial c_{im}}{\partial t} = \omega (c_m - c_{im}) - \mu_2 c_{im} + \gamma_2(x), \end{cases} \tag{1.3}$$

where $R \geq 1$ is retardation factor, μ_1 and μ_2 are degeneration coefficients, and γ_1, γ_2 are production coefficients in the mobile and immobile regions respectively, and other symbols denote the same meanings as in (1.2).

The models (1.1)-(1.3) are integer-order transport equations which have been studied and applied widely by hydrogeologists in lab and field experiments. Nevertheless, quite a few research studies have shown that fractional diffusion equations are more effective than the classical equations in modeling and describing solute transport behaviors with heavier (power law) tails in recent decades. We only refer to Metzler et al. [24], Metzler and Klafter [25], Zaslavsky [36], Zhang et al. [37] for some early work on the non-instantaneous dynamical models, and recently see [3], [8], [9], [31] for fractional mobile-immobile models and [1], [26] for numerical solutions of fractional differential equations.

It is noted that Schumer et al. [30] proposed a fractional mobile-immobile model by choosing a power-law memory function, which was referred to as the FMIM equation:

$$c_t + r\partial_t^\gamma c = \mathcal{L}(x) c + s(x, t), \tag{1.4}$$

where c denotes the solute concentration in the mobile/immobile region, $r > 0$ is fractional water storage coefficient, and $s(x, t)$ also denotes the source term, and $\partial_t^\gamma c$ is the Caputo's fractional derivative of c on t with the order

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C. Y. Yu is a graduate student of Shandong University of Technology, Zibo, Shandong, 255000 China (e-mail: ycy2783741626@163.com).

W. Y. Liu is a PhD student of Hohai University, Nanjing, Jiangsu 211100, China (e-mail: wenyiliu@hhu.edu.cn).

G. S. Li is a professor of School of Mathematics and Statistics, Shandong University of Technology, Zibo, Shandong, 255000, China (corresponding author to provide phone: 86-533-2782308; e-mail: ligs@sdut.edu.cn).

of $\gamma \in (0,1)$, defined by [15], [28]

$$\partial_t^\gamma c = \frac{1}{\Gamma(1-\gamma)} \int_0^t (t-s)^{-\gamma} \frac{\partial c}{\partial s} ds, \tag{1.5}$$

where $\Gamma(\cdot)$ denotes the Gamma function. The FMIM equation (1.4) is a basic model leading to follow-up studies on anomalous diffusion of solute transport in porous media, see [6], [10], [13], [23], [35] for instance.

Based on the models (1.2)-(1.4), we will consider an integer-fractional two-region solute transport system in the mobile-immobile porous media. This system is a deformation of the FMIM equation (1.4), where the classical hydrologic advection-dispersion transport occurs in the mobile region and the solute variations in the immobile region result from the first-order mass transfer between the mobile and the immobile regions with time-memory effect. By the method of Laplace transform, a unique solution to the integer-fractional two-region solute transport system is deduced, which gives mathematical foundation for further studies of the integer-fractional solute transport model.

On the other hand, some parameters in the model are always unknown in advance, such as the mass transfer rate, the initial distribution of the solute ions, the source term, etc. In these cases, we have to encounter some inverse problems related to the corresponding model. As for inverse problems in fractional diffusion equations, we refer to [7], [29] for early typical work, and recently see [5], [14], [17], [34], etc. To the authors' best knowledge, there are few studies on inverse problems associated with a system of fractional differential equations [2], [18]. In this paper we will deal with an inverse source problem for the integer-fractional two-region solute transport system from numerics.

As we know it is tough to study an inverse coefficient problem in PDEs from theory and numerics when the unknown coefficient is space-time-dependent, or space-state-dependent, or time-state-dependent. This work aims to reconstruct two space-time-dependent sources in the integer-fractional two-region solute transport system. It is still meaningful to investigate such inverse source problems from the viewpoint of engineering applications.

It is noted that ordinary methodologies, such as gradient-type optimal algorithms, are not good and effective for inverse space-time-dependent coefficient problems. Fortunately, a boundary functional energy method was proposed to solve inverse coefficient problems numerically arising in science and engineering, see [21], [22] for instance. This method does not need to solve the forward problem repetitiously and does not need to compute the gradient of the cost functional. However, this method lacks mathematical analysis and basis to some extent. We will develop this method to solve the inverse source problem for the integer-fractional two-region solute transport system, and give some theoretical analysis based on the variational method, which is the main contribution of this paper. By utilizing the variational method, the undetermined parameters in our inversion algorithm can be solved uniquely and the algorithm's implementation becomes easy compared with the previous work [21], [22]. In addition, regularization strategy is always employed to solve inverse coefficient problems in order to overcome the ill-posedness [4], [16]. The inverse source problem here is approximated and transformed to a linear system by discretization, and Tikhonov regularization is utilized to solve the discretized system uniquely, which is another contribution of this paper.

The rest of the paper is organized as follows.

In section 2, the integer-fractional two-region solute transport system with space-time-dependent sources is introduced, and the unique existence of a solution to the forward problem is obtained using the method of Laplace transform. In section 3, the inverse space-time-dependent source problem is set forth by overposing all of Dirichlet-Neumann boundary data, and it is reduced to a dynamical system by the variational method and boundary homogeneity. In section 4, the dynamical system is discretized to a linear system by alternative iterations for the sources and the solutions of the forward problem, and the inversion algorithm with Tikhonov regularization is proposed. In section 5, numerical experiments are performed, and concluding remarks are given in section 6.

II. The integer-fractional two-region model and its solution

A. The mathematical model

Consider a heterogeneous porous media divided into mobile and immobile regions, and the space domain is set to be $\Omega = (0,1)$ by simplification and dimensionless.

Assume that the solute migration and diffusion begin in the mobile region, and some mass transfer occurs between the mobile and the immobile regions. Further assume that the solute transport behavior in the mobile region is governed by the classical hydrologic advection-dispersion and reaction-diffusion actions, and it becomes a dynamic process with memory-effect in the immobile region. Thus an integer-fractional mobile-immobile two-region solute transport system is obtained, where the solute variations in the immobile region is described by a time-fractional differential equation, and the solute transport in the mobile region is described by the classical convection-diffusion equation. By introducing space-time-dependent sources in the two regions respectively, we have

$$\begin{cases} u_t &= Du_{xx} - u_x - \omega(u-v) + s_1, \\ \tau\, \partial_t^\gamma v &= \omega(u-v) + s_2, \end{cases} \tag{2.1}$$

where $u = u(x,t)$ and $v = v(x,t)$ denote the solute concentrations, and $s_1 = s_1(x,t)$ and $s_2 = s_2(x,t)$ denote the sources in the mobile and immobile regions respectively, and $(x,t) \in \Omega \times (0,\infty)$, and ∂_t^γ denotes the Caputo fractional operator on $t > 0$ of the γ-order $(0 < \gamma < 1)$; $\tau > 0$ is a constant related with the partition parameter, the retardation factor and the fractional time scale, and $D > 0$ is a constant related with the hydrodynamical parameters, and $\omega > 0$ also denotes the first-order mass transfer rate between the mobile and immobile regions.

The model (2.1) is an integer-fractional system combining the hydrologic advection-dispersion transport in the mobile with the fractional diffusion in the immobile, which can be regarded as a deformation of the FMIM equation. In fact, by (2.1) there holds

$$u_t + \tau\, \partial_t^\gamma v = Du_{xx} - u_x + s_1 + s_2, \tag{2.2}$$

which induces the same equation as (1.4) if considering the solute transport in the given mobile/immobile region. From the viewpoint of engineering application, the system model (2.1) seems more practical than the FMIM equation (1.4).

For the system (2.1), the initial condition is given as:

$$u(x,0)=1, \quad v(x,0)=0, \quad 0 \le x \le 1, \tag{2.3}$$

which means that there is a constant distribution of the considered solute in the mobile region, and the solute concentration in the immobile is zero at the initial stage. The boundary condition at $x=0$ is given as

$$u(0,t)=1, \quad v(0,t)=0, \quad t>0, \tag{2.4}$$

which implies that the left-hand side of the region in the mobile keeps a constant same as the initial. The boundary condition at $x=1$ is impermeable, which given as

$$u_x(1,t)=v_x(1,t)=0, \quad t>0. \tag{2.5}$$

As a result we get a determined system composed by (2.1) with (2.3)-(2.5) which is called forward problem of the mobile-immobile two-region solute transport system.

In what follows we first prove the unique existence of the solution to the forward problem by using the Laplace transform, and then set forth an alternative iteration algorithm based on variational method and boundary homogenization to determine the two source functions in the system (2.1).

B. Existence of the solution

Assume that for given $x \in \Omega$, any possible solutions $u(x,t)$ and $v(x,t)$ to the system (2.1) and source functions $s_1(x,t)$ and $s_2(x,t)$ satisfy the growth condition on $t>0$:
(A1) $|u(x,t)|, |v(x,t)|,\ |s_1(x,t)|, |s_2(x,t)| \le M\exp(c_0 t)$ as $t \to \infty$, and M, c_0 are positive constants.

In addition, assume that the source functions $s_1(x,t)$ and $s_2(x,t)$ are continuous on $x \in \bar{\Omega}$ for any given $t>0$. By performing Laplace transform for the system (2.1), and thanks to the initial condition (2.3), we get

$$\begin{cases} p\ \hat{u} - 1 = D\hat{u}_{xx} - \hat{u}_x - \omega(\hat{u}-\hat{v}) + \hat{s}_1, \\ \tau p^\gamma\ \hat{v} = \omega(\hat{u}-\hat{v}) + \hat{s}_2, \end{cases} \tag{2.6}$$

where $\hat{u}=\hat{u}(x;p)$, $\hat{v}=\hat{v}(x;p)$ denote the Laplace transforms of $u(x,t)$ and $v(x,t)$ on $t>0$ for fixed $x\in\Omega$ respectively, which are defined by

$$\begin{cases} \hat{u}(x;p) = \int_0^\infty \exp(-pt)u(x,t)dt, \\ \hat{v}(x;p) = \int_0^\infty \exp(-pt)v(x,t)dt, \end{cases} \tag{2.7}$$

here p is the Laplace transform parameter satisfying the convergent condition $\mathrm{Re}(p) > c_0$, and $c_0>0$ is given in the growth condition (A1); $\hat{s}_1=\hat{s}_1(x;p)$, $\hat{s}_2=\hat{s}_2(x;p)$ denote the Laplace transforms of $s_1(x,t)$ and $s_2(x,t)$ on $t>0$ also for fixed $x\in\Omega$ respectively, which are defined like (2.7). From the second equation of (2.6) there is

$$\hat{v} = \frac{\omega}{\tau p^\gamma + \omega}\hat{u} + \frac{\hat{s}_2}{\tau p^\gamma + \omega}. \tag{2.8}$$

Thus we have by the first equation of (2.6)

$$D\hat{u}_{xx} - \hat{u}_x + b\hat{u} = d(x), \tag{2.9}$$

where $b = -\omega - p + \frac{\omega^2}{\tau p^\gamma + \omega}$, and $d(x) = -1 - \hat{s}_1(x) - \frac{\omega \hat{s}_2(x)}{\tau p^\gamma + \omega}$.

Eq.(2.9) is a second-order inhomogeneous ordinary differential equation on $x\in\Omega$ with constant coefficients. By (2.3) and (2.4) the boundary conditions are given as

$$\hat{u}(0) = 1/p,\ \hat{u}'(1) = 0. \tag{2.10}$$

By the theory of the second-order inhomogeneous ODE, there holds

Lemma 1([33]) Assume that the growth condition (A1) is valid for the functions $u(x,t)$, $v(x,t)$ and $s_1(x,t)$, $s_2(x,t)$ on $t>0$, and the source functions are continuous on $x\in\bar{\Omega}$; and the coefficients $D>0$, $\tau>0$, $\omega>0$ and $\gamma\in(0,1)$, and the Laplace transform parameter p satisfies $\mathrm{Re}(p)>c_0>0$, then the problem (2.9)-(2.10) has a unique, bounded solution.

Nevertheless, following the method used in [18], we can get the unique existence of the solution to the forward problem (2.1), (2.3)-(2.5).

Theorem 1 Under the conditions of Lemma 1, the forward problem (2.1), (2.3)-(2.5) has a unique solution in $L^\infty(\Omega_\infty)$.

Proof Under the conditions of the theorem, and by the method of inverse Laplace transform, the contour integral

$$\frac{1}{2\pi i}\int_{p_0-i\infty}^{p_0+i\infty} \hat{u}(x,p)e^{pt}dp,$$

is convergent for $(x,t)\in\Omega_\infty$, which is the solution $u(x,t)$, i.e., there is

$$u(x,t) = \frac{1}{2\pi i}\int_{p_0-i\infty}^{p_0+i\infty} \hat{u}(x;p)e^{pt}dp, \tag{2.11}$$

where $p_0 = \mathrm{Re}(p) > c_0$. Similarly, we can get the expression of the solution $v(x,t)$.

This theorem gives the unique existence of solution to the forward problem in the bounded space of $L^\infty(\Omega_\infty)$, and the solution's regularity is still open due to the complexity of the contour integral. However, it is still meaningful in mathematics to obtain the existence and the expression of the solution to the forward problem.

III. Inverse source problem and dynamical system

A. The inverse source problem

The source terms $s_1(x,t)$ and $s_2(x,t)$ in the system (2.1) are essential issues characterizing some physical/chemical/biological actions in the solute transportation, which are always unknown for real-life problems. At this point, if having some additional measurable data on the solution, we can determine them by utilizing the method of inverse source problems.

Assume that the two sources s_1 and s_2 are both space-time-dependent and continuous functions on $x\in\Omega$ and $t>0$. Noting the known boundary conditions given by (2.4)-(2.5), we give the following additional boundary conditions:

$$u_x(0,t), v_x(0,t);\ u(1,t), v(1,t),\ t>0; \tag{3.1}$$

$$s_1(0,t), s_1(1,t),\ \frac{\partial s_1}{\partial x}(0,t), \frac{\partial s_1}{\partial x}(1,t),\ t>0; \tag{3.2}$$

and

$$s_2(0,t), s_2(1,t),\ \frac{\partial s_2}{\partial x}(0,t), \frac{\partial s_2}{\partial x}(1,t),\ t>0. \tag{3.3}$$

Therefore, an inverse source problem is formulated by the system (2.1), the initial boundary value conditions (2.3)-(2.5), together with the additional boundary conditions (3.1)-(3.3), which is to determine the two source functions $s_1(x,t)$ and $s_2(x,t)$ in (2.1) simultaneously.

It is feasible from the viewpoint of engineering to measure the boundary values and the boundary fluxes for the state variables and the sources, in other words, the additional conditions (3.1)-(3.3) are reasonable and acceptable.

B. The dynamical system

In what follows we set forth a dynamical system connecting the known data with the unknown sources, which plays an important role in the inversion algorithm.

Theorem 2 For the inverse source problem of determining $s_1(x,t)$ and $s_2(x,t)$ in (2.1), there exist third-order polynomials $H_1(\cdot,t)$ and $H_2(\cdot,t)$ on $x\in\Omega$ such that there holds for any given $t>0$:

$$\left\{\begin{array}{rcl} \int_\Omega s_1\tilde{u}dx &=& \int_\Omega \frac{\partial}{\partial t}(\tilde{u}+H_1)\tilde{u}dx \\ &-& D\int_\Omega(\tilde{u}+H_1)\tilde{u}_{xx}dx-\int_\Omega(\tilde{u}+H_1)\tilde{u}_x dx \\ &+& \omega\int_\Omega(\tilde{u}-\tilde{v}+H_1-H_2)\tilde{u}dx, \\ \int_\Omega s_2\tilde{v}dx &=& \tau\int_\Omega \partial_t^\gamma(\tilde{v}+H_2)\tilde{v}dx \\ &-& \omega\int_\Omega(\tilde{u}-\tilde{v}+H_1-H_2)\tilde{v}dx, \end{array}\right. \tag{3.4}$$

where $\tilde{u},\tilde{v}$ are prescribed functions on $x\in\Omega$ and $t>0$, which satisfy the homogeneous Dirichlet and Neumann boundary conditions.

Proof By smooth functions $\varphi(x,t)$ and $\psi(x,t)$ multiplying the mobile and immobile equations of (2.1), and integrating on Ω respectively, there is

$$\left\{\begin{array}{l} \int_\Omega[u_t-Du_{xx}+u_x+\omega(u-v)]\varphi(x,t)dx \\ =\int_\Omega s_1(x,t)\varphi(x,t)dx; \\ \int_\Omega[\tau\partial_t^\gamma v-\omega(u-v)]\psi(x,t)dx \\ =\int_\Omega s_2(x,t)\psi(x,t)dx. \end{array}\right. \tag{3.5}$$

Let φ and φ_x are homogeneous at the boundary of Ω, i.e., there are $\varphi|_{\partial\Omega}=0$ and $\varphi_x|_{\partial\Omega}=0$. There holds by integration by part

$$\left\{\begin{array}{l} \int_\Omega[u_t\varphi-Du\varphi_{xx}-u\varphi_x+\omega(u-v)\varphi]dx=\int_\Omega s_1\varphi dx; \\ \int_\Omega[\tau\partial_t^\gamma v\ \psi-\omega(u-v)\psi]dx=\int_\Omega s_2\psi dx. \end{array}\right. \tag{3.6}$$

Next, let $H_1(x,t)$ satisfy the following boundary conditions on $x\in\Omega$:

$$H_1|_{x=0,1}=u|_{x=0,1},\ \frac{\partial H_1}{\partial x}|_{x=0,1}=\frac{\partial u}{\partial x}|_{x=0,1}. \tag{3.7}$$

By the method of undetermined coefficients, there exists a unique third-order polynomial of x given as

$$\begin{array}{rcl} H_1(x,t) &=& x^3[2-2u(1,t)+u_x(0,t)]-x^2[3-3u(1,t) \\ &+& 2u_x(0,t)]+xu_x(0,t)+1, \end{array} \tag{3.8}$$

Similarly one can determine the function $H_2(x,t)$ given as:

$$\begin{array}{rcl} H_2(x,t) &=& x^3[-2v(1,t)+v_x(0,t)]-x^2[-3v(1,t) \\ &+& 2v_x(0,t)]+xv_x(0,t). \end{array} \tag{3.9}$$

Henceforth by setting

$$\tilde{u}=u-H_1,\ \tilde{v}=v-H_2, \tag{3.10}$$

we get two functions $\tilde{u}$ and $\tilde{v}$, which satisfy the homogeneous Dirichlet-Neumann boundary conditions, respectively. Combining with (3.6) and choosing $\varphi=\tilde{u}$ and $\psi=\tilde{v}$, we obtain the dynamical system (3.4). The proof is completed.

It is noted that (3.4) is a group of integral equations on the unknown sources, and it is also a dynamical system on the time $t>0$, and the two source functions must satisfy the system (3.4). Furthermore, the system is also valid for the series of time $t=t_j$, $j=1,2,\cdots$. From this viewpoint, the dynamical system is discretized on the time, and the sources s_1 and s_2 can be reconstructed by alternative iterations with the aids of regularization strategy.

IV. The inversion algorithm

A suitable approximate space is always needed to implement an inversion algorithm. If fixing $t=t_j\in(0,T]$, $j=1,2,\cdots$ in the dynamical system (3.4) for any given $T>0$, the solutions u, v and the source functions s_1 and s_2 can be regarded as functions of the space variable $x\in\Omega$. Let $\mathcal{V}$ be an approximate space composed by basis functions $B_j(x)$, $j=1,2,\cdots$, i.e., $\mathcal{V}=\text{span}\{B_j(x),j\geq 1\}$, and there holds the homogeneous condition:

$$B_j(0)=B_j(1)=0,\ B_j'(0)=B_j'(1)=0,\ j\geq 1, \tag{4.1}$$

and $\|B_j\|_{L^2(\Omega)},\|B_j'\|_{L^2(\Omega)}\not\equiv 0$ for any $j\geq 1$.

Now let $t=t_j$ ($j=1,2,\cdots$) in (3.4), and $\tilde{u}$ and $\tilde{v}$ be expressed at such t_j by

$$\left\{\begin{array}{l} \tilde{u}|_{t=t_j}=\lambda_1^j B_j(x), \\ \tilde{v}|_{t=t_j}=\lambda_2^j B_j(x), \end{array}\right. \tag{4.2}$$

where λ_1^j and λ_2^j are undetermined parameters dependent upon t_j, $j=1,2,\cdots$.

Assume that the source terms s_1 and s_2 are prescribed given, then by substituting (4.2) into (3.4), a linear system of the parameters λ_1^j and λ_2^j is deduced and we can get:

$$\left\{\begin{array}{l} \lambda_1^j=\frac{c+d}{b-a}, \\ \lambda_2^j=\frac{ad+bc}{b(b-a)}, \end{array}\right. \tag{4.3}$$

where the coefficients a,b and c,d are given as follows:

$$\left\{\begin{array}{ll} a &=D\int_\Omega(B_j')^2dx+\omega\int_\Omega(B_j)^2dx; \\ b &=\omega\int_\Omega(B_j)^2dx; \\ c &=\int_\Omega B_j(\frac{\partial H_1}{\partial t})_{t=t_j}dx+D\int_\Omega B_j'\frac{\partial H_1}{\partial x}dx \\ &\quad+\int_\Omega B_j\frac{\partial H_1}{\partial x}dx+\omega\int_\Omega B_j(H_1-H_2)dx-\int_\Omega B_js_1dx; \\ d &=\tau\int_\Omega B_j(\partial_t^\gamma H_2)_{t=t_j}dx-\omega\int_\Omega B_j(H_1-H_2)dx \\ &\quad-\int_\Omega B_js_2dx. \end{array}\right. \tag{4.4}$$

For convenience of writing, denote

$$z_1^j=\lambda_1^jB_j(x),\ z_2^j=\lambda_2^jB_j(x),j\geq 1. \tag{4.5}$$

Take a fixed integer $K\geq 1$, which is called discretized dimension of the source functions in the approximate space. With a completely similar method as used for u and v, the sources s_1 and s_2 are homogenized and expressed in terms of functions in $\mathcal{V}$ via

$$\left\{\begin{array}{l} s_1(x,t)=f_1(x,t)+\sum\limits_{k=1}^K c_1^kz_1^k(x); \\ s_2(x,t)=f_2(x,t)+\sum\limits_{k=1}^K c_2^kz_2^k(x), \end{array}\right. \tag{4.6}$$

where c_1^k and c_2^k ($k=1,2,\cdots,K$) are coefficients undetermined, and $f_1(x,t)$ and $f_2(x,t)$ are determined by the additional boundary data (2.7) and (2.8) as done in determining $H_1(x,t)$ and $H_2(x,t)$, which are expressed as below:

$$\begin{array}{l} f_i(x,t) \\ =\frac{x^3}{l^3}[2s_i(0,t)-2s_i(l,t)+l\frac{\partial s_i}{\partial x}(0,t)+l\frac{\partial s_i}{\partial x}(l,t)] \\ +\frac{x^2}{l^2}[-3s_i(0,t)+3s_i(l,t)-2l\frac{\partial s_i}{\partial x}(0,t)-l\frac{\partial s_i}{\partial x}(l,t)] \\ +x\frac{\partial s_i}{\partial x}(0,t)+s_i(0,t),\ i=1,2. \end{array} \tag{4.7}$$

As done in the above, let $t = t_j (j \geq 1)$ in (3.4), and substitute (4.6) into (3.4), and choose $\tilde{u}$ and $\tilde{v}$ at $t = t_j$ as z_1^j and z_2^j respectively, we get a linear system on $c_1 = (c_1^1, \cdots, c_1^K)^T$ and $c_2 = (c_2^1, \cdots, c_2^K)^T$, which is given via:

$$\begin{cases} \sum\limits_{k=1}^{K} c_1^k \int_\Omega z_1^j z_1^k dx = y_1^j, \\ \sum\limits_{k=1}^{K} c_2^k \int_\Omega z_2^j z_2^k dx = y_2^j, \end{cases} \tag{4.8}$$

where y_1^j, y_2^j $(j \geq 1)$ are computed by

$$\begin{array}{rcl} y_1^j &=& \int_\Omega z_1^j (\frac{\partial H_1}{\partial t})_{t_j} dx + D \int_\Omega [\frac{\partial z_1^j}{\partial x}]^2 dx \\ &-& D \int_\Omega z_1^j \frac{\partial^2 H_1}{\partial x^2} dx + \int_\Omega z_1^j \frac{\partial H_1}{\partial x} dx \\ &+& \omega \int_\Omega z_1^j (z_1^j - z_2^j + H_1 - H_2) dx \\ &-& \int_\Omega z_1^j f_1(x, t_j) dx; \end{array} \tag{4.9}$$

and

$$\begin{array}{rcl} y_2^j &=& \tau \int_\Omega z_2^j (\partial_t^\gamma H_2)_{t_j} dx - \int_\Omega z_2^j f_2(x, t_j) dx \\ &-& \omega \int_\Omega z_2^j (z_1^j - z_2^j + H_1 - H_2) dx, \end{array} \tag{4.10}$$

respectively.

Take an integer $J \geq 1$, which is called discretized dimension of the dynamical system (3.4), and let $j = 1, 2, \cdots, J$, we rewrite (4.8) in a matrix form:

$$GC = Y, \tag{4.11}$$

where

$$\begin{cases} G = \begin{pmatrix} G_1 & 0 \\ 0 & G_2 \end{pmatrix};\ C = (c_1, c_2)^T; Y = (y_1, y_2)^T; \\ G_1 = \left(g_{jk}^1\right)_{J \times K},\ g_{jk}^1 = \int_\Omega z_1^j z_1^k dx; \\ G_2 = \left(g_{jk}^2\right)_{J \times K},\ g_{jk}^2 = \int_\Omega z_2^j z_2^k dx; \\ Y_1 = \left(y_1^1, y_1^2, \ldots, y_1^K\right)^T, Y_2 = \left(y_2^1, y_2^2, \ldots, y_2^K\right)^T. \end{cases} \tag{4.12}$$

Now we give the solvability of the linear system (4.11).

Noting that the coefficient matrix G and the right-hand term Y are generated by the additional data (3.1)-(3.3), they have random perturbations in the production. Assume that the upper bound of the noises is $\delta > 0$, and we have a disturbed equation:

$$G^\delta C = Y^\delta, \tag{4.13}$$

where G^δ, Y^δ are the noised matrix and the right-hand term. There holds

Theorem 3 For any given $\delta > 0$, there exists an optimal parameter α^*, and a unique regularized solution, denoted as $C^{\alpha^*,\delta}$, to the system (4.11), which can be expressed by

$$C^{\alpha^*,\delta} = (\alpha^* I + (G^\delta)^T G^\delta)^{-1} (G^\delta)^T Y^\delta, \tag{4.14}$$

here I denotes the identity matrix, $(G^\delta)^T$ denotes the transpose of G^δ.

Proof By the general theory of Tikhonov regularization [16], a regularized solution of (4.11), denoted as $C^{\alpha,\delta}$, should satisfy the normal equation:

$$(G^\delta)^T G^\delta C^{\alpha,\delta} + \alpha C^{\alpha,\delta} = (G^\delta)^T Y^\delta, \tag{4.15}$$

where $\alpha > 0$ is the regularization parameter. Henceforth, for any given $\delta > 0$, there must have an optimal regularization parameter $\alpha^* = \alpha^*(\delta, Y^\delta) > 0$ such that the matrix $\alpha^* I + (G^\delta)^T G^\delta$ is symmetric positive definite, and the equation (4.15) has a unique solution expressed by (4.14). This solution is called regularized solution of the system (4.11), and there holds $C^{\alpha^*,\delta} \to C$ as $\delta \to 0$ and $\alpha^* \to 0$, here C denotes the exact solution of (4.11).

The procedure of the algorithm is summarized as follows.

Inversion Algorithm:

Step 1. Give the basis functions $B_j(x) (j \geq 1)$, the time $T > 0$, the discretized dimensions $K, J \geq 1$, the convergent precision ε and the noise level δ. For each $t_j \in (0, T]$ $(j = 1, 2, \cdots, J)$, set initial values of λ_1^j and λ_2^j be zero, and initial guess of C^0 be zero vector;

Step 2. For $k = 0, 1, \ldots K$, calculate z_1^j and z_2^j by (4.5) and s_1 and s_2 by (4.6) respectively;

Step 3. Get the updated coefficients λ_1^j and λ_2^j by (4.3), and then update z_1^j and z_2^j by (4.5) again;

Step 4. Calculate the coefficient matrix G, and the right-hand term Y by (4.12) using the updated z_1^j and z_2^j;

Step 5. For given $\delta > 0$, by choosing the regularization parameter $\alpha > 0$, to get an optimal solution by (4.14) as the updated C, denoted by $C^{(k)} = (c_1^{(k)}, c_2^{(k)})^T$;

Step 6. If $\|C^{(k+1)} - C^{(k)}\|_2 < \varepsilon$, the algorithm terminates and an optimal source solution is obtained by (4.6); Otherwise, go on by turning to Step 2.

V. Numerical experiments

A. *Example 1*

For $(x, t) \in (0, 1) \times (0, 1)$ let the exact solution of the forward problem be

$$u(x, t) = (x^2 - 2x)t + 1;\ v(x, t) = (\frac{1}{2}x^2 - \frac{1}{3}x^3)t, \tag{5.1}$$

and the exact source functions be:

$$\begin{cases} s_1(x, t) &=& -\frac{t}{2}(-\frac{x^3}{3} + \frac{x^2}{2}) - 2x - 2t + (2x - 2)t \\ &+& \frac{t}{2}(x^2 - 2x) + x^2 + \frac{1}{2}, \\ s_2(x, t) &=& \frac{t^{(1-\gamma)}(\frac{x^2}{2} - \frac{x^3}{3})}{\Gamma(2-\gamma)} - \frac{t}{6}x^3 - \frac{t}{4}x^2 + xt - \frac{1}{2}. \end{cases} \tag{5.2}$$

By the above exact solutions we have the additional data at the boundaries, and then the two source functions are reconstructed with noisy data by the inversion algorithm.

On the concrete implementation of the inversion algorithm, take $T = 1$, $\tau = 1$, and $\gamma = 0.5$, and $D = 1$, $\omega = 0.5$ as the model parameters, and take $B_j(x) = x^2(1 - x)^2 x^{j-1}$ $(j = 1, 2, \cdots)$ as the basis functions of the approximate space, and choose $K = J = 3$, $\varepsilon = 1e - 4$ as the inversion parameters. As for the regularization parameter, we choose $\alpha = 0.1$ due to the severe ill-posedness of the system (4.11).

Noting the random noises of the additional data, the inversion result for given noise is an average value of continuous ten-time computations. The inversion errors in the solutions are listed in Tables I-III, where Err_1^1 and Err_1^2 denote the relative errors of s_1 and s_2 at (x, t), Err_2^1 and Err_2^2 denote the relative errors of s_1 and s_2 in L^2-norm at the time $T = 1$, respectively. Moreover, the inversion sources of s_1 and s_2 with the noise level $\delta = 5\%$, and the exact sources are plotted in Figures 1-2, respectively.

Tables I-III and Figs 1-2 show that the inversion sources give good approximations to the exact sources, and the solution errors become small as the noise level goes to small demonstrating that the inversion algorithm is stable against the data noises.

TABLE I
INVERSION RESULTS OF s_1 WITH $\delta = 1\%$ IN EX.1

(x,t)	Inversion Solu.	Exact Solu.	Err_1^1
(0.2, 0.2)	-0.617964766	-0.617733333	3.75e-4
(0.4, 0.4)	-1.559694139	-1.559733333	2.51e-5
(0.6, 0.6)	-2.305021734	-2.304400000	2.70e-4
(0.8, 0.8)	-2.824795065	-2.823733333	3.76e-4
(1.0, 1.0)	-3.084363139	-3.083333333	3.34e-4

TABLE II
INVERSION RESULTS OF s_2 WITH $\delta = 1\%$ IN EX.1

(x,t)	Inversion Solu.	Exact Solu.	Err_1^2
(0.2, 0.2)	-0.454182226	-0.453519807	1.46e-3
(0.4, 0.4)	-0.318797420	-0.318399221	1.25e-3
(0.6, 0.6)	-0.121471238	-0.121203816	2.21e-3
(0.8, 0.8)	0.094182394	0.094448449	2.82e-3
(1.0, 1.0)	0.271006467	0.271396528	1.44e-3

TABLE III
INVERSION ERRORS WITH NOISES AT $T = 1$ IN EX.1

δ	Err_2^1	Err_2^2
5%	7.31e-3	9.52e-2
1%	1.35e-3	2.38e-2
0.1%	8.44e-5	1.59e-3

TABLE IV
INVERSION RESULTS OF s_1 WITH $\delta = 1\%$ IN EX.2

(x,t)	Inversion Solu.	Exact Solu.	Err_1^1
(0.2, 0.2)	1.281899585	1.290420514	6.60e-3
(0.4, 0.4)	2.258525546	2.286362652	1.22e-2
(0.6, 0.6)	3.240805701	3.278301363	1.14e-2
(0.8, 0.8)	4.022861172	4.043684529	5.15e-3
(1.0, 1.0)	4.384496670	4.384067767	9.78e-5

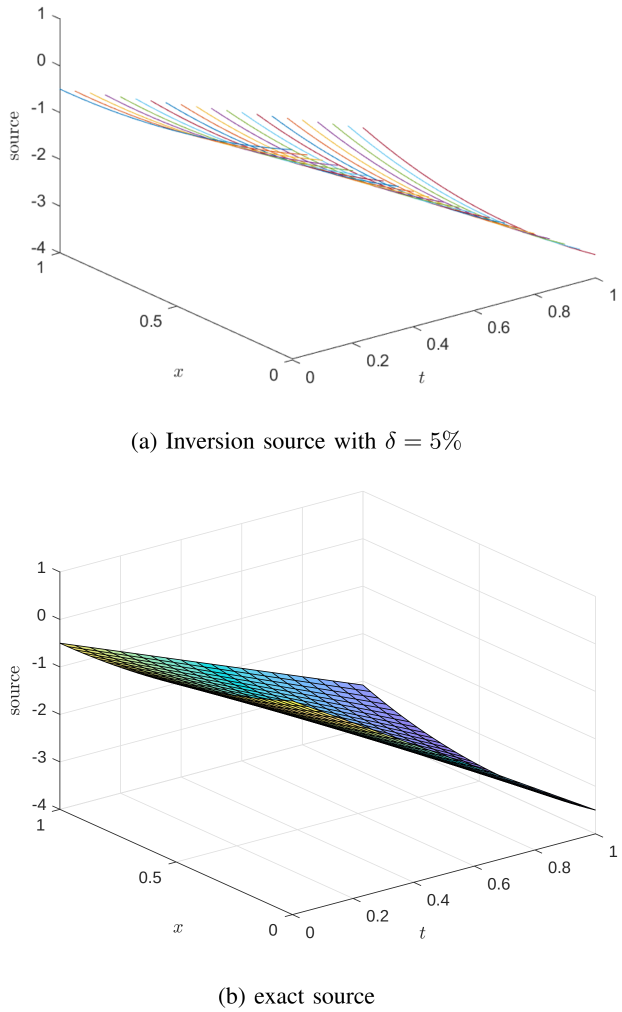


Fig. 1. Inversion and exact sources of $s_1(x,t)$ in Ex.1

TABLE V
INVERSION RESULTS OF s_2 WITH $\delta = 1\%$ IN EX.2

(x,t)	Inversion Solu.	Exact Solu.	Err_1^2
(0.2, 0.2)	-0.517134842	-0.525518149	1.60e-2
(0.4, 0.4)	-0.569710443	-0.578941051	1.59e-2
(0.6, 0.6)	-0.621167632	-0.631466909	1.63e-2
(0.8, 0.8)	-0.658408639	-0.668183624	1.46e-2
(1.0, 1.0)	-0.685812165	-0.695109935	1.34e-2

TABLE VI
INVERSION ERRORS WITH NOISES AT $T = 1$ IN EX.2

δ	Err_2^1	Err_2^2
5%	1.08e-2	3.82e-2
1%	9.27e-3	9.28e-3
0.1%	9.16e-3	5.06e-3

B. Example 2

Let the exact solution of the forward problem be

$$\begin{cases} u(x,t) = \sin(\frac{\pi x}{2})t + 1, \\ v(x,t) = (\frac{x^2}{2} - \frac{x^3}{3})t^{1+\gamma}, \end{cases} \tag{5.3}$$

and the exact source functions are given below:

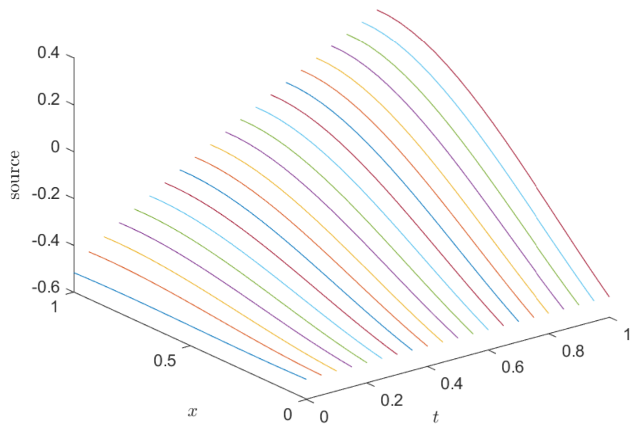
$$\begin{cases} s_1(x,t) &= \sin(\frac{\pi x}{2})[1 + \frac{\pi^2 t}{4} + \frac{t}{2}] + \cos(\frac{\pi x}{2})\frac{\pi t}{2} \\ &- \frac{x^2}{4}t^{1+\gamma} + \frac{x^3}{6}t^{1+\gamma} + \frac{1}{2}, \\ s_2(x,t) &= \Gamma(2+\gamma)(\frac{x^2}{2} - \frac{x^3}{3})t - \sin(\frac{\pi x}{2})\frac{t}{2} \\ &+ \frac{x^2}{4}t^{1+\gamma} - \frac{x^3}{6}t^{1+\gamma} - \frac{1}{2}. \end{cases} \tag{5.4}$$

Choose $K = J = 5$ in this example, and other parameters are the same as used in Ex.1. As done in Ex.1, the inversion results are listed in Tables IV-VI, where Err_1^i $(i = 1, 2)$ and Err_2^i $(i = 1, 2)$ denote the same meanings as in Ex.1.

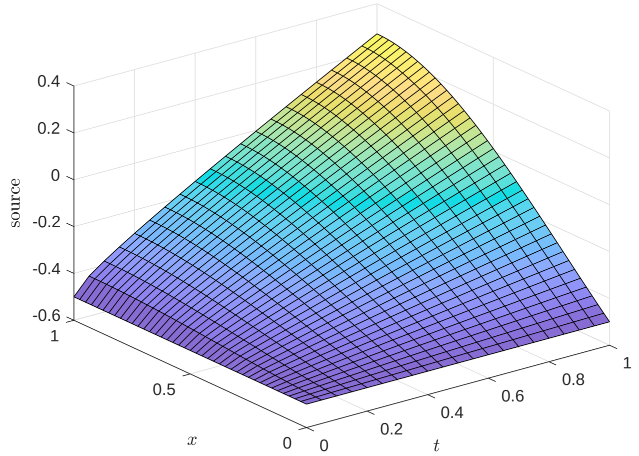
From Tables IV-VI, it can be seen again that the inversion sources are in good approximation to the exact sources as observed in Ex.1. Although the inversion for s_2 is not so good as for s_1, it is still acceptable from numerics.

VI. CONCLUSION

The inverse problem of determining two space-time-dependent sources in the integer-fractional two-region solute transport system is investigated form numerics. A unique bounded solution to the forward problem is obtained by the Laplace transform, and the alternative iteration inversion algorithm is set forth to reconstruct the sources successfully. The inversion algorithm is not only independent of solving the forward problem but also independent of computation



(a) Inversion source with $\delta = 5\%$



(b) exact source

Fig. 2. Inversion and exact sources of $s_2(x,t)$ in Ex.1

of the gradient of the cost functional, which can be utilized to other inverse coefficient problems arising from a system of partial differential equations where the unknowns are in forms of space-time-dependent.

We are concerned with the theoretical analysis of the inverse source problem, and pay attention to the choices of the basis functions and the discretized dimensions in the realization of the inversion algorithm in the near future.

References

[1] A. K. Alomari and Y. Massoun, "Numerical solution of time fractional coupled Korteweg-de Vries equation with a Caputo fractional derivative in two parameters", *IAENG International Journal of Computer Science*, vol. 50, no. 2, pp388-393, 2023.

[2] R. Ashurov and S. Umarov, "An inverse problem of determining orders of systems of fractional pseudo-differential equations", *Fract. Calc. Appl. Anal.*, vol. 25, no. 1, pp109-127, 2022.

[3] E. Awad, T. Sandev, R. Metzler and A. Chechkin, "From continuous-time random walks to the fractional Jeffreys equation: Solution and properties", *Int. J. Heat Mass Tran.*, vol. 181, 121839, 2021.

[4] M. Baati, N. Chakhim, M. Louzar and A. Lamnii, "Numerical approximation of the one-dimensional inverse Stefan problem using a meshless method", *Engineering Letters*, vol. 32, no. 1, pp112-122, 2024.

[5] I. M. Batiha, A. Benguesmia, T.-E. Oussaeif, I. H. Jebril, A. Ouannas and S. Momani, "Study of a superlinear problem for a time fractional parabolic equation under integral over-determination condition", *IAENG International Journal of Applied Mathematics*, vol. 54, no. 2, pp187-193, 2024.

[6] D. A. Benson and M. M. Meerschaert, "A simple and efficient random walk solution of multi-rate mobile/immobile mass transport equations", *Adv. Water Resour.*, vol. 32, no. 4, pp532-539, 2009.

[7] J. Cheng, J. Nakagawa, M. Yamamoto and T. Yamazaki, "Uniqueness in an inverse problem for a one-dimensional fractional diffusion equation", *Inverse Probl.*, vol. 25, no. 11, 115002, 2009.

[8] T. J. Doerries, A. V. Chechkin, R. Schumer and R. Metzler, "Rate equations, spatial moments, and concentration profiles for mobile-immobile models with power-law and mixed waiting time distributions", *Phys. Rev. E*, vol. 105, no. 1, 014105, 2022.

[9] T. J. Doerries, A. V. Chechkin and R. Metzler, "Apparent anomalous diffusion and non-Gaussian distributions in s simple mobile-immobile transport model with Poissonian switching", *J. Royal Soc. Interface*, vol. 19, 20220233, 2022.

[10] G. Y. Gao, H. B. Zhan, S. Y. Feng, B. J. Fu and G. H. Huang, "A mobile-immobile model with an asymptotic scale-dependent dispersion function", *J. Hydrol.*, vol. 424-425, pp172-183, 2012.

[11] R. Haggerty, S. A. McKenna and L. C. Meigs, "On the late-time behavior of tracer test breakthrough curves", *Water Resour. Res.*, vol. 36, no. 12, pp3467-3479, 2000.

[12] R. Haggerty, S. M. Wondzell and M. A. Johnson, "Power-law residence time distribution in the hyporheic zone of a 2nd-order mountain stream", *Geophys. Res. Lett.*, vol. 29, no.13, 1640, 2002.

[13] J. F. Kelly and M. M. Meeschaert, "Space-time duality and high-order fractional diffusion", *Phys. Rev. E*, vol. 99, no.2, 022122, 2019.

[14] Y. Kian, Z. Y. Li, Y. K. Liu and M. Yamamoto, "The uniqueness of inverse problems for a fractional diffusion equation with a single measurement", *Math. Ann.*, vol. 380, no. 3-4, pp1465-1495, 2021.

[15] A. A. Kilbas, H. M. Srivastava and J. J. Trujillo, *Theory and Applications of Fractional Differential Equations*, Amsterdam: Elsevier, 2006.

[16] A. Kirsch, *An Introduction to the Mathematical Theory of Inverse Problems* (Seccond Edition), New York: Springer, 1999.

[17] G. S. Li, Z. Wang, X. Z. Jia and Y. Zhang, "An inverse problem of determining the fractional order in the TFDE using themeasurement at one space-time point", *Fract. Calc. Appl. Anal.*, vol. 26, no. 4, pp1770-1785, 2023.

[18] G. S. Li, W. Y. Liu,X. Z. Jia and Z. Y. Li, "Unique identification of fractional orders in the fractional mobile-immobile solute transport system", *Appl. Math. Sci. Eng.*, vol. 31, no. 1, 2243375, 2023.

[19] X. Li, Z. Wen, Q. Zhu and H. Jakada, "A mobile-immobile model for reactive solute transport in a radial two-zone confined aquifer", *J. Hydrol.*, vol. 580, 124347, 2020.

[20] Y. F. Lin, J. Q. Huang and E. J. Carr, "A temporally relaxed theory of physically or chemically non-equilibrium solute transport in heterogeneous porous media", *J. Hydrol.*, vol. 620, 129432, 2023.

[21] C.-S. Liu, "Solving inverse coefficient problems of non-uniform fractionally diffusive reactive material by a boundary functional method", *Int. J. Heat Mass Tran.*, vol. 116, pp587-598, 2018.

[22] C.-S. Liu, B. T. Li and S. L. Liu, "Solving a nonlinear inverse Sturm-Liouville problem with nonlinear convective term using a boundary functional method", *Inverse Probl. Sci. Eng.*, vol. 28, pp1135-1153, 2020.

[23] M. M. Meerschaert, Y. Zhang and B. Baeumer, "Tempered anomalous diffusion in heterogeneous systems", *Geophy. Res. Lett.*, vol. 35, no.17, L17403, 2008.

[24] R. Metzler, W. G. Glockle and T. F. Nonnenmacher, "Fractional model equation for anomalous diffusion", *Phycia A: Statistical Mechanics and its Applications*, vol. 211, no. 1, pp13-24, 1994.

[25] R. Metzler and J. Klafter, "The random walk's guide to anomalous diffusion: a fractional dynamics approach", *Phys. Rep.*, vol. 339, no. 1, pp1-77, 2000.

[26] N. M. Noor, S. A. M. Yatim and I. S. M. Zawawi, "The design of the new fractional block method in the solution of the three-compartment Pharmacokinetics model", *Engineering Letters*, vol. 32, no. 2, pp252-261, 2024.

[27] L. P. Pang and M. E. Close, "Non-equilibrium transport of Cd in alluvial gravels", *J. Contam. Hydrol.*, vol. 36, no. 1-2, pp185-206, 1999.

[28] I. Podlubny, *Fractional Differential Equations*, New York: Academic Press, 1999.

[29] K. Sakamoto and M. Yamamoto, "Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems", *J. Math. Anal. Appl.*, vol. 382, no. 1, pp426-447, 2011.

[30] R. Schumer, D. A. Benson, M. M. Meerschaert, B. Baeumer, ”Fractal mobile/immobile solute transport”, *Water Resour. Res.*, vol. 39, no.10, pp1296-1308, 2003.
[31] L. Y. Sun, J. Niu, F. Huang, J.-C. Feng, C. H. Wu, H. Qiu and B. X. Hu, ”An efficient fractional-in-time transient storage model for simulating the multi-peaked breakthrough curves”, *J. Hydrol.*, vol. 600, 126570, 2021.
[32] M. T. Van Genuchten and R. J. Wagenet, ”Two-site/two-region models for pesticide transport and degradation: Theoretical development and analytical solutions”, *Soil Sci. Soc. AM. J.*, vol. 53, no. 5, pp1303-1310, 1989.
[33] G. X. Wang, Z. M. Zhou, S. M. Zhu and S. S. Wang, *Ordinary Differential Equation* (in Chinese), Beijing: Higher Education Press, 1982.
[34] M. Yamamoto, ”Uniqueness in determining fractional orders of derivatives and initial values”, *Inverse Probl.*, vol. 37, no. 9, 095006, 2021.
[35] M. S. Yin, R. Ma, Y. Zhang, S. Wei, G. R. Tick, J. Q. Wang, Z. Y. Sun, H. G. Sun and C. M. Zheng, ”A distributed-order time fractional derivative model for simulating bimodal sub-diffusion in heterogeneous media”, *J. Hydrol.*, vol. 591, 125504, 2020.
[36] G. M. Zaslavsky, ”Chaos, fractional kinetics, and anomalous transport”, *Phys. Rep.*, vol. 371, no. 6, pp461-580, 2002.
[37] Y. Zhang, D. A. Benson and D. M. Reeves, ”Time and space nonlocalities underlying fractional-derivative models: Distinction and literature review of field applications”, *Adv. Water Resour.*, vol. 32, no. 4, pp561-581, 2009.