Numerical Solution and Parameters Identification for the Integer-Fractal MIM Solute Transport Model

Haoming Lv, Chengyuan Yu, Wenyi Liu and Gongsheng Li

Abstract—An integer-fractal mobile-immobile (MIM) model for reactive solute transport in a heterogeneous porous media is investigated, where the transport in the mobile zone is given by an advection-dispersion equation, and the diffusion in the immobile zone is described by a time fractional differential equation. A finite difference scheme is put forward to solve the MIM model, and convergence and stability of the scheme are proved based on the spectrum estimation of the coefficient matrix. An inverse problem of identifying the fractional order and the degradation coefficient is considered with the measured data in the mobile zone, and uniqueness of the inverse problem is proved by the method of Laplace transform. Numerical inversions with noisy data are presented to demonstrate a numerical stability of the inverse problem.

Index Terms—MIM solute transport, integer-fractal model, inverse problem, finite difference scheme, Laplace transform, uniqueness, numerical inversion.

I. INTRODUCTION

S OIL and groundwater pollution has become a serious threat to sustainable development throughout the world. It is important to characterize transport and diffusion behaviors in mathematics for solute transport in heterogeneous porous media. Assume that the porous media is divided into mobile and immobile zones due to the heterogeneity, and there is the first-order kinetic mass transfer between the two zones, and no adsorption and degeneration in the transportation, then there holds (see [10], [11] for instance):

$$\begin{cases} \theta_m \frac{\partial c_m}{\partial t} + \theta_{im} \frac{\partial c_{im}}{\partial t} = L(x)c_m, \\ \theta_{im} \frac{\partial c_{im}}{\partial t} = \omega(c_m - c_{im}), \end{cases}$$
(1.1)

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

The system (1.1) is called a mobile-immobile (MIM)

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W. Y. Liu is a PhD student of Hohi 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).

solute transport model in the case of no sources in the porous media. If denoting $\beta = \theta_m/\theta$ as a partition parameter of the mobile water zone, there is $1 - \beta = \theta_{im}/\theta$. Furthermore, considering linear adsorption, first-order degeneration reactions in the process, and one gets a MIM solute transport model (see [20], [21], [27], [33], for instance)

$$\begin{cases} \beta R \frac{\partial c_m}{\partial t} + (1-\beta) R \frac{\partial c_{im}}{\partial t} = L(x)c_m - \mu_1 c_m, \\ (1-\beta) R \frac{\partial c_{im}}{\partial t} = \omega(c_m - c_{im}) - \mu_2 c_{im}, \end{cases}$$
(1.2)

where $R \ge 1$ is retardation factor due to the adsorption, and μ_1 and μ_2 are degeneration coefficients in the mobile and immobile zones respectively, and other symbols denote the same meanings as in (1.1).

The equations (1.1) and (1.2) are integer-order MIM solute transport models which have been studied and applied widely by hydrogeologists not only in lab but also in field tests. However, fractional diffusion equations have been reported to be more effective than the integer-order equations in modeling and describing solute transport behaviors with heavier tails, or earlier breakthrough phenomena during the last three decades. We only refer to Metzler et al. [24], Metzler and Klafter [25], Zaslavsky [37] for some early work. Actually, it is always not a instantaneous process but a longtime dynamic process for solute mass transfer and/or chemical reactions in heterogeneous media. This non-instantaneous dynamic process can be described by fractional diffusion equations [3], [13], [39]. Recently, transient anomalous diffusions and power-law relations of solute transport were observed under suitable conditions by employing the fractional MIM models [7], [8], [32].

It is noted that Schumer et al. [30] proposed a fractional MIM equation by choosing a suitable power-law memory function, which was referred to as the FMIM model. Following the research in [30], there have had quite a few of studies for anomalous diffusion of solute transport in heterogeneous porous media, see [4], [9], [22], [23], [32], [35] for instance. Very recently, the authors considered an integer-fractal solute transport system with source terms in a two-zone porous media, and an inverse source problem of determining two space-time-dependent sources in the model was investigated from numerics [36]. Based on the models (1.1)-(1.2) and the work in [36], this paper will deal with numerical solution and multi-parameters inversion for the integer-fractal solute transport system, which is different from that work in [36].

It is known that research on fractional diffusion models lies mainly in numerical methods and applications [1], [26], and the first work of this paper is to give numerical solutions to the integer-fractal solute transport model. By discretizing the time-fractional derivative and the integer-order derivatives as

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H. M. Lv is a graduate student of Shandong University of Technology, Zibo, Shandong, 255000 China (e-mail: a2993732764@163.com).

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

done in [22], a finite difference scheme to the integer-fractal MIM system is proposed, and its stability and convergence are proved under natural conditions of the model parameters which is one of the contributions of this paper.

On the other hand, some parameters in the model are always unknown or can not be measured directly, such as the order of the fractional derivative, the mass transfer rate, and the initial distribution of the solute ions, etc., in which cases we have to encounter with inverse problems for the MIM solute transport system. As for inverse problems in fractional diffusion equations, we refer to [6], [29] for early typical work, and recently see [5], [14], [18], [34], etc. Nevertheless, to the authors' best knowledge, there are few studies on inverse problems associated with a system of fractal differential equations [2], [19], [36].

The fractional order is an essential parameter to describe the anomalous diffusion behavior which is always unknown in advance, and the degradation coefficient of the solute in the mobile zone is also unknown in most cases. So it is meaningful to study the inverse problem of determining these two parameters. Recently the authors studied an inverse problem of determining two orders in a fractional MIM model [19], and the uniqueness was proved by the method of Laplace transform.

In this paper, we will consider with an inverse problem of identifying the fractional order and the degradation coefficient in the integer-fractal MIM solute transport system also utilizing the method of Laplace transform. We aim to prove the uniqueness of the inverse problem by the maximum principle of elliptic operator in the positive real-space of Laplace transform, which is the main contribution of this paper. Furthermore, numerical inversions are performed by using a modified Levenberg-Marquart (LM in short) algorithm to support the theoretical analysis.

The rest of this paper is organized as follows.

In Section 2, an integer-fractal MIM solute transport model is introduced, and a finite difference scheme for the forward problem is put forward. In Section 3, stability and convergence of the difference scheme are proved by spectral analysis of the coefficient matrix. In Section 4, an inverse problem of identifying the factional order and the degradation coefficient is investigated, and the uniqueness is proved by Laplace transform. Numerical inversions with noisy data are presented in Section 5, and concluding remarks are given in Section 6.

II. THE INTEGER-FRACTAL MIM MODEL AND THE DIFFERENCE SCHEME

Consider a modification of the integer-order transport model (1.2) in a finite domain in 1D case. Suppose that there are no sources in the domain, and the solute transport begins in the mobile phase by the left boundary input, and there are no solute ions in the immobile at the beginning. So the mass transfer happens from the mobile to the immobile along with a classical hydrodynamic advection-dispersion in the mobile and a dynamical process in the immobile. If the porous media is of low-permeability, the dynamical diffusion in the immobile can be described by a time-fractional differential equation, which leads to the integer-fractal mobile-immobile solute transport model.

A. The integer-fractal MIM model

By dimensionless we denote $\Omega = (0,1)$ and $\Omega_{\infty} = \Omega \times (0,\infty)$. Based on (1.2) and the dynamic diffusion in the immobile, an integer-fractal MIM solute transport model is given as follows:

$$\begin{cases} \beta R \frac{\partial u_1}{\partial t} = \frac{1}{P} \frac{\partial^2 u_1}{\partial x^2} - \frac{\partial u_1}{\partial x} - \omega(u_1 - u_2) - \lambda u_1, \\ (1 - \beta) R \partial_t^\gamma u_2 = \omega(u_1 - u_2) - \mu u_2, \end{cases}$$
(2.1)

where $(x,t) \in \Omega_{\infty}$, and $u_1 = u_1(x,t)$ and $u_2 = u_2(x,t)$ denote the solute concentrations in the mobile and immobile zones respectively; P > 0 is the Pelect number, $\omega > 0$ also denotes the mass transfer rate from the mobile to the immobile, and $\lambda, \mu > 0$ are the degradation coefficients in the mobile and the immobile zones respectively, and $\beta \in (0,1)$ and $R \ge 1$ denote the same meanings as in (1.2), and $\partial_t^{\gamma} u_2$, $0 < \gamma < 1$, denotes the Caputo fractional derivative of u_2 on time t > 0 which is defined by [15], [28]

$$\partial_t^{\gamma} u_2 = \frac{1}{\Gamma(1-\gamma)} \int_0^t (t-s)^{-\gamma} \frac{\partial u_2(x,s)}{\partial s} ds, \qquad (2.2)$$

where $\Gamma(\cdot)$ denotes the Gamma function.

The model (2.1) is a system combining the hydrologic advection-dispersion transport in the mobile with a fractional diffusion in the immobile zone, which can be regarded as the deformation of the FMIM equation. Here the system model (2.1) can be utilized directly to describe the diffusion and mass transfer processes in the mobile and immobile zones, and it should be more practical than that of the FMIM equation from the viewpoint of engineering applications.

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

$$u_1(x,0) = 1, \quad u_2(x,0) = 0, \quad 0 \le x \le 1,$$
 (2.3)

which means that the solute concentration in the immobile zone is zero at the initial stage. The boundary conditions are given as

$$u_1(0,t) = 1, \quad u_2(0,t) = 0, \quad 0 \le t < \infty,$$
 (2.4)

and

$$\frac{\partial u_1}{\partial x}(1,t) = 0, \quad \frac{\partial u_2}{\partial x}(1,t) = 0, \quad 0 \le t < \infty, \quad (2.5)$$

which imply that the left-hand side of the region in the mobile keeps a constant same as the initial distribution, and the right-hand boundary is impermeable.

As a result, we get a determined system composed by (2.1) with (2.3)-(2.5) which is called the forward problem. The solution of the forward problem can be expressed by the inverse of Laplace transform, however, it is very difficult to work out the solution due to the complexity of the inverse Laplace transformation.

In what follows we give a finite difference solution to the forward problem for $(x,t) \in \Omega \times (0,T)$ for any given time T > 0, and prove its stability and convergence by the estimation of the spectral radius of the coefficient matrix.

B. The finite difference scheme

For any finite time T > 0, let m, n be positive integers, and h = 1/m, $\tau = T/n$ be grid steps to discretize the domain $(0, 1) \times (0, T)$. Denote $x_i = ih(i = 0, \dots, m)$, $t_k = k\tau(k = 0, \dots, n)$ as the grid points, and $u_1^{i,k} \approx u_1(x_i, t_k)$, $u_2^{i,k} \approx u_2(x_i, t_k)$ as the approximations.

Assume that the solutions u_1 and u_2 are suitably smooth, then by using ordinary finite difference method to discretize the derivatives in (2.1) at (x_i, t_{k+1}) , there hold:

$$\frac{\partial u_1}{\partial t}|_{(x_i,t_{k+1})} = \frac{u_1^{i,k+1} - u_1^{i,k}}{\tau} + O(\tau), \qquad (2.6)$$

$$\frac{\partial u_1}{\partial x}|_{(x_i,t_{k+1})} = \frac{u_1^{i,k+1} - u_1^{i-1,k+1}}{h} + O(h), \qquad (2.7)$$

$$\frac{\partial^2 u_1}{\partial x^2}|_{(x_i,t_{k+1})} = \frac{u_1^{i+1,k+1} - 2u_1^{i,k+1} + u_1^{i-1,k+1}}{h^2} + O(h^2),$$
(2.8)

and

$$\partial_t^{\gamma} u_2|_{(x_i, t_{k+1})} = \frac{1}{\tau^{\gamma} \Gamma(2-\gamma)} \sum_{j=0}^k [u_2^{i,j+1} - u_2^{i,j}] \\ \cdot [(k+1-j)^{1-\gamma} - (k-j)^{1-\gamma}] + O(\tau).$$
(2.9)

Denote $r = \frac{\tau}{\beta B P h^2}$ as the grid ratio, and denote

$$\begin{cases} A = \frac{\tau}{\beta R h} + r, \ C = r, \ D = \frac{\omega \tau}{2\beta R}, \ E = \frac{\omega \tau^{\gamma} \Gamma(2-\gamma)}{2(1-\beta)R}; \\ B = 1 + A + C + 2D + \frac{\tau}{\beta R} \lambda, \ F = 1 + 2E + \frac{2E}{\omega} \mu. \end{cases}$$
(2.10)

By utilizing the above notations and omitting the remainder terms in (2.6)-(2.8) and (2.9), the system (2.1) is discretized as

$$\begin{cases} -Au_{1}^{i-1,k+1} + Bu_{1}^{i,k+1} - Cu_{1}^{i+1,k+1} - Du_{2}^{i-1,k+1} \\ -Du_{2}^{i+1,k+1} = u_{1}^{i,k}, \\ -Eu_{1}^{i-1,k+1} - Eu_{1}^{i+1,k+1} + Fu_{2}^{i,k+1} = u_{2}^{i,k} \\ -\sum_{j=0}^{k-1} (u_{2}^{i,j+1} - u_{2}^{i,j})[(k+1-j)^{1-\gamma} - (k-j)^{1-\gamma}]. \end{cases}$$

$$(2.11)$$

The initial boundary value conditions are discretized as

$$U^{(0)} = (1, 1, \dots, 1; 0, 0, \dots, 0)^T$$

and

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$$u_1^{0,k} = 1, \quad u_2^{0,k} = 0, \quad k = 0, 1, \cdots, n;$$

and

$$u_1^{m-1,k} = u_1^{m,k}, \quad u_2^{m-1,k} = u_2^{m,k}, \quad k = 0, 1, \cdots, n,$$

respectively. By rearranging (2.11) we get an implicit difference scheme in the matrix form:

$$\begin{cases} MU^{1} = U^{0}, \\ MU^{k+1} = NU^{k} + \sum_{j=1}^{k-1} \Psi_{j}^{k} U^{j} + N_{0} U^{0}, k = 1, \cdots, n-1, \end{cases}$$
(2.12)

where $U^k = (u_1^{1,k}, \dots, u_1^{m-1,k}, u_2^{1,k}, \dots, u_2^{m-1,k})^T$ for $k = 1, \dots, n$. The matrices in the difference scheme (2.12) are given as follows.

Firstly, M is a 2(m-1)-order matrix defined by

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}, \qquad (2.13)$$

where M_{11}, M_{12}, M_{21} and M_{22} are all m-1-order matrices given by

$$M_{11} = \begin{pmatrix} B & -C & 0 & \cdots & 0 \\ -A & B & -C & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & -A & B & -C \\ 0 & \cdots & 0 & -A & B - C \end{pmatrix},$$

$$M_{12} = \begin{pmatrix} 0 & -D & 0 & \cdots & 0 \\ -D & 0 & -D & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & -D & 0 & -D \\ 0 & \cdots & 0 & -D & -D \end{pmatrix},$$
$$M_{21} = \begin{pmatrix} 0 & -E & 0 & \cdots & 0 \\ -E & 0 & -E & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & -E & 0 & -E \\ 0 & \cdots & 0 & -E & -E \end{pmatrix},$$
$$M_{22} = \begin{pmatrix} F & 0 & 0 & \cdots & 0 \\ 0 & F & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & F & 0 \\ 0 & \cdots & 0 & 0 & F \end{pmatrix}$$

respectively. Secondly, N and N_0 in (2.12) are both 2(m-1)-order matrices and defined by

$$N = \begin{pmatrix} \mathbf{I} & \mathbf{O} \\ \mathbf{O} & (2-2^{1-\gamma})\mathbf{I} \end{pmatrix}, N_0 = \begin{pmatrix} \mathbf{O} & \mathbf{O} \\ \mathbf{O} & a_k \mathbf{I} \end{pmatrix}, \quad (2.14)$$

respectively, where I is the m-1-order identity matrix, O denotes the m-1-order zero matrix, and

$$a_k = (k+1)^{1-\gamma} - k^{1-\gamma}, k = 1, \cdots, n-1.$$
(2.15)

Finally, the matrix Ψ_i^k is defined by

$$\Psi_j^k = \begin{pmatrix} \mathbf{O} & \mathbf{O} \\ \mathbf{O} & b_j^k \mathbf{I} \end{pmatrix}, \qquad (2.16)$$

where

$$b_j^k = 2(k+1-j)^{1-\gamma} - (k-j)^{1-\gamma} - (k-j+2)^{1-\gamma}, \quad (2.17)$$

for $j = 1, \dots, k - 1$ and $k = 2, \dots, n - 1$.

By solving the difference equation (2.12), numerical solutions of the forward problem can be obtained, and we need to prove the solvability, stability and convergence of the difference scheme.

III. STABILITY AND CONVERGENCE OF THE DIFFERENCE SCHEME

According to the background of solute transport in porous media and the physical/chemical laws, the parameters in the system (2.1) should satisfy the condition:

$$0 < \gamma < 1, 0 < \beta < 1, R \ge 1, P > 0, \omega > 0, \lambda > 0, \mu > 0,$$
(3.1)

with which we will prove the solvability, stability and convergence of (2.12). Therefore we need some preliminaries on the coefficient matrix.

A. Preliminaries on the coefficient matrix

Lemma 3.1([12]) For $k = 1, 2, \dots$, and $0 < \gamma < 1$, there holds

$$2k^{\gamma} - (k-1)^{\gamma} - (k+1)^{\gamma} > 0, \qquad (3.2)$$

and then the coefficients b_j^k $(j = 1, \dots, k - 1, k = 2, 3, \dots)$ given in (2.17) are all positive.

By direct computations we get the following assertion.

Lemma 3.2 Let $0 < \gamma < 1$, and the coefficients a_k (k =

 $1, 2, \dots$) and b_{j}^{k} $(j = 1, \dots, k - 1, k = 2, 3, \dots)$ be defined by (2.15) and (2.17) respectively, there hold $0 < a_k < 1$, and $a_k + \sum_{j=1}^{k-1} b_j^k = 2^{1-\gamma} - 1.$

Proposition 3.1 For the matrix M defined by (2.13), there holds

$$M_{ii} > 1 + \sum_{j=1, j \neq i}^{2m-2} |M_{ij}|, \qquad (3.3)$$

with $\sum_{j=1, j \neq i}^{2m-2} M_{ij} < 0$ for $i = 1, 2, \dots, 2m-2$. **Proof** Öbviously, the coefficients A, B, C, D and E, Fdefined in (2.10) are all positive under the natural condition (3.1), and the assertion is valid by the following verifications. (i) i = 1. Noting $M_{11} = B > 0$ and $\sum_{j=2}^{2m-2} M_{1j} = -C - D < 0$ 0, there is

$$M_{11} = 1 + A + C + 2D + \frac{\tau}{\beta R}\lambda > 1 + \sum_{j=2}^{2m-2} |M_{ij}|.$$

(ii) $i = 2, \dots, m - 1$. Noting $M_{ii} = B > 0$ and $\sum_{j=1, j \neq i}^{2m-2} M_{ij} = -A - C - 2D < 0$, we get

$$M_{ii} = 1 + A + C + 2D + \frac{\tau}{\beta R} \lambda > 1 + \sum_{j=1, j \neq i}^{2m-2} |M_{ij}|.$$

(iii) i = m. Since $M_{mm} = F > 0$ and $\sum_{j=1, j \neq m}^{2m-2} M_{mj} = 0$ On the other hand, by the definitions of N, N_0 and Ψ_j^k given in (2.14) and (2.16), and noting $2 - 2^{1-\gamma} < 1$, we -E < 0, there is

$$M_{mm} = 1 + 2E + \frac{2E}{\omega}\mu > 1 + \sum_{j=1, j \neq m}^{2m-2} |M_{mj}|.$$

(iv) $i = m + 1, \dots, 2m - 2$. Noting $M_{ii} = F > 0$ and $\sum_{j=1, j \neq i}^{2m-2} M_{ij} = -2E < 0$, we get

$$M_{ii} = 1 + 2E + \frac{2E}{\omega}\mu > 1 + \sum_{j=1, j \neq i}^{2m-2} |M_{ij}|.$$

The proof is completed.

Corollary 3.1 By this proposition, the coefficient matrix Mof the difference scheme (2.12) is strictly diagonal dominant, and the difference scheme is uniquely solvable.

Based on (3.3) it is not difficult to get the estimate of the spectral radius of the coefficient matrix with the same method as used in [12], [17].

Lemma 3.3 For the coefficient matrix M there holds

$$\frac{1}{2\|M\|_{\infty} - 1} < \rho(M^{-1}) < 1, \tag{3.4}$$

and there exists a matrix norm $\|\cdot\|_*$ such that

$$\|M^{-1}\|_* < 1, \tag{3.5}$$

here $||M||_{\infty} = \max_{1 \le i \le 2m-2} \{M_{ii}\}$, and $\rho(M^{-1})$ is the spectral radius of M^{-1} , and M^{-1} denotes the inverse matrix of M.

B. Stability and convergence

We discuss the stability and convergence of the difference scheme (2.12) by the norm $\|\cdot\|_*$ given in Lemma 3.3, and we denote it as $\|\cdot\|$ for convenience of writing.

Theorem 3.1 Assume that the solutions u_1 and u_2 are suitably smooth, and the model parameters satisfy the natural condition (3.1), then the finite difference scheme (2.12) is stable.

Proof By linearity of the scheme (2.12), we get

$$\begin{cases} ME^{1} = E^{0}, \ E^{0} = \tilde{U}^{0} - U^{0}, \\ ME^{k+1} = NE^{k} + \sum_{j=1}^{k-1} \Psi_{j}^{k} E^{j} + N_{0} E^{0}, \end{cases}$$
(3.6)

where \widetilde{U}^0 denotes the initial function with noises, $E^k=\widetilde{U}^k-U^k$ denotes the solutions' difference at the k-th level, and $k = 0, 1, \cdots$.

By (3.6) and Lemma 3.3, there holds

$$||E^{1}|| \le ||M^{-1}|| ||E^{0}|| < ||E^{0}||.$$
(3.7)

Suppose that there are $||E^j|| < ||E^0||$ for $j = 1, 2, \dots, k$. Then we get also by (3.6) and Lemma 3.3

$$\begin{split} \|E^{k+1}\| &\leq \|M^{-1}\| \|NE^{k} + \sum_{j=1}^{k-1} \Psi_{j}^{k} E^{j} + N_{0} E^{0}\| \\ &< \|NE^{k} + \sum_{j=1}^{k-1} \Psi_{j}^{k} E^{j} + N_{0} E^{0}\| \\ &< (\|N\| + \sum_{j=1}^{k-1} \|\Psi_{j}^{k}\| + \|N_{0}\|)\|E^{0}\|. \end{split}$$

$$||N||_{\infty} = 1, ||N_0||_{\infty} = a_k, ||\Psi_j^k||_{\infty} = b_j^k (j = 1, \dots, k-1)$$
(3.9)

for $k = 1, 2, \cdots$. Thus by Lemma 3.2 there holds

$$\|N\|_{\infty} + \|N_0\|_{\infty} + \sum_{j=1}^{k-1} \|\Psi_j^k\|_{\infty} = 1 + a_k + \sum_{j=1}^{k-1} b_j^k = 2^{1-\gamma}.$$
(3.10)

Henceforth by (3.8), and thanks to the equivalence of the norm in finite-dimensional space, there exists a positive constant c > 0 independent of $k \in \mathbf{N}$ such that

$$||E^{k+1}|| \le c||E^0||, \tag{3.11}$$

which implies that the assertion of this theorem is valid by the inductive principle. The proof is over.

Denote the errors in the solutions by

$$e^{k} = (u_{1}(x_{1}, t_{k}) - u_{1}^{1,k}, \cdots, u_{1}(x_{m-1}, t_{k}) - u_{1}^{m-1,k}, u_{2}(x_{1}, t_{k}) - u_{2}^{1,k}, \cdots, u_{2}(x_{m-1}, t_{k}) - u_{2}^{m-1,k})^{T},$$
(3.12)

for $k = 1, 2, \dots, n$, where $u_j(x_i, t_k)$ and $u_j^{i,k}$, j = 1, 2, are the exact and numerical solutions at (x_i, t_k) of the forward problem respectively. Now we prove the convergence of the finite difference scheme (2.12).

Theorem 3.2 Under the conditions of Theorem 3.1, the difference solution of (2.12) is convergent to the exact solution with the order of $O(h\tau^{1-\gamma}+\tau)$ as $h,\tau \to 0$ for any finite time $T < \infty$, and there holds

$$\|e_k\| \le c_{\gamma} T^{\gamma} (h\tau^{1-\gamma} + \tau), \qquad (3.13)$$

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 TABLE I

 Solution errors and convergence rates with grids ratios

h	$\tau = h^2$	Err1	Rat1	Err2	Rat2
1/4	1/16	3.87549e-2		2.25301e-1	
1/10	1/100	1.44610e-2	2.680	6.55298e-2	3.438
1/20	1/400	7.00629e-3	2.064	2.74381e-2	2.388
1/40	1/1600	3.45238e-3	2.029	1.22166e-2	2.246
1/80	1/6400	1.71439e-3	2.014	5.70225e-3	2.142

where c_{γ} is a positive constant related with the order $\gamma \in (0,1)$ but independent of $k \in \mathbf{N}$.

Proof Also by the linearity of the scheme (2.12), we have $Me^1 = R^1$.

$$\begin{cases}
Me^{k+1} = Ne^k + \sum_{j=1}^{k-1} \Psi_j^k e^j + R^{k+1}, \\
(3.14)
\end{cases}$$

where R^k denotes the truncated term in the solutions' approximation for $k = 1, 2, \cdots$.

By the difference approximations (2.6)-(2.9), there holds

$$||R^k|| \le c(h\tau + \tau^{1+\gamma}), k = 1, 2, \cdots,$$
(3.15)

here c > 0 also denotes a positive constant independent of $k \in \mathbb{N}$. Thus by a similar method as used in Theorem 3.1, one can get

$$\begin{aligned} \|e^{k+1}\| &\leq (\|N\| \|e^{k}\| + \sum_{j=1}^{k-1} \|\Psi_{j}^{k}\| \|e^{j}\|) / \|N_{0}\| + \|R^{k+1}\| \\ &\leq \frac{c}{a_{k}} (\|N\| + \sum_{j=1}^{k-1} \|\Psi_{j}^{k}\| + \|N_{0}\|) (h\tau + \tau^{1+\gamma}) \\ &\leq \frac{c \cdot 2^{1-\gamma}}{a_{k}} \tau^{\gamma} (h\tau^{1-\gamma} + \tau). \end{aligned}$$

$$(3.16)$$

Noting $\tau = T/n$ and $n \ge k$, there holds

$$\|e^{k+1}\| \le \frac{c \cdot 2^{1-\gamma}}{a_k k^{\gamma}} T^{\gamma} (h\tau^{1-\gamma} + \tau).$$
(3.17)

By the limitation $\lim_{k\to\infty} a_k k^{\gamma} = 1 - \gamma$, we get the assertion (3.13), where $c_{\gamma} = \frac{c \cdot 2^{1-\gamma}}{1-\gamma}$. The proof is over.

C. Numerical experiment

Let the analytic solution of the forward problem be

$$\begin{cases} u_1(x,t) = (x^2 - 2x)t + 1, \\ u_2(x,t) = (\frac{1}{2}x^2 - \frac{1}{3}x^3)t, \end{cases}$$
(3.18)

for $(x,t) \in (0,1) \times (0,1)$. The model parameters are chosen as $\gamma = 0.75$, P = 10, $\beta = 0.5$, $\omega = 1$, R = 2 and $\lambda = 0.05$, $\mu = 0.01$. Using the scheme (2.12) to solve the system, the errors in the solutions with the grid ratios are listed in Table 1, where h, τ are the space and time steps, Rat1 and Rat2 denote the convergence rates of u_1 and u_2 respectively, and Err1, Err2 denote the solutions errors for u_1 and u_2 at t = 0.5respectively, where Err1 is given by

$$\operatorname{Err1} = \frac{\|u_1(x, 0.5) - u_1^*(x, 0.5)\|_2}{\|u_1(x, 0.5)\|_2}, \quad (3.19)$$

here u_1^* denotes the numerical solution, and Err2 is given similarly to (3.19).

From Table 1 it can be seen that the difference solutions give good approximations to the exact solution. The convergent rates for u_1 and u_2 are basically in accordance with each other as the grid goes to fine with $\tau = h^2$.

IV. INVERSE PROBLEM OF IDENTIFYING MODEL PARAMETERS

A. The inverse problem

Suppose that the fractional order γ and the degradation coefficient λ in the model (2.1) are unknown, we aim to identify and determine them with some additional information based on the forward problem.

The additional observation is given for the solute concentration in the mobile zone at one space-point $x_0 \in \Omega$:

$$u_1(x_0, t), \ 0 < t < \infty,$$
 (4.1)

with which an inverse problem is formulated composed by (2.1), (2.3)-(2.5) together with (4.1).

An inverse problem is often investigated in an admissible set of the unknowns. For the considered inverse problem, assume that $(\gamma, \lambda) \in S_{ad}$, where S_{ad} is given by

$$S_{ad} = \{ (\gamma, \lambda) : 0 < \gamma < 1, 0 < \lambda < K \},$$
(4.2)

and K is a positive constant. In addition, assume that the solutions of the forward problem belong to $C^{2,1}(\Omega_{\infty})$, and they satisfy growth condition as $t \to \infty$ such that Laplace transform can be performed for the system (2.1).

For proof of the uniqueness of the inverse problem, we also need the following lemmas.

Lemma 4.1 Suppose that the Laplace transforms of $u_1(\cdot, t)$ and $u'_1(\cdot, t)$ on t > 0 exist, then there holds

$$s\hat{u}_1(\cdot, s) \to u_1(\cdot, 0), \qquad \operatorname{Re}(s) \to \infty.$$
 (4.3)

where $\hat{u}_1(\cdot, s)$ denotes the Laplace transform of $u_1(\cdot, t)$ on t > 0.

For the Caputo fractional derivative $\partial_t^{\gamma} u_2(\cdot, t)$ (0 < γ < 1), there holds the Laplace transform formula:

$$\mathcal{L}\{\partial_t^{\gamma} u_2(\cdot, t); s\} = s^{\gamma} \hat{u}_2(s) - s^{\gamma - 1} u_2(\cdot, 0), \qquad (4.4)$$

where $\hat{u}_2(\cdot, s)$ denotes the Laplace transform of $u_2(\cdot, t)$ on t > 0.

Lemma 4.2 ([31])) Let *I* be a bounded interval in **R**, and u = u(x) be a nonconstant solution of

$$a(x)u'' + b(x)u' + h(x)u \ge 0, \ x \in I,$$
(4.5)

where the coefficients a(x), b(x) and h(x) are bounded and $h(x) \le 0$ in *I*, and there exists a constant $a_0 > 0$ such that $a(x) \ge a_0 > 0$ in *I*. Then a nonnegative maximum of *u* can only occur on ∂I , and $du/d\nu > 0$ there, where ν denotes a normal vector pointing outward at the boundary.

Corollary 4.1 Let I = (0, 1). Under the conditions of Lemma 4.2, suppose further that u(0) = 0 and u'(1) = 0, then there must have u(x) < 0, $x \in I$.

B. The uniqueness

For any given $(\gamma, \lambda) \in S_{ad}$, denote $u_1^{\gamma, \lambda}(x, t)$, $u_2^{\gamma, \lambda}(x, t)$ as the smooth solutions of the forward problem in the mobile and immobile zones respectively.

Theorem 4.1 For given $\lambda > 0$, let u_1^{γ} , u_2^{γ} be the solutions of the forward problem in the mobile and immobile zones, corresponding to the factional order $\gamma \in (0, 1)$ respectively, and $x_0 \in \Omega$ be the measured point. If $u_1^{\gamma_1}(x_0, t) = u_1^{\gamma_2}(x_0, t)$ for $t \in (0, \infty)$ and $\gamma_1, \gamma_2 \in (0, 1)$, then there holds $\gamma_1 = \gamma_2$. **Proof** By using Laplace transform for the model (2.1), and

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utilizing the initial conditions $u_1|_{t=0} = 1$ and $u_2|_{t=0} = 0$, there hold

$$\beta R(s\hat{u_1}^{\gamma} - 1) = \frac{1}{P} \frac{d^2 \hat{u_1}^{\gamma}}{dx^2} - \frac{d\hat{u_1}^{\gamma}}{dx} - \omega(\hat{u_1}^{\gamma} - \hat{u_2}^{\gamma}) - \lambda \hat{u_1}^{\gamma},$$
(4.6)

and

$$(1-\beta)R(s^{\gamma}\hat{u}_{2}^{\gamma}) = \omega(\hat{u}_{1}^{\gamma} - \hat{u}_{2}^{\gamma}) - \mu\hat{u}_{2}^{\gamma}.$$
 (4.7)

From (4.7) there is

$$\hat{u}_2^{\gamma} = \frac{\omega \hat{u}_1^{\gamma}}{(1-\beta)R \ s^{\gamma} + \omega + \mu}.$$
 (4.8)

Substituting (4.8) into (4.6) we get

$$\frac{\frac{1}{P}\frac{d^2\hat{u}_1^{\gamma}}{dx^2} - \frac{d\hat{u}_1^{\gamma}}{dx}}{+\left\{\frac{\omega^2}{(1-\beta)Rs^{\gamma}+\omega+\mu} - \omega - \lambda - \beta Rs\right\}}\hat{u}_1^{\gamma} + \beta R = 0.$$
(4.9)

Now for $\gamma_1, \gamma_2 \in (0, 1)$, there hold the expressions for $\hat{u_1}^{\gamma_1}$ and $\hat{u_1}^{\gamma_2}$ corresponding to (4.9). Let $U(x) = \hat{u_1}^{\gamma_1} - \hat{u_1}^{\gamma_2}$ and $\gamma_1 > \gamma_2$. There holds for $x \in \Omega$

$$\frac{1}{P}\frac{d^{2}U}{dx^{2}} - \frac{dU}{dx} + cU = d,$$
(4.10)

where

$$c = -\omega - \lambda - \beta Rs + \frac{\omega^2}{(1-\beta)Rs^{\gamma_1} + \omega + \mu}, \quad (4.11)$$

and

$$d = \hat{u_1}^{\gamma_2} \frac{\omega^2 (1-\beta) R \left(s^{\gamma_1} - s^{\gamma_2}\right)}{\left[(1-\beta) R s^{\gamma_1} + \omega + \mu\right] \left[(1-\beta) R s^{\gamma_2} + \omega + \mu\right]},$$
(4.12)

and the boundary conditions are U(0) = 0 and U'(1) = 0.

Let us consider the case of s > 0 and large enough. Thanks to the priori conditions of $\omega > 0, \lambda > 0, \mu > 0$ and $R \ge 1, 1 - \beta > 0$, there holds

$$c = -\omega - \lambda - \beta Rs + \frac{\omega^2}{(1-\beta)Rs^{\gamma_1} + \omega + \mu}$$

$$\leq -\omega - \lambda - \beta Rs + \omega$$

$$= -\lambda - \beta Rs < 0, \quad s > 0.$$

Rewrite (4.12) as

$$d = s\hat{u_1}^{\gamma_2} \frac{\omega^2 (1-\beta) R \left(s^{\gamma_1 - 1} - s^{\gamma_2 - 1}\right)}{\left[(1-\beta) R s^{\gamma_1} + \omega + \mu\right] \left[(1-\beta) R s^{\gamma_2} + \omega + \mu\right]},$$
(4.13)

for s > 0. Since $s\hat{u}_1^{\gamma_2} \to u_1(x,0) = 1, s \to \infty$ by Lemma 4.1, there exists $s_0 > 0$ large enough such that

$$s\hat{u_1}^{\gamma_2} > 0, \ s \ge s_0.$$
 (4.14)

On the other hand, by the assumption $\gamma_1 > \gamma_2$, there is $s^{\gamma_1} > s^{\gamma_2}$ for $s \ge s_0$, and we have

$$s^{\gamma_1-1} > s^{\gamma_2-2}, \ s \ge s_0.$$

Then by (4.13) together with (4.14) follows that $d \ge 0$ for $s \ge s_0 > 0$.

Henceforth, by using Corollary 4.1 for the equation (4.10), we deduce that U(x) < 0 for $x \in \Omega$ and there holds $U(x_0) < 0$ for $s \ge s_0 > 0$. On the other hand, by performing the Laplace transform on the overposed condition $u_1^{\gamma_1}(x_0, t) = u_1^{\gamma_2}(x_0, t)$, there holds

$$U(x_0) = \hat{u}_1^{\gamma_1}(x_0, s) - \hat{u}_1^{\gamma_2}(x_0, s) = 0.$$
 (4.15)

This is a contradiction and there must have $\gamma_1 \leq \gamma_2$. Similarly, $\gamma_1 < \gamma_2$ is impossible. Therefore $\gamma_1 = \gamma_2$. The proof is completed.

Furthermore, the fractional order and the degradation coefficient in (2.1) can be uniquely determined also by the additional measurement $u_1(x_0, t)$, $0 < t < \infty$.

Theorem 4.2 Let $u_1^{\gamma,\lambda}, u_2^{\gamma,\lambda}$ be the solutions of the forward problem in the mobile and immobile zones, corresponding to $\gamma \in (0,1)$ and $\lambda > 0$ respectively, and $x_0 \in \Omega$ be the measured point. If $u_1^{\gamma_1,\lambda_1}(x_0,t) = u_1^{\gamma_2,\lambda_2}(x_0,t)$ for $t \in (0,\infty)$ and $(\gamma_i,\lambda_i) \in S_{ad}$ (i = 1,2), then there hold $\lambda_1 = \lambda_2$ and $\gamma_1 = \gamma_2$.

Proof Assume that $\lambda_1 > \lambda_2$. Denote $\hat{u}_1^{\gamma,\lambda}(x,s)$ as the Laplace transform of the solution $u_1^{\gamma,\lambda}(x,t)$ on t > 0 for $(\gamma,\lambda) \in S_{ad}$, and let $V(x,s) = \hat{u}_1^{\gamma_2,\lambda_2}(x,s) - \hat{u}_1^{\gamma_1,\lambda_1}(x,s)$ for $x \in \Omega$ and s > 0. With a similar method as used in Theorem 4.1, there holds

$$\frac{1}{P}\frac{d^2V}{dx^2} - \frac{dV}{dx} + \bar{c}V = \bar{d},$$
(4.16)

where

$$\bar{c} = -\omega - \lambda_1 - \beta Rs + \frac{\omega^2}{(1-\beta)Rs^{\gamma_1} + \omega + \mu}, \quad (4.17)$$

and

and the boundary conditions are V(0) = 0 and V'(1) = 0.

Also consider the case of s > 0 and large enough. Obviously there is $\bar{c} \leq -\lambda_1 - \beta Rs < 0$. Let us analyze the sign of the coefficient \bar{d} . Also as done in the above, rewrite (4.18) as

$$\bar{d} = s \hat{u}_1^{\gamma_2,\lambda_2} \{ \frac{\lambda_1 - \lambda_2}{s} + \frac{\omega^2 (1 - \beta) R(s^{\gamma_1 - 1} - s^{\gamma_2 - 1})}{[(1 - \beta) Rs^{\gamma_1} + \omega + \mu][(1 - \beta) Rs^{\gamma_2} + \omega + \mu]} \},$$

$$(4.19)$$

for s > 0. As done in Theorem 4.1, there exists $s_0 > 0$ large enough such that $s\hat{u_1}^{\gamma_2,\lambda_2} > 0$ as $s \ge s_0$. By the a priori conditions for the known parameters we have

$$\frac{\frac{\omega^{2}(1-\beta)R(s^{\gamma_{1}-1}-s^{\gamma_{2}-1})}{[(1-\beta)Rs^{\gamma_{1}}+\omega+\mu][(1-\beta)Rs^{\gamma_{2}}+\omega+\mu]}}{\sim \frac{\omega^{2}}{(1-\beta)R}\frac{s^{-\gamma_{2}}-s^{-\gamma_{1}}}{s}, s \to \infty.}$$
(4.20)

Since $\gamma_1, \gamma_2 \in (0, 1)$, and $s^{-\gamma_2} - s^{-\gamma_1} \to 0$ as $s \to \infty$, there holds

$$\frac{s^{-\gamma_2}-s^{-\gamma_1}}{s}=O(s^{-1-\gamma^*}),s\to\infty,$$

where $\gamma^* = \min{\{\gamma_1, \gamma_2\}}$. By the assumption $\lambda_1 > \lambda_2$, there holds

$$\frac{\lambda_1 - \lambda_2}{s} + \frac{\omega^2 (1 - \beta) R(s^{\gamma_1 - 1} - s^{\gamma_2 - 1})}{[(1 - \beta) Rs^{\gamma_1} + \omega + \mu][(1 - \beta) Rs^{\gamma_2} + \omega + \mu]} \ge 0$$
(4.21)

for $s \ge s_0$. Then there holds $\overline{d} \ge 0$ for $s \ge s_0$ by (4.19). So by applying Corollary 4.1 for the equation (4.16), there must have V(x,s) < 0 for $x \in \Omega$ and $s \ge s_0 > 0$.

With a completely same arguments as stated in Theorem 4.1, we get a contradiction which gives the assertion $\lambda_1 \leq \lambda_2$. Consequently we can get $\lambda_1 \geq \lambda_2$. Thus there must have $\lambda_1 = \lambda_2$.

Denote $\lambda_1 = \lambda_2 := \lambda$, and by the same arguments as given in Theorem 4.1, we get $\gamma_1 = \gamma_2$. The proof is over.

V. NUMERICAL INVERSIONS

In this section, we present numerical inversions for simultaneously identifying the fractional order and the degradation coefficient in the model (2.1) by the modified Levenberg-Marquart (LM) algorithm. We refer to [12], [38] for detailed procedures of the inversion algorithm.

A. The inversion algorithm

Here and henceforth, we denote $z := (\gamma, \lambda) \in S_{ad}$ as the exact solution to the inverse problem, and S_{ad} is given by (4.2), and we write the solution of the forward problem in the mobile zone as $u_1[z]$ for any prescribed $z \in S_{ad}$. We firstly introduce the LM method.

Consider a nonlinear least square problem

$$\min_{x \in X} \|F(x) - y\|_2^2, \tag{5.1}$$

where F(x) is always a nonlinear function on $x \in X$, X is a bounded domain in \mathbb{R}^d , and y is a vector of measurements. For given x_n , by setting

$$x_{n+1} = x_n + s_n, \ n = 0, 1, \cdots,$$
(5.2)

and choosing a suitable parameter μ_n , and work out s_n by the normal equation

$$(F'(x_n)^*F'(x_n) + \mu_n I)s_n = F'(x_n)^*(y - F(x_n)), \quad (5.3)$$

where $F'(x_n)$ denotes the Jacobi matrix of $F(x_n)$, $F'(x_n)^*$ is the adjoint matrix of $F'(x_n)$, I is the identity matrix, and $\mu_n > 0$ is the so-called LM parameter. This is the main idea of the LM method.

Based on the LM method, we consider the following minimization problem by involving with the regularization strategy and homotopy idea:

$$\min_{x \in X} \{ (1 - \alpha) \| F(x) - y \|_2^2 + \alpha \| x \|_2^2 \},$$
 (5.4)

where $\alpha \in (0, 1)$ is the homotopy parameter which decreases continuously from 1 to 0. By the same induction as for the LM method, we can get a normal equation for given x_n

$$\begin{array}{l} ((1 - \alpha_n)F'(x_n)^*F'(x_n) + \alpha_n I) \, s_n \\ = (1 - \alpha_n)F'(x_n)^*(y - F(x_n)), \end{array}$$
(5.5)

by which an optimal perturbation s_n is solved and we get x_{n+1} also by (5.2).

A key problem on performing the inversion algorithm is how to choose the homotopy parameter. As done in [16], [38], we choose the Sigmoid-type function as the homotopy parameter given as

$$\alpha_n = \frac{1}{1 + e^{\sigma(n - n_0)}},\tag{5.6}$$

where *n* is the number of iterations, n_0 is the preestimated number of iterations, and $\sigma > 0$ is the adjust parameter. The procedures of the inversion algorithm are given as follows: Step 1. Give the target function F(x) and the data vector y, and the control precision eps;

Step 2. Give initial guess $x_n(n = 0, 1, \dots)$, and work out $\overline{F(x_n)}$ and the Jacobi matrix $F'(x_n)$;

Step 3. Work out an optimal perturbation s_n by (5.5) where the homotopy parameter is chosen by (5.6);

<u>Step 4.</u> If $||s_n||_2 \le eps$, then $x_{n+1} = x_n + s_n$ is the inversion solution, and the algorithm terminates; Otherwise, replacing x_n with x_{n+1} , and turn to Step 2 to go on.

 TABLE II

 The inversion results in Ex.5.1

δ	\bar{z}^{inv}	$\bar{E}rr$	\bar{n}
5%	(0.54286268, 0.021777354)	8.89e-2	46.5
1%	(0.50355608, 0.0098008279)	7.12e-3	45
0.1%	(0.49982613, 0.0096872755)	7.15e-4	45
0.01%	(0.49996940, 0.010017620)	7.06e-5	45
0	(0.49999999, 0.0099999979)	1.56e-8	44

B. Numerical examples

For the considered inverse problem, denote the target function as $F(z)(t) = u_1[z](x_0, t), t \in (0, T]$ for any given time T > 0, and the additional data function is supposed to be contaminated by random noises, which satisfies

$$\|u_1^{\delta}(x_0, t) - u_1(x_0, t)\|_{L^2(0,T)} \le \delta, \tag{5.7}$$

and $\delta > 0$ denotes the noise level. By utilizing the modified LM algorithm to solve the nonlinear equation

$$F(z)(t) = u_1^{\delta}(x_0, t), t \in (0, T],$$
(5.8)

we get numerical inversions for each given noise level. On performing the inversion algorithm, the forward problem is solved numerically by the finite difference scheme (2.12), where T = 1 and the time and space grid steps are h = 1/20and $\tau = 1/20$ respectively; and the initial iteration is always chosen as zero, and the measured point is fixed at $x_0 = 0.5$. In addition, we choose $n_0 = 4$ and $\sigma = 0.3$ in (5.6) in the following computations.

Example 5.1 Let $\gamma = 0.5$ and $\lambda = 0.01$ be the exact fractional order and the degradation coefficient, respectively. In other words, the exact solution of the inverse problem is z = (0.5, 0.01). The other known parameters are given as P = 1, R = 2, $\beta = 0.5$, $\omega = 0.5$ and $\mu = 0.5$ in this example. By substituting the exact parameters into the forward problem, the solution is computed and the additional data at $x_0 = 0.5$ are obtained, with which the two parameters are reconstructed using the inversion algorithm.

The inversion results with noisy data and exact data are listed in Table 2, where δ denotes the random noise level and $\delta = 0$ denotes the inversion with exact data, and $\bar{z}^{inv} := (\bar{\gamma}^{inv}, \bar{\lambda}^{inv})$ denotes the average inversion solution with 10-time inversions, and $\bar{E}rr$ denotes the relative error, which is given by $\bar{E}rr = ||z - \bar{z}^{inv}||/||z||$, and \bar{n} denotes the average number of iterations.

Example 5.2 In this example, we choose the known parameters as P = 5, R = 2, $\beta = 0.5$, $\omega = 1.5$ and $\mu = 0.1$. Let $\gamma = 0.75$ and $\lambda = 0.05$, i.e., the exact solution of the inverse problem is z = (0.75, 0.05). As done in Ex.5.1, the inversion results with noisy data and exact data are listed in Table 3, where δ , \bar{z}^{inv} , $\bar{E}rr$ and \bar{n} are the same notations as in Ex.5.1.

From Table 2 and Table 3 it can be seen that the inversion solutions approximate and converge to the exact solution as the noise level goes to zero, and the inversion algorithm is of numerical stability against noises in the measured data.

VI. CONCLUSION

The integer-fractal MIM solute transport model is studied from numerical solution and system identification. An effective finite difference scheme to solve the forward problem

TABLE IIITHE INVERSION RESULTS IN EX.5.2

δ	$ar{z}^{inv}$	$\bar{E}rr$	\bar{n}
5%	(0.81434955, 0.080588152)	9.48e-2	45.5
1%	(0.75121139, 0.043785104)	8.42e-3	43.7
0.1%	(0.75044171, 0.050252851)	6.77e-4	43.3
0.01%	(0.75003291, 0.050032150)	6.12e-5	43
0	(0.74999999, 0.049999994)	1.19e-8	40

is proposed, and the uniqueness of identifying the fractional order and the degradation coefficient is proved by the method of Laplace transform, and numerical inversions with noisy data are presented based on the difference solution. We will give regularity analysis for the solution of the forward problem, and focus on inverse problems of determining other parameters in the model, such as the partition parameter and the mass transfer rate in the near future.

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