

# Simultaneous inversion for dispersion coefficients and space-dependent source magnitude in 2D solute transportation

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*Abstract:* This paper deals with an inverse problem of simultaneously determining the dispersion coefficients and the space-dependent source magnitude in 2D advection dispersion equation with finite observations at the final time. The forward problem is solved by using the alternating direction implicit (ADI) finite difference scheme, and then the optimal perturbation algorithm with the regularization parameter chosen by a Sigmoid-type function is introduced to solve the simultaneous inversion problem numerically. Numerical inversions are presented, and several factors having influences on realization of the algorithm are discussed. The inversion solutions are in good approximations to the exact solutions demonstrating that the optimal perturbation algorithm with the Sigmoid-type regularization parameter is efficient for the simultaneous inversion problem in 2D solute transportation.

*Key-Words:* 2D advection dispersion equation, simultaneous inversion, optimal perturbation algorithm, regularization parameter, numerical simulation

## 1 Introduction

In the process of solute transport and transformation in the soils and groundwater, it is always involving some complicated physical and/or chemical reactions. By the mass conservation law, the process can often be described by mathematical models of advection dispersion and/or reaction diffusion equations with source/sink terms. In many cases for the solute transport model, the dispersion/diffusion coefficient, the source/sink term characteristics and other physical quantities are often unknown and cannot be measured easily. So, the method of inverse problem and parameter identification has had widely applications in the research of soil and groundwater pollution. See, e.g., [1-16].

It is noticeable that most of the research works are focused on the inverse problems of determining one kind of parameter based on the model and some additional information of the solution. If there are more than one different kinds of parameters to be identified by the model and some additional information from the view point of numerics, which can be called multi-parameters simultaneous inversion problem, there seem to have few studies not only in the 1D model but also in the multi-dimensional cases. Ma-

har and Datta [8] studied an inverse problem for determining the source term and the hydrologic parameters simultaneously arising from the 2D groundwater pollution by applying the optimization method, and Rodrigues et al [17] ever considered an inverse problem of simultaneously identifying the diffusion coefficient and the source magnitude but in the 1D diffusion equation by the conjugate gradient method with aids of an adjoint problem.

In this paper, we will deal with a simultaneous inversion problem for a solute transport in a homogeneous unit section  $\Omega = (0, 1) \times (0, 1)$  with final observations. Let  $T > 0$ , the model considered here is the 2D advection dispersion equation given as [5, 18]

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} + D_T \frac{\partial^2 c}{\partial y^2} - v \frac{\partial c}{\partial x} + \mu(t) f(x, y), \quad (1)$$

for  $(x, y) \in \Omega$  and  $0 < t < T$ , where  $c = c(x, y, t)$  is the solute concentration at time  $t$ , and space point  $(x, y)$ ;  $D_L > 0$  is the longitudinal dispersion coefficient, and  $D_T > 0$  is the transverse dispersion coefficient;  $v > 0$  is the average pore-water velocity;  $\mu(t) > 0$  is the attenuation factor depending on the time-variable;  $f(x, y)$  is the space-dependent continuous source/sink magnitude which reflecting some

capabilities of solute dissolution, adsorption, and ion transformation in the porous media.

For Eq.(1), what we want to do is to determine the dispersion coefficients  $D_L$ ,  $D_T$  and the source magnitude function  $f(x, y)$  by utilizing the optimal perturbation algorithm with the regularization parameter chosen as a Sigmoid-type function. The inversion problem here for simultaneously identifying the two dispersion coefficients and the space-dependent source magnitude becomes severely ill-posed as compared with the problems of determining one single unknown. On one hand, the ordinary optimal perturbation algorithm [19-22] has to be modified to suit for the simultaneous inversion problem. On the other hand, the inversion algorithm here could lose effectiveness if still utilizing empirical choice method on the regularization parameter as done in the previous works [23-25]. Fortunately, sigmoid-type functions are usually utilized to construct variable step-size algorithm which can give a possible approach to suitable choice of the regularization parameter, and we can see that if regularization parameter is taken as the Sigmoid-type function depending on the number of iterations, then it will continuously decrease and approach to zero by which an optimal regularization parameter can be determined, and then an optimal solution to the inverse problem is obtained.

Furthermore, three numerical examples are presented, and several factors having important influences on realization of the inversion algorithm are discussed, which are the additional data, the numerical differential step, and the initial iteration, etc. In particular, we will investigate how many additional data are needed to determine the multi-parameters from the view point of optimality, which is few reported in the literature to our knowledge. The inversion solutions are in good agreements with the exact solutions demonstrating that the optimal perturbation algorithm with the Sigmoid-type regularization parameter is efficient for the simultaneous inversion problem arising from the 2D solute transport phenomena.

The paper is organized as follows. In Section 2, the Peaceman-Rachford ADI difference scheme for solving the forward problem is introduced, and a numerical testification is presented to support the difference scheme. In Section 3, the inverse problem of simultaneously determining the dispersion coefficients and the space-dependent source magnitude is formulated, and the modified optimal perturbation algorithm with the Sigmoid-type regularization parameter is given. In Section 4, numerical inversions are carried out, and the factors that having important influences on the inversion algorithm are discussed. Finally, several concluding remarks are given in Section 5.

## 2 The forward problem and the ADI scheme

Consider numerical solution to Eq.(1) with the following initial boundary value conditions

$$c(x, y, 0) = c_0(x, y), \quad (2)$$

and

$$\begin{aligned} c(0, y, t) &= g_0(y, t), \quad c(1, y, t) = g_1(y, t), \\ c(x, 0, t) &= h_0(x, t), \quad c(x, 1, t) = h_1(x, t), \end{aligned} \quad (3)$$

where the functions  $c_0(x, y)$ , and  $g_0(y, t)$ ,  $g_1(y, t)$ , and  $h_0(x, t)$ ,  $h_1(x, t)$  are supposed to be continuous, and satisfy data compatibilities.

If all the model parameters are known, including the dispersion coefficients, the average velocity, the source term and the initial boundary values functions, the problem (1)-(3) is called the forward problem, which is just an ordinary determinate problem of 2D parabolic partial differential equation. We give the alternating direction implicit (ADI) finite difference scheme to solve the forward problem numerically [26, 27].

### 2.1 The ADI scheme

Denote the grid points in the space domain  $[0, 1] \times [0, 1]$  as  $x_i = ih$  and  $y_j = jh$ ,  $i, j = 0, 1, 2, \dots, M$  with the uniform space step size  $h = 1/M$ , and the grid points in the time interval  $[0, T]$  are labeled as  $t_n = n\Delta t$ ,  $n = 0, 1, 2, \dots, N$ , where the time step size  $\Delta t = T/N$ . The values of the functions  $c(x, y, t)$  at the grid points are denoted as  $c_{i,j}^n = c(x_i, y_j, t_n)$ . The Peaceman-Rachford ADI difference scheme is given as follows.

Firstly, introducing the intermediate layer  $t_{n+1/2}$  between  $t_n$  and  $t_{n+1}$ , and discretizing Eq.(1) at  $(x_i, y_j, t_{n+1/2})$ , and using central difference methods, we have

$$\begin{aligned} &\frac{\partial^2 c}{\partial x^2} \Big|_{(x_i, y_j, t_{n+1/2})} \\ &= \frac{1}{2h} [c_{i+1,j}^{n+1} - 2c_{i,j}^{n+1} + c_{i-1,j}^{n+1} + c_{i+1,j}^n \\ &\quad - 2c_{i,j}^n + c_{i-1,j}^n] + O(h^2 + (\Delta t)^2), \end{aligned} \quad (4)$$

and

$$\begin{aligned} &\frac{\partial^2 c}{\partial y^2} \Big|_{(x_i, y_j, t_{n+1/2})} \\ &= \frac{1}{2h} [c_{i,j+1}^{n+1} - 2c_{i,j}^{n+1} + c_{i,j-1}^{n+1} + c_{i,j+1}^n \\ &\quad - 2c_{i,j}^n + c_{i,j-1}^n] + O(h^2 + (\Delta t)^2); \end{aligned} \quad (5)$$

and for the first-order derivatives in Eq.(1), there are

$$\frac{\partial c}{\partial t} \Big|_{(x_i, y_j, t_{n+1/2})} = \frac{1}{\Delta t} [c_{i,j}^{n+1} - c_{i,j}^n] + O((\Delta t)^2), \quad (6)$$

and

$$= \frac{\partial c}{\partial x} \Big|_{(x_i, y_j, t_{n+1/2})} \\ = \frac{1}{4h} [c_{i+1,j}^{n+1} - c_{i-1,j}^{n+1} + c_{i+1,j}^n - c_{i-1,j}^n] \\ + O(h^2 + (\Delta t)^2). \quad (7)$$

Next, based on the above discretizing expressions (4)-(7), denoting  $r = \frac{\Delta t}{h^2}$ , the Crank-Nicolson scheme for solving Eq.(1) is given as

$$\begin{aligned} & \left(-\frac{vrh}{4} - \frac{rD_L}{2}\right)c_{i-1,j}^{n+1} + (1 + rD_L)c_{i,j}^{n+1} \\ & + \left(\frac{vrh}{4} - \frac{rD_L}{2}\right)c_{i+1,j}^{n+1} \\ & - \frac{rD_T}{2}c_{i,j-1}^{n+1} + rD_Tc_{i,j}^{n+1} - \frac{rD_T}{2}c_{i,j+1}^{n+1} \\ & = \left(\frac{vrh}{4} + \frac{rD_L}{2}\right)c_{i-1,j}^n - rD_Lc_{i,j}^n \\ & + \left(\frac{rD_L}{2} - \frac{vrh}{4}\right)c_{i+1,j}^n \\ & + \frac{rD_T}{2}c_{i,j-1}^n + (1 - rD_T)c_{i,j}^n + \frac{rD_T}{2}c_{i,j+1}^n \\ & + \Delta t f_{i,j} \mu^{n+1/2}, \end{aligned} \quad (8)$$

where  $f_{i,j} = f(x_i, y_j)$ , and  $\mu^{n+1/2} = \mu(t_{n+1/2})$ .

It is noted that the above scheme is of high computational complexity, and it requires much more extra computational labor. So we should seek for other numerical schemes for the 2D advection dispersion equation. The alternating direction implicit (ADI) method is often utilized to modify the Crank-Nicolson scheme in two-dimensional case. The idea of the ADI method is to split the scheme (8) into two, one with the  $x$ -derivative taken implicitly and the next with the  $y$ -derivative taken implicitly by introducing the intermediate layer  $t_{n+1/2}$  between  $t_n$  and  $t_{n+1}$ . According to (8), from  $t_n$  to  $t_{n+1/2}$ , there is

$$\begin{aligned} & \left(-\frac{vrh}{4} - \frac{rD_L}{2}\right)c_{i-1,j}^{n+1/2} + (1 + rD_L)c_{i,j}^{n+1/2} \\ & + \left(\frac{vrh}{4} - \frac{rD_L}{2}\right)c_{i+1,j}^{n+1/2} \\ & = \frac{rD_T}{2}c_{i,j-1}^n + (1 - rD_T)c_{i,j}^n + \frac{rD_T}{2}c_{i,j+1}^n \\ & + \frac{\Delta t}{2} f_{i,j} \mu^n. \end{aligned} \quad (9)$$

And from  $t_{n+1/2}$  to  $t_{n+1}$ , there is

$$\begin{aligned} & -\frac{rD_T}{2}c_{i,j-1}^{n+1} + (1 + rD_T)c_{i,j}^{n+1} - \frac{rD_T}{2}c_{i,j+1}^{n+1} \\ & = \left(\frac{rD_L}{2} + \frac{vrh}{4}\right)c_{i-1,j}^{n+1/2} + (1 - rD_L)c_{i,j}^{n+1/2} \\ & + \left(\frac{rD_L}{2} - \frac{vrh}{4}\right)c_{i+1,j}^{n+1/2} + \frac{\Delta t}{2} f_{i,j} \mu^{n+1}. \end{aligned} \quad (10)$$

The above system of the difference equations (9) and (10) is called the ADI scheme for solving Eq.(1). It is noticeable that both of the coefficient matrices involving in the ADI scheme are symmetric and tridiagonal, and the scheme can be typically solved using tridiagonal matrix algorithm. Moreover, the ADI scheme is of unconditional stability and second-order convergence in time and space [27]. Next, we will give a numerical testification to support the ADI scheme.

## 2.2 Numerical test

Set the exact solution of the forward problem (1)-(3) be  $c(x, y, t) = \exp(-t)(x^2 + y^2)$ , and the dispersion coefficients  $D_L = 1$  and  $D_T = 0.5$ , the average flow velocity  $v = 1$ , and the attenuation factor  $\mu(t) = e^{-t}$ , then the corresponding initial boundary value functions are given as

$$c_0(x, y) = x^2 + y^2; \quad (11)$$

and

$$\begin{aligned} g_0(y, t) &= y^2 e^{-t}, \quad g_1(y, t) = (1 + y^2) e^{-t}, \\ h_0(x, t) &= x^2 e^{-t}, \quad h_1(x, t) = (1 + x^2) e^{-t}, \end{aligned} \quad (12)$$

respectively, and the source magnitude function is expressed by

$$\begin{aligned} f(x, y) &= -2(D_L + D_T) + 2x - x^2 - y^2 \\ &= -3 + 2x - x^2 - y^2. \end{aligned} \quad (13)$$

The solutions errors in the exact solution and the numerical solution at  $T = 1$  with various number of grids are listed in Table 1, where  $M$  is the grids number in space domain, and  $N$  is the grids number in time interval, and  $Err_{\max}$ ,  $Err_{\text{rel}}$  denote the maximum error and the relative error in the solutions, which are defined by  $Err_{\max} = \|c(x, y, 1) - c^*(x, y, 1)\|_2$ , and  $Err_{\text{rel}} = Err_{\max} / \|c(x, y, 1)\|_2$ , respectively.

**Table 1. The solution errors at  $T = 1$  with grids number**

$M$	$N$	$Err_{\max}$	$Err_{\text{rel}}$
20	20	3.66484e-4	6.43209e-4
40	40	9.78912e-5	1.71914e-4
80	80	2.56767e-5	4.44603e-5
100	100	1.66357e-5	2.86494e-5
120	120	4.28650e-6	7.26107e-6

From Table 1, we can see that the solutions error becomes small and small with the space-time mesh refinement showing that the ADI scheme is of numerical convergence, and the convergence order is about  $O(h^2 + (\Delta t)^2)$  with  $h = 1/M$  and  $\Delta t = T/N$ .

## 3 The inverse problem and the inversion algorithm

### 3.1 The inverse problem

Suppose that the dispersion coefficients  $D_L$  and  $D_T$ , and the space-dependent source magnitude  $f(x, y)$  in

Eq.(1) are all unknown, and we have the final observations at  $t = T$  as the overposed condition given as

$$c(x, y, T) = c_T(x, y), (x, y) \in \Omega, \quad (14)$$

with which an inverse problem of simultaneously determining the dispersion coefficients and the source magnitude is formulated by Eq.(1), the initial boundary value conditions (2)-(3) together with the additional condition (14).

Actually for real problems, what we can obtain for the additional information is a finite number of the measured data, given at  $(x_l, y_k)$  for  $l = 1, 2, \dots, L$  and  $k = 1, 2, \dots, K$ . Hence, the real additional data for solving the inverse problem we can utilize are given as

$$c(x_l, y_k, T) = c_{l,k}, (x_l, y_k) \in \Omega, \quad (15)$$

$$l = 1, 2, \dots, L, k = 1, 2, \dots, K.$$

As a result, from the view point of numerical identification, the simultaneous inversion problem here is composed by the model (1)-(3) together with the real additional condition (15).

### 3.2 The inversion algorithm

As we know, most of inversion algorithms are based on regularization strategies so as to overcome ill-posedness of the inverse problem, and different kinds of inverse problems could need different approximate methods on the basis of conditional well-posedness analysis. The optimal perturbation algorithm has been testified to be effective for determining one single unknown in the diffusion equations [13, 14, 20, 23, 28, 29], however, we will still employ it to solve the above simultaneous inversion problem with a little modification to suit for the joint inversion problem here.

Suppose that the dispersion coefficients  $D_L, D_T \in \mathbb{R}^+$ , and the source magnitude  $f(x, y)$  is continuous on the space domain  $\Omega$ , and  $\Phi \subset C(\Omega)$  is an admissible set for the space-dependent source function. A solution to the inverse problem can be represented by  $\langle D_L, D_T, f(x, y) \rangle \in \mathbb{R}^+ \times \mathbb{R}^+ \times \Phi$ .

Thus for any prescribed  $D_L, D_T \in \mathbb{R}^+$  and  $f(x, y) \in \Phi$ , the unique solution of the corresponding forward problem, denoted by  $c(x, y, t; D_L, D_T, f)$ , can be solved by the ADI difference scheme (9)-(10), and then we get the computational data  $c(x_l, y_k, T; D_L, D_T, g)$  for  $l = 1, 2, \dots, L$  and  $k = 1, 2, \dots, K$ , which can be regarded as the output data corresponding to the input  $f \in \Phi$  and  $D_L, D_T \in \mathbb{R}^+$ . So, an optimal idea for solving the inverse problem here is to minimize an error of the unknown function

between the output data and the additional data. The inversion algorithm is stated as follows.

Suppose that  $\{\varphi_s(x, y), s = 1, 2, \dots, \infty\}$  is a group of basis functions of  $\Phi$ , and there has an approximate expansion given as:

$$f(x, y) \approx f^S(x, y) = \sum_{s=1}^S a_s \varphi_s(x, y), \quad (16)$$

where  $f^S(x, y)$  is the  $S$ -dimensional approximate solution to  $f(x, y)$ , and  $S \geq 1$  is the truncated level of  $f(x, y)$ , and  $a_s (s = 1, 2, \dots, S)$  is the expansion coefficient. It is convenient to set a limited dimensional space as

$$\Phi^S = \text{span}\{\varphi_1, \varphi_2, \dots, \varphi_S\}, \quad (17)$$

and a  $S$ -dimensional vector  $\mathbf{a} = (a_1, a_2, \dots, a_S) \in \mathbb{R}^S$ . Therefore, to get an approximate solution  $\langle D_L, D_T, f^S(x, y) \rangle \in \mathbb{R}^+ \times \mathbb{R}^+ \times \Phi^S$  is equivalent to finding a vector  $(D_L, D_T, \mathbf{a}) \in \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^S$ , in which meaning we can say that

$$(D_L, D_T, \mathbf{a}) = \langle D_L, D_T, f^S \rangle.$$

In the follows, we will also utilize  $\mathbf{a} = (D_L, D_T, a_1, \dots, a_S)$  as an approximate solution to the simultaneous inverse problem if there is no specification.

Based on the above discussions, denoting  $c(x, y, t; \mathbf{a}) = c(x, y, t; D_L, D_T, f^S)$  as the unique solution of the forward problem for any admissible source function  $f^S(x, y)$  given by (16) and  $D_L, D_T \in \mathbb{R}^+$ , and taking values at the measured points  $(x_l, y_k)$ , we get the computational data, denoted as a  $L \times K$ -dimensional vector

$$\mathbf{C}_{\text{comp}}^{LK} = (c(x_l, y_k, T; \mathbf{a}))_{l=1,2,\dots,L}^{k=1,2,\dots,K}.$$

Then, combining with the additional condition (15), and denoting the observed data with a  $L \times K$ -dimensional vector given as

$$\mathbf{C}_{\text{obs}}^{LK} = (c_{l,k})_{l=1,2,\dots,L}^{k=1,2,\dots,K},$$

and a feasible way to solve the simultaneous inversion problem numerically is to solve the minimization problem with Tikhonov regularization:

$$\min_{\mathbf{a} \in \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^S} \{ \|\mathbf{C}_{\text{comput}}^{LK} - \mathbf{C}_{\text{obs}}^{LK}\|_2^2 + \alpha \|\mathbf{a}\|_2^2 \}, \quad (18)$$

where  $\|\cdot\|_2$  is the Euclid norm, and  $\alpha > 0$  is the regularization parameter.

Now, for any given  $\mathbf{a}^j \in \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^S$ , set

$$\mathbf{a}^{j+1} = \mathbf{a}^j + \delta \mathbf{a}^j, j = 0, 1, \dots, \quad (19)$$

where  $\delta \mathbf{a}^j$  denotes a perturbation of  $\mathbf{a}^j$  for each  $j$ , and  $j$  is the number of iterations. In the follows for convenience of writing,  $\mathbf{a}^j$  and  $\delta \mathbf{a}^j$  are abbreviated as  $\mathbf{a}$  and  $\delta \mathbf{a}$ , respectively.

Taking Taylor's expansion for  $c(x_l, y_k, T; \mathbf{a} + \delta \mathbf{a})$  at  $\mathbf{a}$ , and ignoring higher-order terms, we have

$$c(x_l, y_k, T; \mathbf{a} + \delta \mathbf{a}) \approx c(x_l, y_k, T; \mathbf{a}) + \nabla_{\mathbf{a}}^T c(x_l, y_k, T; \mathbf{a}) \cdot \delta \mathbf{a}. \quad (20)$$

Denoting  $J_a = (\nabla_{\mathbf{a}}^T c(x_l, y_k, T; \mathbf{a}))_{L \times K}$  as Jacobi matrix, and noting to (18), let us define an error functional for the perturbation given as follows

$$F(\delta \mathbf{a}) = \|J_a \cdot \delta \mathbf{a} - (\mathbf{C}_{\text{obs}}^{LK} - \mathbf{C}_{\text{comp}}^{LK})\|_2^2 + \alpha \|\delta \mathbf{a}\|_2^2. \quad (21)$$

For further computations, we also need to work out the elements of the Jacobi matrix  $J_a$ . Utilizing ordinary one-order forward difference, there is

$$\frac{\partial c(x_l, y_k, T; \mathbf{a})}{\partial a_s} \approx \frac{c(x_l, y_k, T; \mathbf{a} + \tau \mathbf{e}_s) - c(x_l, y_k, T; \mathbf{a})}{\tau}$$

for  $l = 1, 2, \dots, L$ ,  $k = 1, 2, \dots, K$ , and  $s = 1, 2, \dots, S+2$ , where  $\tau > 0$  is the numerical differential step, and  $\mathbf{e}_s$  is basis vector of  $\mathbb{R}^{S+2}$ . If denoting

$$b_{lk,s} = \frac{c(x_l, y_k, T; \mathbf{a} + \tau \mathbf{e}_s) - c(x_l, y_k, T; \mathbf{a})}{\tau}, \quad (22)$$

$$\mathbf{B} = (b_{lk,s})_{LK \times (S+2)},$$

then the error functional (21) can be approximated to:

$$F(\delta \mathbf{a}) = \|\mathbf{B} \delta \mathbf{a} - (\mathbf{C}_{\text{obs}}^{LK} - \mathbf{C}_{\text{comp}}^{LK})\|_2^2 + \alpha \|\delta \mathbf{a}\|_2^2. \quad (23)$$

It is not difficult to testify that minimizing (23) is equivalent to solving the following normal equation [30]:

$$(\mathbf{B}^T \mathbf{B} + \alpha \mathbf{I}) \delta \mathbf{a} = \mathbf{B}^T (\mathbf{C}_{\text{obs}}^{LK} - \mathbf{C}_{\text{comp}}^{LK}). \quad (24)$$

and then an optimal perturbation, denoted by  $\delta \mathbf{a}^\alpha$ , can be worked out via

$$\delta \mathbf{a}^\alpha = (\alpha \mathbf{I} + \mathbf{B}^T \mathbf{B})^{-1} \mathbf{B}^T (\mathbf{C}_{\text{obs}}^{LK} - \mathbf{C}_{\text{comp}}^{LK}). \quad (25)$$

Thus an optimal solution can be approximated by the iteration procedure (19) as long as arriving at the given number of iterations, or the perturbation satisfying the prescribed convergent precision given as

$$\|\delta \mathbf{a}^\alpha\| \leq \text{eps}, \quad (26)$$

here eps is the given convergent precision.

### 3.3 The Sigmoid-type regularization parameter

The key points of performing the above inversion algorithm lie in suitable choices of the approximate space  $\Phi^S$  for the source magnitude function, the regularization parameter, the numerical differential step, the initial iteration, and the convergent precision, etc. Generally speaking, it is a trouble on how to choose an optimal regularization parameter on realization of the algorithm when using regularization strategy. Especially for the solving of the above simultaneous inversion problem, the inversion algorithm could be failure if still utilizing empirical choice method to the regularization parameter due to severe ill-posedness of the joint inversion problem. So, based on the properties of Sigmoid-type functions [31, 32], the regularization parameter here we will utilize on the implementation of the inversion algorithm is given as

$$\alpha = \alpha(j) = \frac{1}{1 + \exp(\beta(j - j_0))}, \quad (27)$$

where  $j$  is the number of iterations, and  $j_0$  is the preestimated number of iterations at which the regularization parameter decreases to 0.5, and  $\beta > 0$  is the adjust parameter. Figure 1 gives some curves of the above regularization parameter function depending on the number of iterations for  $j_0 = 3$  and  $\beta = 0.5$ , respectively.

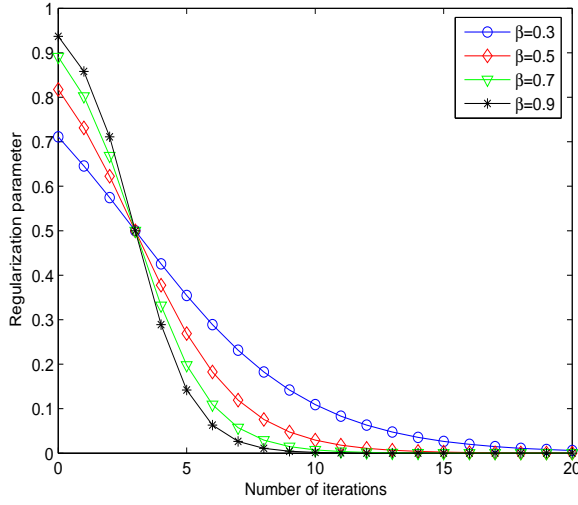
From Figure 1, we can see that the regularization parameter approaches to zero with the number of iterations goes to large whatever for the given preestimated number of iterations, or for the given adjust parameter. In the next section, numerical inversions will be carried out to illustrate implementation of the simultaneous inversion algorithm with the regularization parameter given by (27). The detailed steps to perform the above algorithm are given as follows.

**Step 1.** Give basis functions  $\{\varphi_i(x, y)\}_{i=1}^S$ , initial iteration  $\mathbf{a}^j$ , numerical differentiation step  $\tau$ , convergent precision eps, and the additional data  $\mathbf{C}_{\text{obs}}^{LK}$ ;

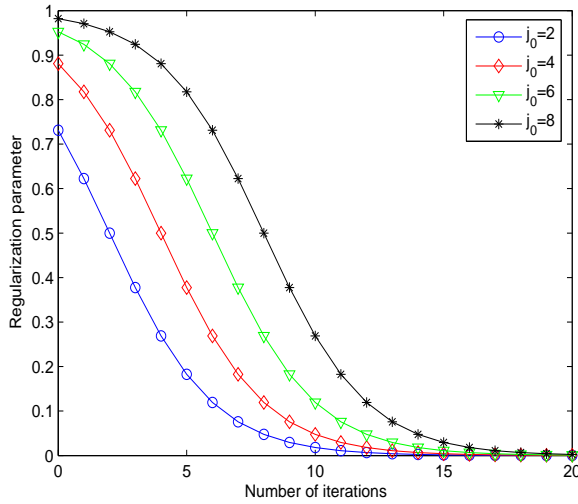
**Step 2.** Set  $\mathbf{a} = \mathbf{a}^j$ , and solve the forward problem with the ADI scheme (9)-(10) to get  $c(x_l, y_k, T; \mathbf{a}^j)$  and  $c(x_l, y_k, T; \mathbf{a}^j + \tau \mathbf{e}_s)$ , and then obtain the vector  $\mathbf{C}_{\text{comp}}^{LK}$  and the matrix  $\mathbf{B} = (b_{lk,s})$  by (22);

**Step 3.** Choose the adjust parameter  $\beta$  and the preestimated iteration number  $j_0$  in (27) to determine the regularization parameter, and work out an optimal perturbation via formula (25);

**Step 4.** If the number of iterations is satisfied, or the stopping rule (26) is valid, then the algorithm is terminated; otherwise, go to Step 2 by replacing  $\mathbf{a}^j$  with



(a)  $j_0 = 3$



(b)  $\beta = 0.5$

Figure 1: Regularization parameter with number of iterations

$\mathbf{a}^{j+1}$  by (19) to go on.

## 4 Numerical inversions

We will choose polynomials as the basis functions, i.e., there are

$$\varphi(x, y) = a_1 + a_2x + a_3y + a_4xy + a_5x^2 + a_6y^2 + \dots, \quad (28)$$

and we will employ lower-order polynomials space as the approximate space on the concrete inversions. For the numerical examples presented in this section, we will utilize the quadratic polynomials space  $\Phi^6$  as the approximate space in Ex.1 and Ex.2, and the cubic polynomials space  $\Phi^{10}$  as the approximate

space in Ex.3, respectively. For instance, the unknown source magnitude function  $f(x, y)$  in  $\Phi^6 = \text{span}\{1, x, y, xy, x^2, y^2\}$  can be regarded as  $\mathbf{a} = (a_1, \dots, a_6) \in \mathbb{R}^6$  as utilized in Subsection 3.2. Together with the two dispersion coefficients  $D_L$  and  $D_T$ , the solution we are to determine is denoted as

$$\mathbf{a} = (D_L, D_T, a_1, \dots, a_6) \in \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^6. \quad (29)$$

also as indicated in Subsection 3.2.

In the sequel, we will take the average flow velocity as  $v = 1$ , the time-dependent attenuation factor as  $\mu(t) = e^{-t}$ , and the final time as  $T = 2$ , and we will always set  $M = 20$  and  $N = 20$  in the computations of the forward problem, and choose  $\text{eps} = 1e - 6$  as the convergent precision for the inversion algorithm if there is no specification. In addition, all computations are performed in a PC of Dell Studio.

### 4.1 Ex.1–Inversion

$$f = -3 + 2x - x^2 - y^2$$

$$D_L = 1, D_T = 0.5$$

for  
with

As given in Subsection 2.2, set the exact solution of the forward problem be  $c(x, y, t) = e^{-t}(x^2 + y^2)$ , and the initial boundary value functions are given by (11) and (12), respectively, and the exact dispersion coefficients are  $D_L = 1$  and  $D_T = 0.5$ , the exact source magnitude is given by (13). Under the above assumptions, the forward problem is solved and the final observations at  $T = 2$  are obtained, which are utilized as the additional data by which the inversion algorithm is applied to reconstruct the dispersion coefficients and the source magnitude simultaneously. If dealing with the source function in the quadratic polynomials space  $\Phi^6$ , then the exact solution of the inverse problem in this example is

$$\mathbf{a}^{\text{exa}} = (1, 0.5, -3, 2, 0, 0, -1, -1). \quad (30)$$

On the concrete computations in this example, we will choose the regularization parameter by (27), where  $\beta = 0.5$  and  $j_0 = 3$ , and the initial iteration as zero, i.e.,  $\mathbf{a}^0 = \mathbf{0}$ , and the numerical differential step as  $\tau = 1e - 4$ . We will investigate several factors having influences on realization of the inversion algorithm, which are the additional data, the initial iteration, and the differential step, respectively.

#### (a) Influence of the additional data on the inversion algorithm

Choose some points on three lines  $(x_l, y)$  for  $x_l = l/4$  ( $l = 1, 2, 3$ ) as the measured points, and noting  $M = 20$  in the computing of the forward problem, so the real measured points are chosen as  $(x_l, y_k)$  for  $x_l = l/4, l = 1, 2, 3$ , and  $y_k = k/20, k =$

0, 1,  $\dots$ , 20. For convenience of writing in the following statement, we denote  $[c(x_l, y_k)]$  where  $l = 1, 2, 3$  and  $k = 0, 1, \dots, 20$  as a  $3 \times 21$ -dimensional vector of the additional data along with the three measured lines, and  $[c(1/4, y_k)]$  where  $k = 0, 1, \dots, 20$  as a 21-dimensional vector of the additional data along the measured line of  $x = 1/4$ , etc. The inversion results varying with different additional data are listed in Table 2, where  $c(x_l, y_k, 2)$  denotes the additional information given at  $T = 2$ ,  $\mathbf{a}^{\text{inv}}$  denotes the inversion solution, and  $Err = \|\mathbf{a}^{\text{inv}} - \mathbf{a}^{\text{exa}}\|_2 / \|\mathbf{a}^{\text{exa}}\|_2$  is the relative error in the solutions, and  $j$  is the number of the iterations.

Furthermore, the exact and the inversion sources at  $x = x_l = l/4$  ( $l = 1, 2, 3$ ) are plotted in Figure 2, respectively.

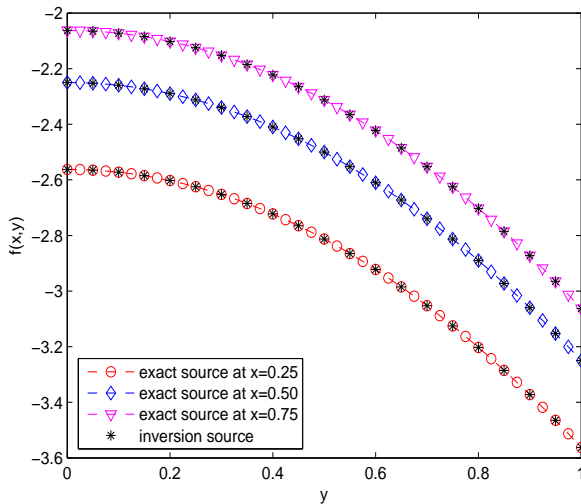


Figure 2: The exact source and the inversion source in Ex.1

From Table 2 and Figure 2, we can see that the inversion solutions perfectly coincide with the exact solutions, however, the choice of the additional data are important to the realization of the inversion algorithm. If choosing the additional data along one measured line, the inversion could always be failure, and the inversion seems to be stable if choosing the additional data along more than one measured lines, and the more of the additional data, the less of the number of the iterations.

**(b) Influence of the initial iterations on the inversion algorithm**

Suppose that the additional data are taken on the three lines of  $(x_l, y)$  for  $x_l = l/4$  ( $l = 1, 2, 3$ ), also noting to  $M = 20$ , here we will choose  $[c(x_l, y_k)]$  for  $l = 1, 2, 3$  and  $k = 0, 1, \dots, 20$  as the additional data to testify influence of the initial iterations on the

inversion algorithm. The inversion results are listed in Table 3, where  $\mathbf{a}^0$  denotes the initial iteration, and  $\mathbf{a}^{\text{inv}}$ ,  $Err$ , and  $j$  all denote the same meanings as in Table 2.

From Table 3, we find that the choice of the initial iterations has small influence on the inversion algorithm, and the inversion solutions give good approximations to the exact solutions with high-precision even in the case of using zero vector as the initial iteration.

**(c) Influence of the numerical differential step on the inversion algorithm**

Also choosing the additional data on the three lines of  $(x_l, y)$  for  $x_l = l/4$  ( $l = 1, 2, 3$ ), and the initial iteration  $\mathbf{a}^0 = \mathbf{0}$ , the inversion results with different numerical differential steps are listed in Table 4, where  $\tau$  denotes the differential step, and  $\mathbf{a}^{\text{inv}}$ ,  $Err$ , and  $j$  also denote the same meanings as in the above.

From Table 4, we find that the inversion algorithm can be performed smoothly for the differential step lying in  $[1e-7, 1e-2]$  except for  $\tau = 1e-3$ , and the inversion solutions are also in good agreement with the exact solutions.

**4.2 Ex.2-Inversion for  $f = -1 + y - xy$  with  $D_L = D_T = 1$**

In this subsection, set the exact solution of the forward problem be  $c(x, y, t) = e^{-t}(1 + xy)$ , and take the dispersion coefficients as  $D_L = 1$  and  $D_T = 1$ , and the initial boundary value functions are given as

$$c_0(x, y) = 1 + xy, \tag{31}$$

and

$$\begin{aligned} g_0(y, t) &= e^{-t}, \quad g_1(y, t) = (1 + y)e^{-t}, \\ h_0(x, t) &= e^{-t}, \quad h_1(x, t) = (1 + x)e^{-t}, \end{aligned} \tag{32}$$

respectively. Under the above assumptions, the exact source magnitude is given as

$$f(x, y) = -1 + y - xy, \tag{33}$$

together with  $D_L = D_T = 1$ , the exact solution in the case of  $f(x, y) \in \Phi^6$  for the inverse problem here is represented by

$$\mathbf{a}^{\text{exa}} = (1, 1, -1, 0, 1, -1, 0, 0). \tag{34}$$

Based on the above inversion computations, we will only perform the inversion algorithm with different additional data in this example still utilizing the Sigmoid-type regularization parameter given by (27),

**Table 2. The inversion results with additional data in Ex.1**

$c(x_l, y_k, 2)$	$\mathbf{a}^{\text{inv}}$	$Err$	$j$
$[c(1/4, y_k)]$	(1.0, 0.5, -3.0, 2.0, 1.9e-9, 4.0e-10, -1.0, -1.0)	1.72e-9	81
$[c(2/4, y_k)]$	failure		
$[c(3/4, y_k)]$	failure		
$[c(1/4, y_k), c(2/4, y_k)]$	(1.0, 0.5, -3.0, 2.0, 6.4e-11, 7.1e-12, -1.0, -1.0)	2.94e-10	70
$[c(1/4, y_k), c(3/4, y_k)]$	(1.0, 0.5, -3.0, 2.0, 3.8e-10, -2.2e-12, -1.0, -1.0)	9.87e-10	69
$[c(2/4, y_k), c(3/4, y_k)]$	(1.0, 0.5, -3.0, 2.0, 2.4e-9, -1.5e-10, -1.0, -1.0)	6.14e-9	68
$[c(x_l, y_k)]$	(1.0, 0.5, -3.0, 2.0, 3.9e-10, -1.2e-11, -1.0, -1.0)	5.32e-9	62

**Table 3. The inversion results with initial iterations in Ex.1**

$\mathbf{a}^0$	$\mathbf{a}^{\text{inv}}$	$Err$	$j$
(0, 0, 0, 0, 0, 0, 0, 0)	(1.0, 0.5, -3.0, 2.0, 3.9e-10, -1.2e-11, -1.0, -1.0)	5.32e-9	62
(1, 1, 1, 1, 1, 1, 1, 1)	(1.0, 0.5, -3.0, 2.0, -1.7e-10, 4.0e-12, -1.0, -1.0)	1.80e-9	63
(2, 2, 2, 2, 2, 2, 2, 2)	(1.0, 0.5, -3.0, 2.0, 2.1e-10, -3.2e-12, -1.0, -1.0)	1.46e-9	64
(3, 3, 3, 3, 3, 3, 3, 3)	(1.0, 0.5, -3.0, 2.0, -1.5e-13, -4.7e-14, -1.0, -1.0)	1.38e-11	68
(4, 4, 4, 4, 4, 4, 4, 4)	(1.0, 0.5, -3.0, 2.0, -1.3e-12, -4.0e-14, -1.0, -1.0)	9.26e-12	69

where  $\beta = 0.5$  and  $j_0 = 3$ , and  $\tau = 1e-4$  and  $\mathbf{a}^0 = \mathbf{0}$  as used in Ex.1. The inversion results are listed in Table 5, where  $c(x_l, y_k, 2)$ ,  $\mathbf{a}^{\text{inv}}$ ,  $Err$ , and  $j$  also denote the same meanings as in the above. Moreover, the exact and the inversion sources at  $x = x_l = l/4$  ( $l = 1, 2, 3$ ) are plotted in Figure 3, respectively.

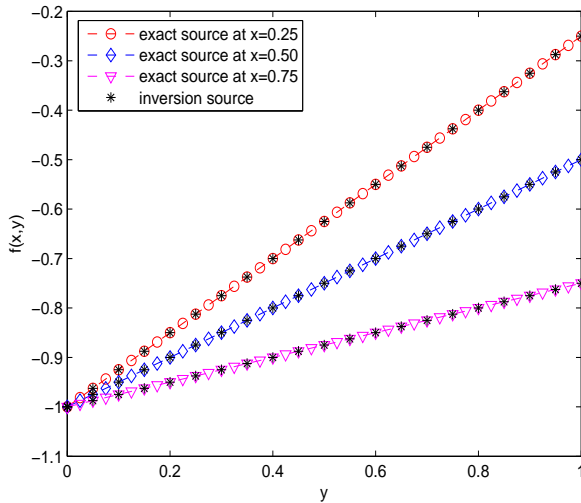


Figure 3: The exact source and the inversion source in Ex.2

From Table 5 and Figure 3, we can find that the inversion solutions perfectly coincide with the exact solutions, and there is the same trend for the choice of the additional data as that observed in Ex.1. The inversion seems to become stable if choosing the additional data along more than one measured lines. On

the other hand, if choosing suitable initial iterations, the inversion can also be performed smoothly. For instance, since the initial iteration is  $\mathbf{a}^0 = \mathbf{0}$  in this example, and the inversion is failure when utilizing the additional data along two lines of  $x = 1/4$  and  $x = 3/4$ , however, the inversion can be realized if choosing  $\mathbf{a}^0 = (0.2, 0.2, 0.2, 0.2, 0.2, 0.2, 0.2, 0.2)$  as the initial iteration, and the inversion error is  $Err = 4.9242e - 10$ , the number of iterations is  $j = 73$ . In the next subsection, we will perform the inversion algorithm on exponential continuous source function which seems to be more complicated as compared with those in Ex.1 and Ex.2.

### 4.3 Ex.3-Inversion for $f = -3e^{x+y}$ with $D_L = 2, D_T = 1$

In this subsection, set the exact solution of the forward problem be  $c(x, y, t) = e^{x+y-t}$ , and take the dispersion coefficients as  $D_L = 2$  and  $D_T = 1$ , and the initial boundary value functions are given as

$$c_0(x, y) = e^{x+y}, \tag{35}$$

and

$$\begin{aligned} g_0(y, t) &= e^{y-t}, \quad g_1(y, t) = e^{1+y-t}, \\ h_0(x, t) &= e^{x-t}, \quad h_1(x, t) = e^{x+1-t}, \end{aligned} \tag{36}$$

respectively, and the exact source magnitude is given as

$$f(x, y) = -3e^{x+y}. \tag{37}$$

Noting that

$$e^{x+y} = 1 + (x+y) + \frac{(x+y)^2}{2!} + \frac{(x+y)^3}{3!} + \dots, \tag{38}$$



**Table 4. The inversion results with differential steps in Ex.1**

$\tau$	$\mathbf{a}^{\text{inv}}$	$Err$	$j$
$1e-2$	(1.0, 0.5, -3.0, 2.0, 3.6e-8, -8.9e-10, -1.0, -1.0)	4.04e-7	85
$5e-3$	(1.0, 0.5, -3.0, 2.0, 4.3e-9, -5.4e-11, -1.0, -1.0)	2.46e-8	67
$1e-3$	failure		
$1e-4$	(1.0, 0.5, -3.0, 2.0, 3.9e-10, -1.2e-11, -1.0, -1.0)	5.32e-9	62
$1e-5$	(1.0, 0.5, -3.0, 2.0, 2.7e-10, -1.3e-11, -1.0, -1.0)	6.14e-9	62
$1e-6$	(1.0, 0.5, -3.0, 2.0, 2.6e-10, -1.4e-11, -1.0, -1.0)	6.24e-9	62
$1e-7$	(1.0, 0.5, -3.0, 2.0, 2.5e-10, -1.4e-11, -1.0, -1.0)	6.22e-9	62

**Table 5. The inversion results with additional data in Ex.2**

$c(x_l, y_k, 2)$	$\mathbf{a}^{\text{inv}}$	$Err$	$j$
$[c(1/4, y_k)]$	failure		
$[c(2/4, y_k)]$	failure		
$[c(3/4, y_k)]$	failure		
$[c(1/4, y_k), c(2/4, y_k)]$	(1.0, 1.0, -1.0, 2.2e-12, 1.0, -1.0, 2.0e-11, 1.1e-11)	9.03e-9	74
$[c(1/4, y_k), c(3/4, y_k)]$	failure		
$[c(2/4, y_k), c(3/4, y_k)]$	(1.0, 1.0, -1.0, -1.3e-11, 1.0, -1.0, 3.6e-11, 8.0e-11)	1.82e-8	71
$[c(x_l, y_k)]$	(1.0, 1.0, -1.0, -2.9e-11, 1.0, -1.0, -2.5e-11, 1.6e-11)	2.55e-8	69

together with  $D_L = 2, D_T = 1$ , the exact solution of the inverse problem here is represented by

$$\mathbf{a}^{\text{exa}} = (2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5), \quad (39)$$

for

$$f(x, y) \in \Phi^{10} = \text{span}\{1, x, y, xy, x^2, y^2, \dots, y^3\}.$$

The above inversion problem becomes severe ill-posed as compared with those of Ex.1 and Ex.2. The inversion algorithm is always failure if still utilizing the same inversion parameters as used in the above, and then the initial iteration and the Sigmoid-type regularization parameter have to be modified to suit for the inversion. The regularization parameter is also chosen by (27), but the adjust parameter is changed to  $\beta = 0.8$ , and the pre-estimated number of iterations is  $j_0 = 5$ , the differential step also given as  $\tau = 1e-4$ , the inversion results varying with various initial iterations in the case of using the additional data in all of the three lines are listed in Table 6, where  $\mathbf{a}^0$  also denotes the initial iteration, and for convenience of writing,  $\mathbf{a}^0 = 0.2, \mathbf{a}^0 = 1$  and so on here represent the initial iteration vectors with equal component 0.2 and 1, respectively.

From Table 6 we can see that there still exists a large range for the choice of the initial iterations, and the inversion solutions perfectly coincide with the exact solutions almost with the same precision and the same number of iterations.

Next, let us perform the algorithm with different additional data as done in Ex.1 and Ex.2. Choosing the initial iteration as  $\mathbf{a}^0 = 0.5$ , and other inversion parameters unchanged as used in the computations of Table 6, the inversion results are listed in Table 7, where  $c(x_l, y_k, 2), \mathbf{a}^{\text{inv}}, Err$ , and  $j$  also denote the same meanings as used in the above. Moreover, the exact and the inversion sources at  $x = x_l = l/4$  ( $l = 1, 2, 3$ ) are plotted in Figure 4, respectively.

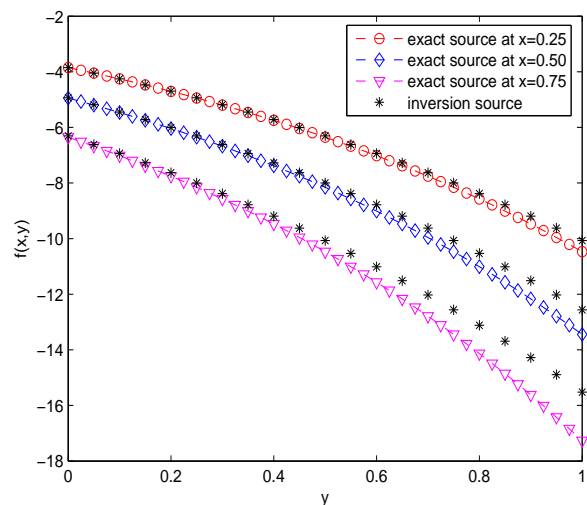


Figure 4: The exact source and the inversion source in Ex.3

**Table 6. The inversion results with initial iterations in Ex.3**

$a^0$	$a^{\text{inv}}$	<i>Err</i>	<i>j</i>
0.2	(2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5)	3.50e-8	47
0.5	(2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5)	2.44e-8	47
1.0	(2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5)	1.06e-9	48
2.0	(2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5)	1.87e-9	48
4.0	(2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5)	1.01e-8	47

**Table 7. The inversion results with additional data in Ex.3**

$c(x_l, y_k, 2)$	$a^{\text{inv}}$	<i>Err</i>	<i>j</i>
$[c(1/4, y_k)]$	failure		
$[c(2/4, y_k)]$	failure		
$[c(3/4, y_k)]$	failure		
$[c(1/4, y_k), c(2/4, y_k)]$	(2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5)	1.34e-8	51
$[c(1/4, y_k), c(3/4, y_k)]$	(2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5)	1.32e-9	52
$[c(2/4, y_k), c(3/4, y_k)]$	(2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5)	3.28e-9	53
$[c(x_l, y_k)]$	(2, 1, -3, -3, -3, -3, -1.5, -1.5, -1.5, -1.5, -0.5, -0.5)	2.44e-8	47

From Table 7, we find that the additional data at least on two measured lines are needed to implement the inversion algorithm smoothly. From Figure 4 we can see that the inversions are not so good as those presented in Figure 2 and Figure 3. The reason comes from the truncated errors for the exact exponential source function according to (38) and (39).

Furthermore, also choosing the inversion parameters as used in Table 7, we will continue to perform the algorithm utilizing more additional data given at the lines of  $x_l$  ( $l = 1, 2, \dots, L$ ) for  $L = 4, 5, \dots, 10$  respectively. It is pleasure that all inversions can be realized successfully, and the inversion solutions are all in good agreement with the exact solution. The inversion errors and the number of iterations corresponding to different additional data are listed in Table 8, where  $L$  is the number of measured lines, and  $[x_l]$  here denotes the measured line with which  $c(x_l, y_k, 2)$  for  $k = 0, 1, \dots, 20$  are chosen as the additional data, and *Err* also denotes the relative error in the solutions,  $j$  is the number of iterations, and  $T_{\text{cpu}}$  denotes the CPU time (unit: second) for each inversion.

From Table 8, we can see that the inversion becomes stable if employing the additional data along more than three lines, and the inversion solutions are good approximations to the exact solutions with almost the same precision, and the required number of iterations and the CPU time are reduced with the number of the measured lines increasing. However, the inversion results can not have significant improvement for  $L \geq 7$  showing that an optimal number for the measured lines here should be  $L = 6$ .

## 5 Conclusion

We give several concluding remarks in this section.

(i) The optimal perturbation algorithm with the regularization parameter chosen by the Sigmoid-type function depending on the number of iterations is suitable for the simultaneous inversion problem of determining the dispersion coefficients and the space-dependent source magnitude in 2D advection dispersion equation. The inversion gives good approximate solutions to the exact solutions for various space-dependent source magnitude functions and dispersion coefficients.

(ii) The choice on the regularization parameter is important to the implementation of the inversion algorithm. The inversion algorithm can not be implemented with traditional choice method to the regularization parameter, however, it can be realized with stability and adaptivity by the Sigmoid-type regularization parameter given by (27). We also find that the inversions are performed successfully for the source function taking on polynomials if utilizing polynomials space as the approximate space, and it becomes complicated when taking the exponential function as the exact source as presented in Ex. 3. More fine regularization parameters should be needed to overcome the ill-posedness of the simultaneous inversion when performing the algorithm in high-dimensional approximate spaces. Another possible approach is to employ orthogonal polynomials space as the approximate space in which the inversion could be expected to get better results.

(iii) The choice of additional data is also important

**Table 8. The inversion results using more additional data in Ex.3**

$L$	$[x_l]$	$Err$	$j$	$T_{cpu}$
4	[1/10, 1/4, 1/2, 3/4]	1.61e-10	40	199.1
5	[1/20, 1/4, 1/2, 3/4, 8/9]	5.24e-10	39	193.7
6	[1/20, 1/10, 1/4, 1/2, 3/4, 8/9]	1.15e-10	39	194.0
7	[1/20, 1/10, 1/5, 1/4, 1/2, 3/4, 8/9]	7.73e-9	38	182.1
8	[1/20, 1/10, 1/5, 1/4, 1/2, 3/4, 4/5, 8/9]	5.66e-9	38	176.0
9	[1/10, 1/5, 3/10, 2/5, 1/2, 3/5, 7/10, 4/5, 9/10]	1.87e-9	38	176.9
10	[1/20, 3/20, 1/4, 7/20, 9/20, 11/20, 13/20, 3/4, 17/20, 19/20]	5.53e-10	38	176.1

to realization of the inversion algorithm especially for inverse problems in multi-dimensional cases. There are plenty of lines which can be chosen as the measured lines to get the additional data. The number of the additional data can not be too few, otherwise the inversion becomes failure, but the inversion seems to have few improvement even though utilizing much more additional data as observed in Ex.3. We will focus our attention on the utilization of orthogonal basis functions, and on the choice of Sigmoid-type regularization parameter and the additional data in our sequent works to deal with multi-parameters simultaneous inversion problems in multi-dimensional cases.

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