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Numerical Inversion of a Time-Dependent Reaction Coefficient in a Soil-Column Infiltrating Experiment

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Abstract: This paper deals with an inverse problem of determining a time-dependent reaction coefficient arising from a disturbed soil-column infiltrating experiment based on measured breakthrough data. A purpose of doing such experiment is to simulate and study transport behaviors of contaminants when they vertically penetrating through the soils. Data compatibility of the inverse problem is discussed showing a sufficient condition to the solution's monotonicity and positivity with the help of an adjoint problem. Furthermore, an optimal perturbation regularization algorithm is applied to solve the inverse problem, and two typical numerical examples are presented to support the inversion algorithm. Finally, transport model of a positive solute ion in the soil-column is investigated based on the researches to the inverse problem. An optimal reaction coefficient is determined by the inversion algorithm, and the inversion is of numerical uniqueness. The inversion results not only coincide with data compatibility of the inverse problem, but also agree with the real breakthrough data.

Keywords: solute transport; advection-dispersion equation; inverse problem; determination of time-dependent reaction coefficient; soil-column experiment; optimal perturbation regularization algorithm; numerical inversion; numerical uniqueness.

1 Introduction

Soil and groundwater pollution has become a serious threat to sustainable development throughout the world. It is important to characterize physical/chemical reactions quantitatively in solutes transport processes in the soils and groundwater [Sun (1996), Atmadja (2001), Zheng (2002), Khlaifi (2009)]. To understand

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transport behaviors of the soil in the presence of infiltrating contaminants, soil-column experiments are often performed in the laboratory. There are disturbed and undisturbed soil-column infiltrating experiments, and the soil-column in a disturbed experiment is often loaded uniformly and orderly with a lucite tube. A primary purpose of doing disturbed soil-column experiment is to simulate and study transport behaviors of contaminants when they vertically penetrating through the soils with artificial chemical liquid.

As we know, there are lots of researches on solutes transportation in soil-column infiltrating experiments since the 1980's. Typical work could belong to the researching group of Nielsen and Van Genuchten. Nielsen [Nielsen, Van Genuchten, and Biggar (1986)] put forward general equations of advection-dispersion type to describe solute transport behaviors, and Van Genuchten [Van Genuchten and Wagenet (1989)] constructed solute transport models of two sites/two regions in the soils. With development of computational tools and techniques, numerical methods and software packages based on convection-dispersion equations are widely utilized on researches of soil-column infiltrating experiments [Toride, Leij and Van Genuchten (1995); Torsten (1998); Pang and Close (1999); Inoue, Simunek, Shiozawa, and Hopmans (2000); Kamra, Lennartz, Van Genuchten, and Widmoser (2001); Cui, Li, Li, and Yang (2004), Köhne, Mohanty, Simunek (2005); Barry (2009); Lewis, Sjöstrom (2010)]. Recently, the authors have even considered an undisturbed soil-column experiment from two different aspects respectively. One aspect is to consider single solute transport and identify source parameters based on linear adsorption model [Li, Cheng, Yao, Liu and Liu (2007)], the other is to deal with multi-components solutes transport and determine multi-parameters based on hydro-chemical analysis with advection dispersion mechanism [Li, Yao, Wang and Jiang (2009)].

It is obvious that researching difficulties for soil-column infiltrating experiments lie in construction of suitable solute transport model and determination of model parameters which always lead to researches of inverse problems. It is noticeable that most of inversion algorithms are based on regularization strategies so as to overcome ill-posedness of the real problem, and different kinds of inverse problems could need different regularization strategies. For example, method of fundamental solutions [Ling and Takeuchi (2008); Marin (2009)], lie-group estimation method and one-step group preserving scheme [Liu, Liu, and Hong (2007); Liu, Chang, and Chang (2008)], level set method [Shim, Ho, Wang, and Tortorelli (2008); Lin, Chen, Cheng, and Wang (2009)], and optimal approximate methods [Su (1995); Amirov and Ustaoglu (2009)] have been testified to be effective methods in dealing with corresponding inverse problems. However, to our knowledge, there are few theoretical analysis on inverse problems of parameter determination arising in

soil-column infiltrating experiments, and it is still a trouble on how to realize an inversion algorithm with high efficiency in concrete computations.

In this paper, we will investigate a disturbed soil-column experiment carried out in Zibo, Shandong Province, China. By analysis to the experiment and experimental data, we find that transport behaviors of the solutes ions in the column are principally dominated by hydromechanical dispersion and possible chemical reactions or ions exchanges in the liquid phase, and physical/chemical reactions between the solid and liquid phases can be ignored due to relatively clean sandy soils in the column. Thus, transport process of each solute ion in the column can be described by a 1-D advection-dispersion model with an unknown first order reaction term depending upon time, and then an inverse problem of determining a time-dependent reaction coefficient based on advection-dispersion equation is encountered with.

Additional information of the inverse problem is given at the outflow hand-side which called breakthrough data of soil-column experiment. Although there are quite a few researches on inverse problems of determining space-dependent or state-dependent functions for diffusion equations [Choulli and Yamamoto (1997); Isakov (1999); Liu, Liu, and Hong (2007); Chi and Li (2010)], but there are few researches for such inverse problems of determining time-dependent reaction coefficient in advection-dispersion equation in the known literatures we have. In paper [Tadi (1997)], an inverse problem with boundary measurement at the right hand-side for heat equation was considered, and in the case of the reaction coefficient being a constant, an iterative algorithm was introduced to determine it successfully. In this paper, we will deal with an inverse problem of determining a reaction coefficient which depends on time variable in an advection-dispersion equation with the boundary measurement too. A similar problem was ever coped with in paper [Li, Cheng, Yao, Liu and Liu (2007)] by the author, but here it is different as compared with that work. This paper will present data compatibility and corresponding numerical testification, and investigate numerical uniqueness of the inversion algorithm, both of which are ignored in that work. In addition, the soil-column infiltrating experiments in the two papers are different, too.

The paper is arranged as follows:

Section 2 gives the forward problem and the inverse problem of determining a time-dependent reaction coefficient, and a sufficient condition to the solution's monotonicity and positivity of the forward problem is discussed with the help of an adjoint problem.In section 3, an optimal perturbation regularization algorithm is applied to solve the inverse problem, and two typical numerical examples are presented to support the inversion algorithm. In section 4, a disturbed soil-column experiment is introduced, and transport model of a positive solute ion through the soil-column is investigated. An optimal reaction coefficient is determined with nu-

merical uniqueness by applying the inversion algorithm. The inversion results not only coincide with data compatibility analysis of the inverse problem, but also agree with the real breakthrough data. Finally, several concluding remarks are presented.

2 The forward problem and the inverse problem

For $l > 0$, $T > 0$, denote $\Omega_T = \{(x,t) : 0 < x < l, 0 < t < T\}$, and consider an initial boundary value problem of equilibrium advection-dispersion equation

$$u_t = Du_{xx} - vu_x + \beta(t)u, \quad (x,t) \in \Omega_T, \tag{1}$$

$$u(x,0) = g(x), \quad 0 \le x \le l, \tag{2}$$

$$u(0,t) = u_0(t), \quad u_x(l,t) = 0, \quad 0 \le t \le T, \tag{3}$$

where $u = u(x,t)$ denotes solute concentration at space point x and time t, $D > 0$ is longitudinal dispersivity, $v > 0$ is average flow velocity, and $\beta = \beta(t)$ represents the first order physical/chemical reaction coefficient depending on the experimental time for the considered solutes ion, which is always unknown in the solute transportation. By general theory of parabolic type of partial differential equation, we know that if the functions $\beta(t)$, $g(x)$, and $u_0(t)$ satisfy suitable conditions, for example, $u_0(t)$, $\beta(t) \in C([0,T])$, and $g(x) \in C([0,l])$, then there exists an unique solution $u(x,t) \in C^{2,1}(\Omega_T)$ for the forward problem (1)-(3).

Now suppose the reaction coefficient function $\beta(t)$ unknown, and the coefficients D and v, the initial function $g(x)$, and the boundary function $u_0(t)$ are all known, an inverse problem here we will deal with is to determine $\beta = \beta(t)$ utilizing the following additional information given at the boundary $x = l$

$$u(l,t) = h(t), \quad 0 \le t \le T. \tag{4}$$

In many cases for real problems, a solution $u = u(x,t)$ of the forward problem should be positive and monotone on time or space variables. In this paper, we will consider a situation of that the concentration solution is positive and monotone on space variable $x \in (0,l)$ at each given time $t \in (0,T)$.

Theorem 1 Suppose that $u = u(x,t)$ is a priori bounded, and the functions $g(x)$, $u_0(t)$, and $\beta(t)$ satisfy suitable conditions given later, we have

(a) If $g'(x) \le 0$ for $x \in (0,l)$, and $u_0'(t) - u_0(t)\beta(t) \ge 0$ for $t \in (0,T)$, then for each $t \in (0,T)$ follows that

$$h(t) = u(l,t) \le u(x,t) \le u(0,t) = u_0(t), \quad x \in (0,l); \tag{5}$$

(b) If $g'(x) \geq 0$ for $x \in (0,l)$, and $u_0'(t) - u_0(t)\beta(t) \leq 0$ for $t \in (0,T)$, then for each $t \in (0,T)$ follows that

$$u_0(t) = u(0,t) \leq u(x,t) \leq u(l,t) = h(t), \quad x \in (0,l). \tag{6}$$

Proof We will only prove assertion (a), and assertion (b) can be proved similarly. For $u = u(x,t)$ satisfying equation (1), and any smooth test function $\varphi(x,t)$, there is

$$\int_{\Omega_T} [u_t - Du_{xx} + vu_x - \beta(t)u]\varphi_x dxdt = 0. \tag{7}$$

Integration by parts leads to

$$\int_{\Omega_T} [\varphi_t + D\varphi_{xx} + v\varphi_x + \beta\varphi]u_x dxdt = \int_0^T [-u_t\varphi + Du_x\varphi_x + \beta u\varphi]_0^l dt + \int_0^l [u_x\varphi]_0^T dx. \tag{8}$$

Now suppose that $\varphi = \varphi(x,t)$ solves the following adjoint problem

$$\begin{cases} \varphi_t + D\varphi_{xx} + v\varphi_x + \beta(t)\varphi = G(x,t), & (x,t) \in \Omega_T, \\ \varphi(x,T) = 0, & 0 \leq x \leq l, \\ \varphi_x(0,t) = 0,\ \varphi(l,t) = 0, & 0 \leq t \leq T, \end{cases} \tag{9}$$

where $G(x,t)$ is a nonnegative but otherwise arbitrary function in Ω_T. Then equality (8) reduces to

$$\int_{\Omega_T} G(x,t)u_x dxdt = \int_0^T [u_0'(t) - \beta(t)u_0(t)]\varphi(0,t)\,dt + \int_0^l -\varphi(x,0)g'(x)dx. \tag{10}$$

By applying maximum principle to the adjoint problem (9), we can get that, if $G(x,t)$ is nonnegative but is otherwise arbitrary, then $\varphi(x,t)$ is negative in Ω_T. Thus, noting the condition of assertion (a) together with equality (10), there is

$$\int_{\Omega_T} G(x,t)u_x(x,t)dxdt \leq 0, \tag{11}$$

which implies that assertion (a) is valid. The proof is over.

By the above theorem, we know that if the solution $u = u(x,t)$ is monotone on space variable at given time, then the following two conditions need to be valid:

(A1) $g(x) \in C^1(0,1)$, and $g'(x)$ keeps symbol unchangeable for $x \in (0,l)$;

(A2) $u_0(t) \in C^1(0,T)$, $\beta(t) \in C(0,T)$, and $u_0'(t) - u_0(t)\beta(t)$ also keeps symbol unchangeable for $t \in (0,T)$.

In other words, we will investigate the inverse problem under conditions (A1) and (A2) together with inequalities (5) and (6) satisfied respectively, in which case data functions of the inverse problem are called compatible. Furthermore, for given $g(x)$ and $u_0(t)$ satisfying (A1) and (A2) respectively, and for given boundary measurement $h(t)$, if there is $0 < h(t) \leq u_0(t)$, then we should seek to solve a possible reaction coefficient in the following admissible set:

$$S_\beta^- = \{\beta \in C(0,T) : u_0' - u_0\beta \geq 0\},$$

with $g'(x) \leq 0$.

Otherwise, if there is $0 < u_0(t) \leq h(t)$, then we should seek to solve the reaction coefficient in a set of

$$S_\beta^+ = \{\beta \in C(0,T) : u_0' - u_0\beta \leq 0\},$$

with $g'(x) \geq 0$.

Remark 1 For real problems arising in soil-column experiments, the boundary condition at the left hand of $x = 0$ is always set to be a constant, i.e. $u_0(t) = \text{const} > 0$, in which case the assumption $u_0'(t) - u_0(t)\beta(t) \geq 0$ in assertion (a) means that $\beta \leq 0$ for $t \in (0,T)$, and $u_0'(t) - u_0(t)\beta(t) \leq 0$ in assertion (b) means that $\beta \geq 0$ for $t \in (0,T)$. In section 4, we can see that a real inverse problem arising from a soil-column experiment just coincides with the case of assertion (a).

3 The inversion algorithm and numerical simulations

It is important to explore uniqueness and stability for an inverse problem, but it still has a long distance from theory to practice. For an inverse problem, one should adopt a suitable inversion algorithm to work out the solution and reconstruct the data. It can be reduced to minimize an error functional of the unknown function between the computational output data and the additional data in solving an inverse problem. However, considering data errors, model errors, and rounding errors, etc., inversion algorithms with regularization terms are often necessary to cut down the noises, and stabilize the minimization problem so as to get a trustable solution. In this paper, an optimal perturbation regularization algorithm is applied to determine the reaction coefficient function $\beta = \beta(t)$, and a numerical uniqueness for the inverse problem will be illustrated by the inversion results.

3.1 The optimal perturbation regularization algorithm

As we know, an unknown function in an inverse problem arising in PDE should often be confined in a suitable set which induces an admissible space of the unknowns. We will assume that $\beta(t) \in \Psi$, where $\Psi \subset C(0,T)$ is an admissible space of the unknowns.

Therefore, for any $\beta(t) \in \Psi$, an unique solution of the corresponding forward problem, denoted by $u(x,t;\beta)$, can be solved numerically, and then computational data at the boundary $x = l$ are obtained, denoted by $u(l,t;\beta)$. So, an optimal idea for solving the inverse problem here is to solve a minimization problem:

$$\min_{\beta\in\Psi} J(\beta), \tag{12}$$

where $J(\beta) = ||u(l,t;\beta) - h(t)||_2^2 = \int_0^T [u(l,t;\beta) - h(t)]^2 dt$.

Generally speaking, it is unstable to solve the above minimization problem (12) numerically, especially in the case of the additional data having noises. Fortunately, the optimal perturbation regularization algorithm is a possible approach to finding an optimal solution to the above problem [Su (1995); Li, Cheng, Yao, Liu and Liu (2007); Li, Yao, Wang and Jiang (2009); Chi and Li (2010)]. If employing Tikhonov regularization, it needs to minimize the following functional with Tikhonov regularization term

$$\min_{\beta\in\Psi}\{||u(l,t;\beta) - h(t)||_2^2 + \alpha||\beta||_2^2\}, \tag{13}$$

where $\alpha > 0$ is regularization parameter. Suppose that $\{\phi_i(t)\}_{i=1}^{\infty}$ is a group of basis functions of Ψ, then there is

$$\beta(t) = \sum_{i=1}^{\infty} a_i \phi_i(t),$$

where $a_i (i = 1,2,\cdots)$ are expansion coefficients. Taking an approximation by choosing limited terms, we have

$$\beta(t) \approx \sum_{i=1}^{N} a_i \phi_i(t), \tag{14}$$

here $N \geq 1$is a truncated level of $\beta(t)$, which can be regarded as dimension of approximate space. It is convenient to set a limited dimensional space as $\Psi^N = \text{span}\{\phi_1, \phi_2, \cdots, \phi_N\}$, and a N-dimension vector $\mathbf{a} = (a_1, a_2, \cdots, a_N)$. Therefore,

to get an approximate reaction coefficient $\beta \in \Psi^N$ is equivalent to find a vector $\mathbf{a} \in R^N$, in which meaning we can say $\beta = \mathbf{a}$.

Now, for given $\beta_j \in \Psi^N$, assume that

$$\beta_{j+1} = \beta_j + \delta\beta_j, j = 0, 1, \cdots. \tag{15}$$

Then in order to get β_{j+1} from β_j, we need to compute an optimal perturbation $\delta\beta_j$. In the follows for convenience of writing, β_j and $\delta\beta_j$ are abbreviated as β and $\delta\beta$.

Paying attention to (14), let us set

$$\delta\beta(t) = \sum_{i=1}^{N} \delta a_i \phi_i(t),$$

by which we only need to work out a vector $\boldsymbol{\delta}\mathbf{a} = (\delta a_1, \delta a_2, \cdots, \delta a_N)$.

Taking Taylor's expansion for $u(l,t;\beta+\delta\beta)$ at β, and ignoring higher order terms, we can get

$$u(l,t;\beta+\delta\beta) \approx u(l,t;\beta) + \nabla^{\mathrm{T}} u(l,t;\beta) \cdot \delta\beta.$$

Thus, define a perturbation functional for $\delta\beta$ (or $\boldsymbol{\delta}\mathbf{a}$) as follows:

$$F(\delta\beta) = ||u(l,t;\beta) + \nabla^{\mathrm{T}} u(l,t;\beta) \cdot \delta\beta - h(t)||_2^2 + \alpha||\delta\beta||_2^2, \tag{16}$$

where

$$\nabla^{\mathrm{T}} u(l,t;\beta) \cdot \delta\beta \approx \sum_{i=1}^{N} \frac{u(l,t;\beta+\tau_i\phi_i) - u(l,t;\beta)}{\tau_i} \delta a_i,$$

here τ_i $(i = 1, 2, \cdots, N)$ is numerical differential step. Next, discretizing the domain $(0,T)$ with $0 = t_1 < t_2 < \cdots t_K = T$, then the above L^2 norm in (16) can be reduced to discrete Euclid norm given as

$$F(\boldsymbol{\delta}\mathbf{a}) = ||\mathbf{G}\boldsymbol{\delta}\mathbf{a} - (\boldsymbol{\eta} - \boldsymbol{\xi})||_2^2 + \alpha||\boldsymbol{\delta}\mathbf{a}||_2^2,$$

where

$$\boldsymbol{\xi} = (u(l,t_1;\beta), u(l,t_2;\beta), \cdots, u(l,t_K;\beta)), \quad \boldsymbol{\eta} = (h(t_1), h(t_2), \cdots, h(t_K));$$

and

$$g_{ki} = [u(l,t_k;\beta+\tau_i\phi_i) - u(l,t_k;\beta)]/\tau_i, \quad \mathbf{G} = (g_{ki})_{K\times N}, \\ k = 1, \cdots, K, \quad i = 1, \cdots, N. \tag{17}$$

It is not difficult to verify that the square minimization problem $\min_{\boldsymbol{\delta}\mathbf{a}\in\mathbf{R}^N} F(\boldsymbol{\delta}\mathbf{a})$ is equivalent to solve the following normal equation [Kirsch, (1996)]:

$$\mathbf{G}^T\mathbf{G}\boldsymbol{\delta}\mathbf{a}+\alpha\boldsymbol{\delta}\mathbf{a}=\mathbf{G}^T(\boldsymbol{\eta}-\boldsymbol{\xi}). \tag{18}$$

Therefore, an optimal perturbation can be worked out by (18) given as

$$\boldsymbol{\delta}\mathbf{a}^\alpha=(\alpha\mathbf{I}+\mathbf{G}^T\mathbf{G})^{-1}\mathbf{G}^T(\boldsymbol{\eta}-\boldsymbol{\xi}), \tag{19}$$

and then an optimal increment $\delta\beta^\alpha$ can be obtained. Furthermore, an optimal coefficient function $\beta=\beta(t)$ can be obtained approximately by iterative procedures (15) as long as the increment satisfying a given convergent precision. The detailed steps to implement the above algorithm are given as follows.

Step 1. Given approximate space $\Psi^N=\text{span}\{\phi_1,\phi_2,\cdots,\phi_N\}$, and initial iteration β (or $\mathbf{a}$), numerical differentiation steps vector $\tau=(\tau_1,\tau_2,\cdots,\tau_N)$, and convergent precision eps, and additional measurement $h(t)$;

Step 2. Solve the forward problem (1)-(3) to get $u(l,t;\beta)$ and $u(l,t;\beta+\tau_i\phi_i)$ for $i=1,2,\cdots,N$, and then obtain the vector $\boldsymbol{\xi}$ and the matrix $\mathbf{G}$ by formula (17);

Step 3. Choosing suitable regularization parameter $\alpha>0$, and get an optimal perturbation vector $\boldsymbol{\delta}\mathbf{a}^\alpha$ by using formula (19), and then get $\delta\beta^\alpha$;

Step 4. If there is $||\delta\beta^\alpha||_2\le eps$, then the inversion algorithm can be terminated, and $\beta+\delta\beta^\alpha$ is taken as the solution what we just want to determine; otherwise, go to Step 2 by replacing β with $\beta+\delta\beta^\alpha$.

In the next subsection, we will give numerical simulations by performing the above inversion algorithm to the inverse problem (1)-(4). All computations are carried out in a PC of Tsinghua Tongfang, China.

3.2 Numerical simulations

Consider inverse problem (1)-(4) again, and take $D=0.2, v=1$, and $l=1, T=5$, and $g(x)=0$, and $u_0(t)=1$ in concrete computations in this subsection. Moreover, in order to support assertions of Theorem 1, we will present here two kinds of numerical examples which correspond to two cases of $\beta(t)\le 0$, and $\beta(t)\ge 0$ for $t\in(0,T)$, respectively.

3.2.1 Example 1

Take a true reaction coefficient function as

$$\beta(t)=-2+0.5t-0.1t^2, \tag{20}$$

and polynomial basis functions space as $\Psi^N = \text{span}\{1, t, \cdots, t^{N-1}\}$. Obviously, it is not difficult to verify that $\beta(t) \leq 0$ for all $t \in \mathbf{R}$, and for each $t \in (0,5)$, it is valid that $u(1,t) \leq u(x,t) \leq u(0,t)$ for $0 < x < 1$. For the true reaction coefficient in approximate space with different dimensionality, it can be regarded as $\beta^{\text{true}} = (-2, 0.5, -0.1)$ in Ψ^3, and $\beta^{\text{true}} = (-2, 0.5, -0.1, 0)$ in Ψ^4, etc.

With the true reaction coefficient, the forward problem is worked out and then the additional data $u(l,t)$ can be obtained. In the follows, we will apply ordinary optimal perturbation algorithm without using explicit regularization terms to reconstruct the reaction coefficient function, i.e., we will utilize formula (19) by setting regularization parameter $\alpha = 0$ in the following computations.

(a) Using accurate data

Set initial iteration be zero, i.e., $\beta_0 = \mathbf{0}$, differential steps vector $\tau = (1e-1, 1e-2, \cdots, 1e-N)$ for approximate dimension N, and convergent precision as $eps = 1e-8$. Table 1 lists inversion results in different approximate space Ψ^N for $N = 3,4,5,6,7$, and Fig.1 plots an inversion coefficient via the true reaction coefficient in the case of $N = 7$. Where β_N^{inv} denotes inversion coefficient in N-dimensional approximate space, and T_{cpu}/I denotes CPU time for each iteration, and T_{cpu} is total CPU time (second), and I is number of iterations. Furthermore, Table 2 gives solutions errors implemented in Ψ^N, where $Err_{\text{abs}} = ||\beta_N^{\text{inv}} - \beta^{\text{true}}||_2$ and $Err_{\text{rel}} = Err_{\text{abs}}/||\beta^{\text{true}}||_2$ denote absolute and relative errors in the solutions, respectively.

Table 1: Numerical inversion results in Ψ^N

N	β_N^{inv}	T_{cpu}/I
3	(-2.00000, 0.500001, -0.100000)	10.6/6
4	(-2.00000, 0.500003, -0.100001, 2.2814e-7)	12.9/6
5	(-2.00003, 0.500073, -0.100054, 1.4935e-5, -1.3839e-6)	31.7/13
6	(-2.00024, 0.500748, -0.100750, 3.2807e-4, -6.4905e-5, 4.7603e-6)	80.8/29
7	(-1.99983, 0.499278, -0.098987, -6.573e-4, 2.155e-4, -3.466e-5, 2.17e-6)	30.1/7

Table 2: Errors in the solutions in different approximate space

N	3	4	5	6	7
Err_{abs}	1.0000e-6	3.1705e-6	9.6799e-5	1.1364e-3	1.4339e-3
Err_{rel}	4.8450e-7	1.5361e-6	4.6899e-5	5.5060e-4	6.9472e-4

(b) Using noisy data

Let us perform the inversion algorithm in the case of using noisy data. Suppose that noisy data are expressed by

$$h^{\varepsilon}(t) = h(t) + \varepsilon\,\theta,$$

where $0 < \varepsilon \leq \varepsilon_0$ is noisy level, ε_0 is a constant, and θ is a random vector ranged in [-1,1]. Noting that random noises of the data, inversion result for each computation is different. Figs.2-3 plot ten-time inversion results in Ψ^3 with noisy level ε =1% and ε =5%, respectively.

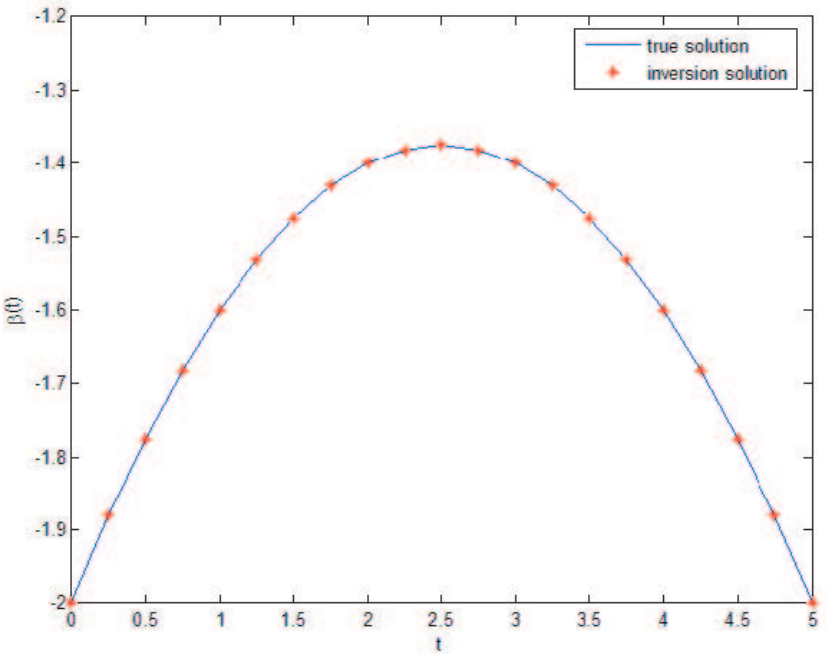

Figure 1: Reconstruction reaction coefficient in Ψ^7 and the true coefficient.

By the above numerical simulations, we can see that the optimal perturbation algorithm not only has accuracy, but also is stable for random noises of the additional data, although explicit regularization strategy has not been utilized here.

3.3 Example 2

In this example, we will take

$$\beta(t) = 2 - 0.5t + 0.1t^2, \tag{21}$$

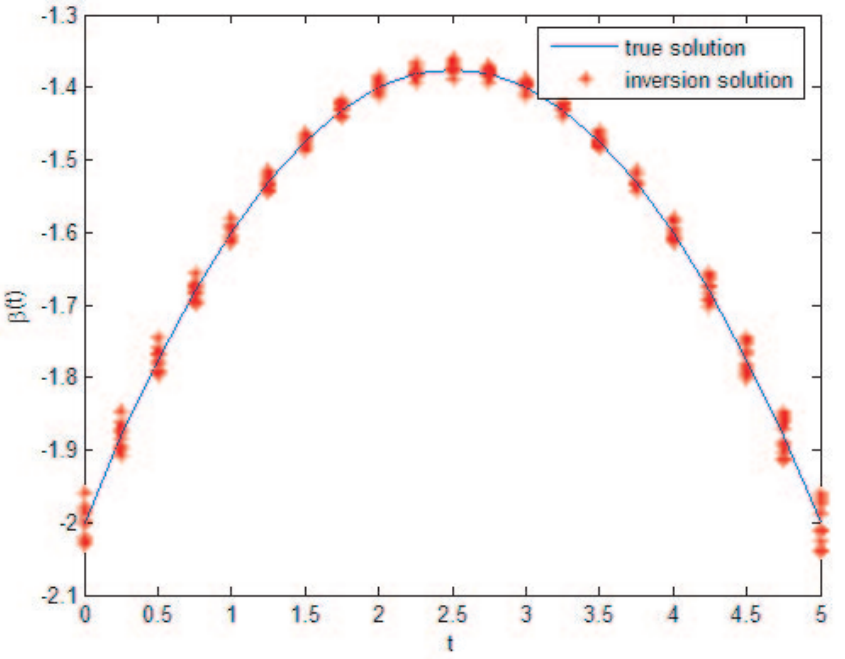

Figure 2: Inversion results of ten-time computations in Ψ^3 for ε =1%

as a true reaction coefficient function, and also take $\Psi^N = \text{span}\{1,t,\cdots,t^{N-1}\}$ as approximate space. We can see that $\beta(t) \geq 0$ for all $t \in \mathbf{R}$. In the case of utilizing accurate data, similarly done as in Example 1, also set $\beta_0 = \mathbf{0}$, $\tau = (1e-1, 1e-2, \cdots, 1e-N)$ for approximate dimension N, and $eps = 1e-8$. Table 3 lists inversion results also for $N = 3,4,5,6,7$, respectively, and Table 4 lists absolute and relative errors of inversion coefficients with the true reaction coefficient, respectively. In addition, Fig.4 also plots an inversion reaction coefficient in Ψ^7 via the true coefficient.

Table 3: Inversion results in Ψ^N for Example 2

N	β_N^{inv}	T_{cpu}/I
3	(2.00000, -0.500001, 0.100000)	35.3/18
4	(2.00000,-0.500001,0.100000,-5.28676e-8)	49.2/20
5	(2.00000,-0.500000,0.100001,-4.63820e-7, 8.16343e-8)	53.1/18
6	(2.00000,-0.500001,0.100000, -3.5786e-8, -3.9885e-8, 8.6359e-9)	75.7/22
7	(2.00000,-0.500000,0.099999, 8.621e-7, -3.694e-7, 7.003e-8, -4.71e-9)	108.2/28

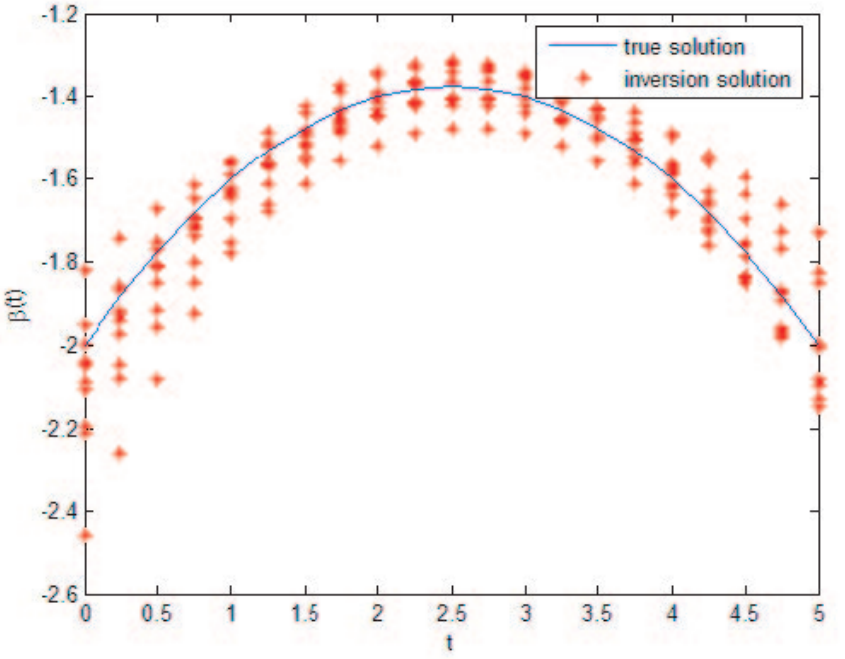

Figure 3: Inversion results of ten-time computations in Ψ^3 for ε =5%

Table 4: Errors in the solutions in different approximate space for Example 2

N	3	4	5	6	7
Err_{abs}	1.0000e-6	1.0014e-6	1.1054e-6	1.0015e-6	1.3728e-6
Err_{rel}	4.8450e-7	4.8518e-7	5.3554e-7	4.8521e-7	6.6513e-7

In the case of coping with noisy data, we will give average inversion results in this example with $N = 3$. By continuously random ten-time computations in Ψ^3, the average inversion results are listed in Table 5 for $\varepsilon = 5\%$ and $\varepsilon = 10\%$ respectively, where $\bar{\beta}_3^{\text{inv}}$ denotes average inversion reaction coefficient, $\bar{T}_{\text{cpu}}/\bar{I}$ denotes average CPU time (second) for each iteration. Moreover, all ten-time inversion results and the true reaction coefficient in Ψ^3 for $\varepsilon = 5\%$ are plotted in Fig.5.

Table 5: Average inversion results with noisy data in Ψ^3 in Example 2

ε	$\bar{\beta}_3^{\text{inv}}$	$\bar{T}_{\text{cpu}}/\bar{I}$
5%	(1.9986, -0.4986, 0.09968)	40.3/20.7
10%	(1.9912, -0.4934, 0.09895)	48.0/26.4

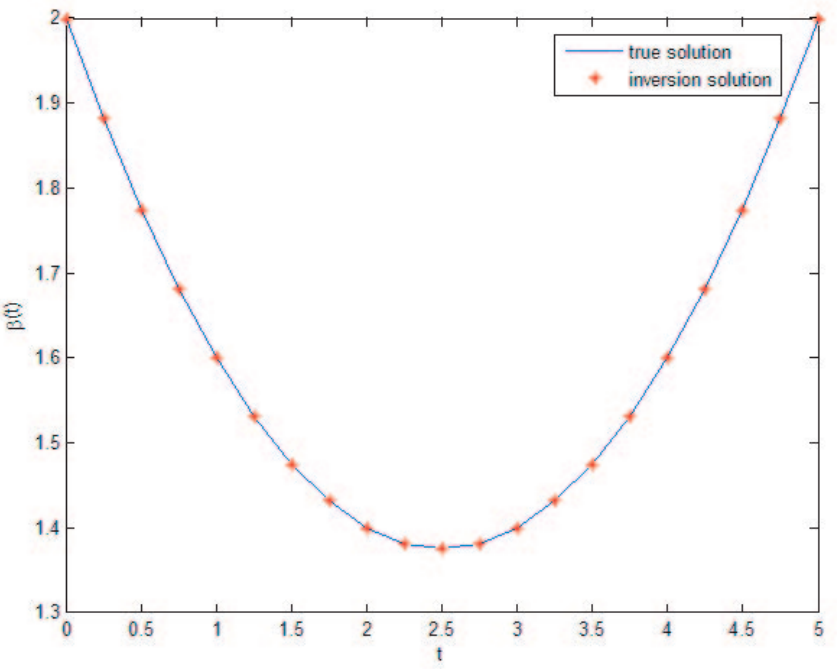

Figure 4: Reconstruction coefficient in Ψ^7 and the true coefficient in Example 2.

By the above computations for the two examples, we can see that the inversion results are satisfactory even not utilizing explicit regularization terms with noisy data, which show that the inverse problem is conditional well-posed at least under the assumptions of Theorem 1. By observing the inversion reaction coefficients and the true coefficient, we find that all relative errors in the solutions are less than 6.9472e-4 in Example 1, and 6.6513e-7 in Example 2, respectively. On the other hand, we can see that high-order terms of β_N^{inv} tend to zero as N goes to large.

However, by Table 1, Table 2, and Table 3, Table 4, we find that the inversion results are not so good in the case of $\beta \leq 0$ in Example 1 as compared with those of Example 2. Maybe the reason results from different ill-posedness of the two examples. As for Example 1, inversion accuracy could be improved if utilizing more accurate convergent precision with suitable regularization than those of Example 2.

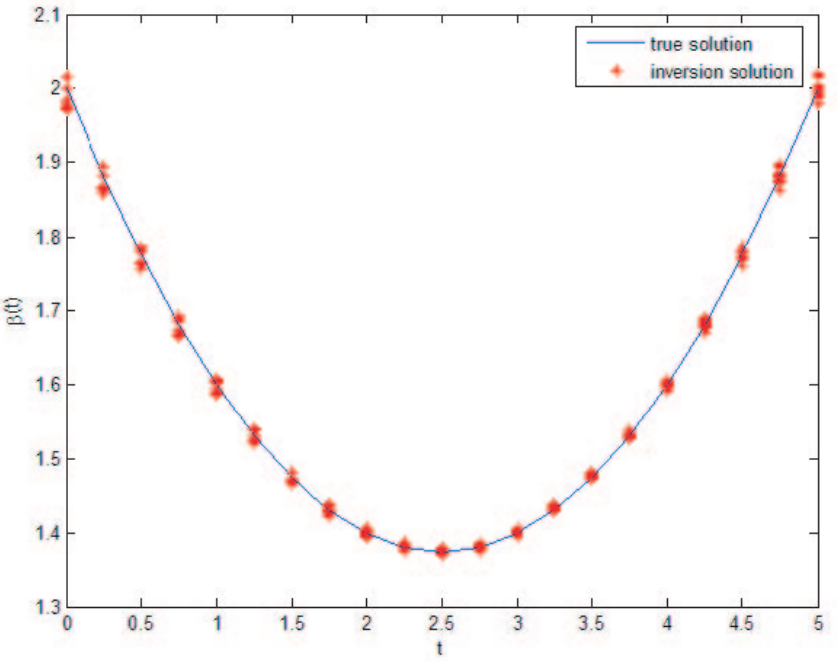

Figure 5: Inversion results of ten-time computations in Ψ^3 for ε =5% in Example 2.

4 Application to a real soil-column infiltrating experiment

4.1 The soil-column experiment and the mathematical model

Consider a disturbed soil-column infiltrating experiment. The experiment was carried out in a simple apparatus in the lab of Shandong University of Technology. The device is installed by three parts: infiltrating system, soil-column system and sample collector system. The soil column is composed by fine sands with diameter of 2mm, the diameter of the lucite tube loading the column is 18.6cm, and the height of the column is about 62cm. After infiltrating the column with distilled water for 24 hours, the experiment was performed at normal temperature of 20 centigrade by infiltrating into the column with artificial coal-mine water.

By collecting water samples at the bottom of the column, 23 samples were collected, and all of them were immediately sent to tested and analyzed in Shandong General Inspecting Station of Geology and Environment. Thus, we get so-called breakthrough data of positive ions of Ca^{2+}, Na^{+}, K^{+} and Mg^{2+}, and negative ions of Cl^{-}, SO_4^{2-}, HCO_3^{-}, and NO_3^{-}.

In this paper, we will take K^+ as an example to illustrate its transport model in the column and deal with an inverse problem of determining time-dependent reaction coefficient. Table 6 gives basic parameters known in the experiment, and Table 7 gives the measured breakthrough data of K^+ from $t_1 = 2/3$[hr] to $T_{\text{tol}} = 20.75$[hr].

Table 6: Basic parameters in the soil-column experiment

l[cm]	a_L[cm]	v[cm/s]	t_1[hr]	T_{tol}[hr]
62	0.88	2.4e-3	2/3	20.75

where l is the length of the column, a_L is the longitudinal dispersivity of the sandy soil which determined by experience according to monogragh [Sun, (1996)], and v is the average flow velocity measured by the experiment, and t_1 is the time at which the first sample collected, after then equilibrium equation (1) could be applied to describe the solute transport behaviors in the column, and T_{tol} denotes total infiltrating time.

Table 7: Breakthrough data of K^+ in the outflow of $x = l$ (t[hr]; u[mg/L])

t	2/3	7/6	3/2	2	2.5	3	4	5	6	7	8	9
u	1.1	1.0	1.4	2.9	3.3	3.6	3.7	3.8	3.9	4.0	4.0	4.1
t	10	11	12	13	14	15	16	17	18	19	20.75	
u	4.2	4.2	4.2	4.2	4.5	4.7	4.8	5.0	5.1	5.2	5.2	

By Table 7, noting that initial concentration of K^+ in the inflow is $u_0 = 17.2$[mg/L], and its concentration at the first outflow is $u(l,t_1) = 1.1$[mg/L], perhaps there are some strong retardation and retention reactions for K^+ during the initial stage of $t \in (0,t_1)$, and after $t = t_1$, the solute concentration goes up rapidly from t_1 to $t = 3$, and it is still in an increasing trend at a slow speed after $t = 3$ until the end of the experiment. Thus, we will utilize the first-order reaction term depending upon time to describe chemical reactions possibly occurring in the liquid phase of the column after $t > t_1$. In other words, we will employ equilibrium equation (1) given in Section 2 with a time-dependent reaction coefficient as transport model of K^+ in the column. However, time domain we are to cope with reduces to $t_1 < t < T_{\text{tol}}$.

In addition, initial boundary value conditions of the forward problem are also given by (2) and (3), here $u_0(t) \equiv u_0 = 17.2$[mg/L], which is just the solute concentration unchangeable in the inflow. As for initial condition (2), there is a trouble that the initial function $u(x,t_1) = g(x)$ for $0 \le x \le l$ is still unknown because we can not stop the experiment at $t = t_1$ to measure space distribution of the solute in the liquid

phase. What we know for $u(x,t_1) = g(x)$ is that $g(0) = u_0$, and $g(l) = u(l,t_1)$. Nevertheless, noting the experimental data and following the method as used in paper [Li, Tan, Yao, Wang, Liu (2008)], we will take on an initial condition given as follows:

$$u(x,t_1) = g(x) = u_0 + (u(l,t_1) - u_0)(x/l)^m, 0 \le x \le l, \tag{22}$$

here $m > 0$ is an index which will be determined later. It needs to point out that for such initial condition (22), there is $g'(x) < 0$ for $x \in (0,l)$ due to $u(l,t_1) < u_0$.

Then, a mathematical model describing the solute transport behaviors in the soil-column is established by equation (1) together with the initial boundary value conditions (22) and (3). For convenience of computation, we will transform the model to a dimensionless form.

Set $U = u/u_0$, $Z = x/l$ and $T = vt/l$, then equation (1) reduces to a dimensionless form:

$$\frac{\partial U}{\partial T} = \frac{a_L}{l}\frac{\partial^2 U}{\partial Z^2} - \frac{\partial U}{\partial Z} + \frac{l}{v}q(T)U, \quad 0 < Z < 1, T_1 < T < \bar{T}, \tag{23}$$

where

$$q(T) = \beta(l/vT), \tag{24}$$

and

$$T_1 = t_1 v/l, \quad \bar{T} = T_{\text{tol}} v/l.$$

The initial and boundary value conditions are transformed to

$$U(Z,T_1) = 1 + (u(l,t_1)/u_0 - 1)Z^m, 0 \le Z \le 1, \tag{25}$$

and

$$U(0,T) = 1,\ U_Z(1,T) = 0, T_1 \le T \le \bar{T}, \tag{26}$$

respectively.

Now the problem remaining here is to determine the unknown initial index m and the reaction coefficient function $q(T)$ by some overposed condition from the experiment. Additional information we will utilize is still given by (4), however, in discrete form, the additional data we can obtain are breakthrough data which are listed in Table 7. Also by dimensionless, we have

$$U(1,T_k) = \bar{U}_k, \quad k = 1,2,\cdots,23. \tag{27}$$

As a result, an inverse problem of determining the reaction coefficient function and the initial index is formulated by dimensionless equation (23) with the initial boundary conditions (25)-(26), and the overposed condition (27).

4.2 Inversion for the real problem

Similarly as done in section 3, we will perform the optimal perturbation regularization algorithm to the above inverse problem (23) with (25)-(27) to determine the unknowns numerically, and then reconstruct the real breakthrough data. Noting that the reaction coefficient function $q(T)$ and the initial index m are both unknown, we will first determine the initial index m by the inversion algorithm, and then we can testify numerical uniqueness of the inverse problem according to Theorem 1 by fixing the initial index unchangeable.

If setting

$$q_N(T) = a_1 + a_2 T + \cdots + a_N T^{N-1}, \tag{28}$$

then it needs to determine a vector given as

$$q_N^m = (a_1, a_2, \cdots, a_N, m),$$

where $m > 0$ is the undetermined initial index. Fortunately, by numerical tests, we find that it is suitable to take $N = 4$ to implement the inversion algorithm. By choosing initial iteration as $q_0 = \mathbf{0}$, and numerical differential step as $\tau = 1e-5$, and convergent precision as $eps = 1e-8$, then reaction coefficient function and initial index can be worked out only by 6-time iterations which costing 2.7 second of CPU time given as follows:

$$q_4^m = (-0.1322, -0.2089, 0.1628, -0.0340, 0.6441). \tag{29}$$

where $m = 0.6441$, and relative error of the inversion is

$$Err_{\text{rel}} = (\sum_{k=1}^{23} \frac{1}{23} |U(1, T_k; q_4^m) - \bar{U}_k|^2)^{1/2} / (\sum_{k=1}^{23} \bar{U}_k^2)^{1/2} = 0.0141, \tag{30}$$

Now, we will focus our attention on testifying numerical uniqueness of determining reaction coefficient function $q = q(T)$ for given initial function based on Theorem 1. By (29), we will take $m = 0.6441$ in initial condition (25), and perform the inversion algorithm to determine $q_N(T)$ given by (28).

The following Table 8 gives numerical inversion results for $N = 4, 5$, and $N = 6$, respectively, where initial iteration, numerical differential step, and convergent precision are all chosen as in the above, and regularization parameter also be zero, and q_N^{inv} denotes inversion coefficient corresponding to N-dimensional approximate space $\Psi^N = \text{span}\{1, T, T^2, \cdots, T^{N-1}\}$, and Err_{rel} denotes relative inversion error defined by (30).

Table 8: Inversion results in Ψ^N for the real problem

N	q_N^{inv}	T_{cpu}/I	Err_{rel}
4	(-0.132151,-0.208952,0.162807,-0.0339806)	2.5/6	0.0141
5	(-0.113888, -0.295902, 0.281387,-0.0948079, 0.0104173)	2.9/6	0.0141
6	(-0.11424, -0.29358, 0.27672, -0.090870, 8.9463e-3, 2.0035e-4)	6.1/11	0.0141

However, in the case of $N = 7$, there are no effective solutions if still not utilizing explicit regularization. We think that the situation becomes very complicated and the ill-posedness of the inverse problem is much severe in the of case of $N \geq 7$. For $N = 7$, by choosing regularization parameter $\alpha = 0.25$, and convergent precision $eps = 6e-8$, and the same initial iteration and numerical differential step as used in the above, we can get an inversion coefficient in Ψ^7 given as

q_7^{inv} =(-0.11427, -0.29314, 0.27023, -0.073739, -7.5728e-3, 6.8557e-3, -9.5002e-4),

and it still remains the same relative error which is Err_{rel}=0.0141. Figure 6 plots the inversion coefficient with the dimensionless time in different approximate space. We can see that all the inversion solutions satisfy condition of taking negative values, i.e., $q(T) \leq 0$ for $T \in [T_1, \bar{T}]$, which just coincide with assertion (a) of Theorem 1.

Furthermore, by the above computational results, we can easily work out solutions' errors in different approximate space given as

$||q_4^{\text{inv}} - q_5^{\text{inv}}||_2 = 7.178\text{e-}2$,

and

$||q_5^{\text{inv}} - q_6^{\text{inv}}||_2 = 2.739\text{e-}3$,

and

$||q_6^{\text{inv}} - q_7^{\text{inv}}||_2 = 9.665\text{e-}3$,

respectively.

By Figure 6 and the above computations, we can deduce that the real inverse problem with suitable initial index is of numerical uniqueness. Nevertheless, if going on performing the inversion algorithm in Ψ^8, we find that larger regularization parameters, and more iterations are needed, but the inversion results are not so good as compared with the above computations. So, we can regard the inversion result of $N = 6$ as an optimal solution to the real inverse problem, i.e., an optimal reaction coefficient function to the real inverse problem in dimensionless form can be given

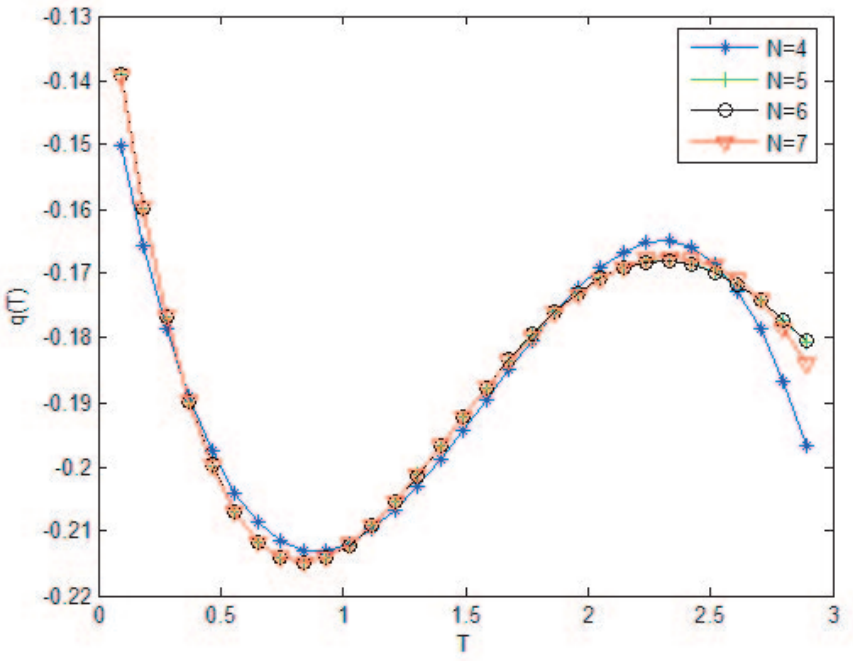

Figure 6: Inversion reaction coefficients via T for $N = 4, 5, 6$ and $N = 7$.

as

$$q(T) = -0.11424 - 0.29358T + 0.27672T^2 - 0.090870T^3 + 8.9463\text{e-}3T^4 + 2.0035\text{e-}4T^5, \quad (31)$$

by which we can reconstruct breakthrough data of K^+ by resolving the corresponding forward problem, which are plotted in Figure 7, as compared with the real breakthrough data.

5 Discussions and conclusions

1) Let us first review and explore properties of the reaction coefficient for the real inverse problem. By the inversion result (31), and noting (24), we can get

$$\beta(t) = -0.11424 - 0.040912t + 5.3738\text{e-}3t^2 - 2.4592\text{e-}4t^3 + 3.3739\text{e-}6t^4 + 1.0529\text{e-}8t^5, \quad (32)$$

which is the reaction coefficient with dimensional time t[hr] for K^+, where $t \in$[2/3, 20.75]. Obviously, it is also valid that $\beta(t) \leq 0$ for $t \in$[2/3, 20.75]; and by (32)

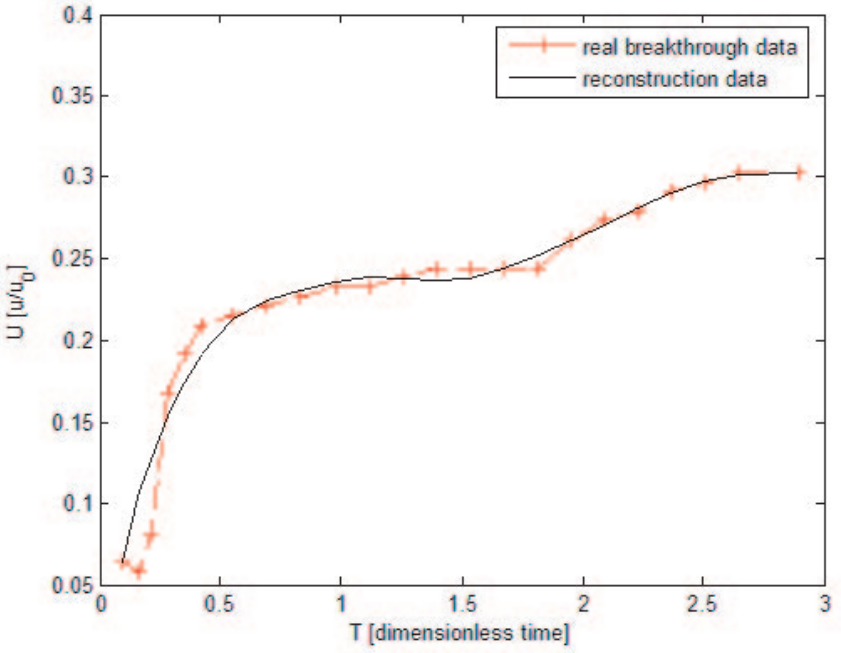

Figure 7: Reconstruction data and real breakthrough data of K^+.

we can also see very clearly that high-order expansion coefficients of $\beta(t)$ become small and go to zero as N goes to large.

On the other hand, by numerical inversion simulations listed in Tables 1-5 for Examples 1-2, and inversion results for the real inverse problem given in Table 8 and Fig.6, we can deduce that it is of conditional uniqueness for the inverse problem of determining $\beta(t)$ (or $q(T)$) not only in the numerical simulations but also in the real inversions. In other words, in the meaning of point of optimal view, an optimal reaction coefficient we want to determine for the real problem is just given by (31) in dimensionless form or (32) in real dimensional space.

2) By computations for the real problem, we find that if the reaction coefficient takes negative values for $t \in [t_1, T_{\text{tol}}]$, then concentration distribution of K^+ is monotone decreasing on space variable at each given time, which just agrees with assertion (a) of Theorem 1. In order to see that clearly, we plot Figures 8-9 in the follows, which are concentration surface and concentration distribution curves of K^+ in dimensionless space by solving the forward problem with the inversion coefficient $q(T)$ given by (31), respectively.

3) Generally speaking, there are several factors impacting the inversion algorithm's

realization, which are approximate space, regularization parameter, convergent precision or number of iteration times, numerical differential step, initial iteration, and computation of the forward problem, etc. However, by inversions for the inverse problem studied here, we find that numerical differential steps and initial iterations both have little impacts on the algorithm, and regularization parameter and convergent precision have some impacts on the algorithm's realization, but their actions can be ignored when performing the algorithm in lower approximate space $\Psi^N(N \leq 6)$. Moreover, regularization parameters should not be too small especially in high-dimensional approximate space, and in order to get a stable solution with high accuracy in the case of using large regularization parameters, convergent precision must be chosen small enough.

4) As stated in subsection 4.1, during the initial interval of $t \in (0, t_1)$ in the real soil-column infiltrating experiment, it is still a trouble to describe solute transport behaviors in mathematics due to lacking of measured data. Maybe better experimental devices, and other mathematical tools and methods are needed. In addition, stability analysis and theoretical uniqueness for the inverse problem here is our another work in the near future.

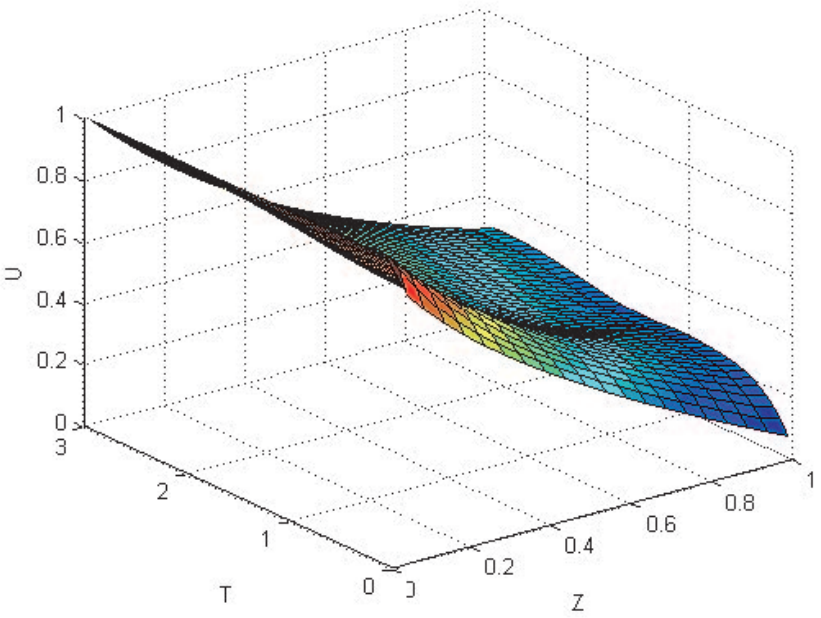

Figure 8: Concentration surface of K^+ in dimensionless space.

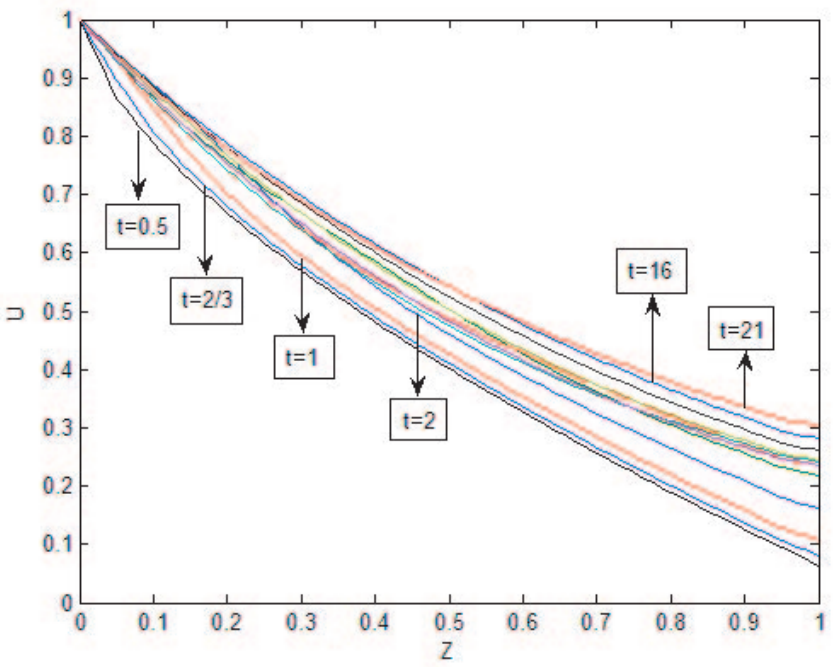

Figure 9: Concentration surface of K^+ in dimensionless space.

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