

# A Quasi-Boundary Semi-Analytical Method for Backward in Time Advection-Dispersion Equation

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**Abstract:** In this paper, we take the advantage of an analytical method to solve the advection-dispersion equation (ADE) for identifying the contamination problems. First, the Fourier series expansion technique is employed to calculate the concentration field  $C(x,t)$  at any time  $t < T$ . Then, we consider a direct regularization by adding an extra term  $\alpha C(x,0)$  on the final condition to carry off a second kind Fredholm integral equation. The termwise separable property of the kernel function permits us to transform it into a two-point boundary value problem. The uniform convergence and error estimate of the regularized solution  $C^\alpha(x,t)$  are provided and a strategy to select the regularized parameter is suggested. The solver used in this work can recover the spatial distribution of the groundwater contaminant concentration. Several numerical examples are examined to show that the new approach can retrieve all past data very well and is good enough to cope with heterogeneous parameters' problems, even though the final data are noised seriously.

**Keywords:** Inverse problem, Groundwater contaminant distribution, Advection-dispersion equation, Fredholm integral equation, Two-point boundary value problem

## 1 Introduction

With the development of society and economics, groundwater contamination has become a very critical issue. Most of groundwater pollution cases usually occur in industrial zones, highly developed areas, and agricultural zones. Reliable and quantitative predictions of pollutant movement can be made only if we are able to realize the source characteristics [Mahar and Datta (2001)], such as contaminant concentration, pollutant location, categories of pollution and so forth. Because

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the data cannot be measured by direct methods in lots of cases, some additional data are needed to determine the unknown sources in accordance with the analytical models, which always result in the inverse problems [Sun (1994)]. For the mathematical model of the problem, many researchers use the backward in time advection-dispersion equation (ADE) to govern the problem. By accurately identifying those groundwater pollution source properties, one can tackle the problem effectively.

Over the last few decades, many researches have been done to deal with the backward in time ADE for identifying the groundwater pollution source problem. One often employs an optimization approach to obtain the best fitted solution due to the nonuniqueness of the solution and the infinite number of plausible combinations. Gorelick et al. (1983) first formulated the problem as the forward simulations together with a linear optimization model by using the linear programming and multiple regression. The optimization model provides an effective method for identifying the time release history of groundwater pollution source and the location in homogeneous medium. However, the classical optimization scheme spent much computational time, produced large numerical errors, and was limited to cases where the data were available in the form of breakthrough curves. Because the groundwater pollution source problem is a nonlinear problem, Wagner (1992) has proposed a combination of the nonlinear optimization model and the nonlinear maximum likelihood estimation to cope with the groundwater contaminant source characterizations and parameter estimations in homogeneous medium simultaneously. It is reported that the nonlinear optimization approach is more accurate than the linear optimization method for solving the reconstruction of the release history and the location of a pollution source since the model parameter uncertainty is considered. Nevertheless, the nonlinear maximum likelihood estimation has so many confinements that its application is limited, and its complex procedures require to be tackled. In general, the above-mentioned optimization approaches encounter complicated procedures and large numerical errors in dealing with the problem in heterogeneous media.

To solve the groundwater pollution source problem in heterogeneous media, a non-optimization approach, namely the marching-jury backward beam equation (MJBBE) method, was proposed by Atmadja (2001) and Atmadja and Bagtzoglou (2001a, 2001b, 2003) to cope with the recovery of the spatial distribution of contaminant concentration. From calculating the recovery of the spatial distribution of contaminant concentration in homogeneous media, the MJBBE method obtains smaller numerical errors than those in heterogeneous media. However, the scheme retrieves the problem merely in a short time period between the initial and final time (it is impossible to retrieve the plume at times near  $t = 0$ ), and it transforms

the backward in time ADE (second-order partial differential equation (PDE)) into the fourth-order PDE. This not only increases the complexity of the computational procedures, where two artificial boundary conditions are needed, and also takes much computational time. In addition, the numerical errors of the MJBBE method are larger than those calculated by the forward numerical scheme. Subsequent to Atmadja and Bagtzoglou (2003), Liu et al. (2009) have proposed a simple and explicit one-step backward group preserving scheme (BGPS) to solve the backward in time ADE. Although the numerical errors of the BGPS are much smaller than those of the MJBBE method, there still has room to increase the accuracy of the BGPS.

In this paper, we propose a direct regularization technique to transform the ADE into a second kind Fredholm integral equation by employing the quasi-boundary method. By using the separating kernel function and eigenfunctions expansion techniques, we can derive a closed-form solution of the second kind Fredholm integral equation, which is a major contribution of this paper. Another one is the application of the Fredholm integral equation to develop an effective numerical scheme, whose accuracy is much better than the MJBBE method proposed by Atmadja and Bagtzoglou (2001b). Particularly, the proposed approach is time-saving and easy to implement. A similar second kind Fredholm integral equation regularization method was first used by Liu (2007a) to solve a direct problem of elastic torsion in an arbitrary plane domain, where it was called a meshless regularized integral equation method. Liu (2007b, 2007c) extended it to solve the Laplace direct problem in arbitrary plane domains. Based on those good results and experiences, Liu (2009) used this new method to treat the inverse Robin coefficient problem of Laplace equation.

The present paper is organized as follows. Section 2 illustrates the backward in time ADE and its final condition and boundary conditions, and then we derive the second kind Fredholm integral equation by a direct regularization in Section 3. In Section 4, we derive a two-point boundary value problem, which helps to derive a closed-form solution of the second kind Fredholm integral equation in Section 5. Section 6 offers a selection principle of the regularized parameter and presents some numerical examples to demonstrate and validate the proposed approach. A summary with some concluding remarks is drawn in Section 7.

## 2 Contaminant source identification problem

Let us consider the following one-dimensional backward in time ADE:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left[ D \frac{\partial C}{\partial x} \right] - v \frac{\partial C}{\partial x}, \quad (1)$$

$$C(0,t) = C(l,t) = 0, \quad 0 \leq t \leq T, \tag{2}$$

$$C(x,T) = C_T(x), \quad 0 \leq x \leq l, \tag{3}$$

where  $C$  is the solute concentration,  $D$  is the dispersion coefficient,  $v$  is the transport velocity in the  $x$  direction, and  $C_T(x)$  is the observed plume’s spatial distribution at a time  $T$ . The domain is assumed to be sufficiently large that the plume has not reached the boundary.

The contaminant source identification problem is to identify the initial profile  $C(x, 0)$ , and is known to be highly ill-posed. One way to solve an ill-posed problem is by perturbation it into a well-posed one. Many perturbing techniques have been proposed, including a biharmonic regularization developed by Lattés and Lions (1969), a pseudo-parabolic regularization proposed by Showalter and Ting (1970), a stabilized quasi-reversibility proposed by Miller (1973), the method of quasi-reversibility proposed by Mel’nikova (1992), a hyperbolic regularization proposed by Ames and Cobb (1997), the Gajewski and Zacharias quasi-reversibility proposed by Huang and Zheng (2005), a quasi-boundary value method by Denche and Bessila (2005), and an optimal regularization proposed by Boussetila and Rebbani (2006). Showalter (1983) first regularized the inverse problem by considering a quasi-boundary-value approximation to the final value problem, which is for our problem, to supersede Eq. (3) by

$$\alpha C(x,0) + C(x,T) = C_T(x). \tag{4}$$

Eqs. (1), (2) and (4) can be shown to be well-posed for each  $\alpha > 0$  as that done by Clark and Oppenheimer (1994) for the heat conduction inverse problem. Ames and Payne (1999) have investigated those regularizations from the continuous dependence of solution on the regularized parameter.

In our previous paper, Chang et al. (2007) have tackled the above quasi-boundary two-point boundary value problem for the case of  $D = 1$  and  $v = 0$  by an extension of the Lie-group shooting method, which was originally developed by Liu (2006) to resolve second-order boundary value problems.

### 3 The Fredholm integral equation

The use of the technique for separation of variables can yield a formal series expansion of  $C(x,t)$ , satisfying Eqs. (1) and (2):

$$C(x,t) = \sum_{k=1}^{\infty} a_k e^{vx/2D - [(v/2D)^2 + (k\pi/l)^2]Dt} \sin \frac{k\pi x}{l}, \tag{5}$$

where  $a_k$  are coefficients to be determined. By imposing the two-point boundary condition (4) on the above equation, we obtain

$$C(x, T) = \sum_{k=1}^{\infty} a_k e^{v x / 2 D - [(v / 2 D)^2 + (k \pi / l)^2] D T} \sin \frac{k \pi x}{l} = C_T(x) - \alpha C(x, 0). \quad (6)$$

Fixing any  $t < T$  and applying the eigenfunctions expansion to Eq. (5), we obtain

$$a_k = \frac{2 e^{[(v / 2 D)^2 + (k \pi / l)^2] D t}}{l} \int_0^l e^{-v \xi / 2 D} \sin \frac{k \pi \xi}{l} C(\xi, t) d \xi. \quad (7)$$

Substituting Eq. (7) for  $a_k$  into Eq. (6) and assuming that the order of summation and integral can be interchanged, it follows that

$$\left(K_x^{T-t} C(\cdot, t)\right)(x) := \int_0^l K(x, \xi; T-t) C(\xi, t) d \xi = C_T(x) - \alpha C(x, 0), \quad (8)$$

where

$$K(x, \xi; t) = \frac{2}{l} \sum_{k=1}^{\infty} e^{-[(v / 2 D)^2 + (k \pi / l)^2] D t} e^{v(x-\xi) / 2 D} \sin \frac{k \pi x}{l} \sin \frac{k \pi \xi}{l} \quad (9)$$

is a kernel function,  $\alpha$  is a regularized parameter, and  $K_x^{T-t}$  is an integral operator generated from  $\mathbf{K}(x, \xi; T-t)$ . Corresponding to the kernel  $K(x, \xi; t)$ , the operator is denoted by  $\mathbf{K}_x^t$ .

In order to recover the concentration  $C(x, 0)$ , we have to solve the second kind Fredholm integral equation:

$$\alpha C(x, 0) + \int_0^l K(x, \xi; T) C(\xi, 0) d \xi = C_T(x), \quad (10)$$

which is obtained from Eq. (8) by taking  $t = 0$ .

#### 4 Two-point boundary value problem

We assume that the kernel function in Eq. (10) can be approximated by  $m$  terms with

$$K(x, \xi; T) = \frac{2}{l} \sum_{k=1}^m e^{-[(v / 2 D)^2 + (k \pi / l)^2] D T} e^{v(x-\xi) / 2 D} \sin \frac{k \pi x}{l} \sin \frac{k \pi \xi}{l}, \quad (11)$$

because of  $T > 0$ . The above kernel is termwise separable, which is also called the degenerate kernel or the Pincherle-Goursat kernel [Tricomi (1985)].

By the inspection of Eq. (11), we have

$$K(x, \xi; T) = \mathbf{P}(x; T) \cdot \mathbf{Q}(\xi), \tag{12}$$

where  $\mathbf{P}$  and  $\mathbf{Q}$  are  $m$ -vectors given by

$$\mathbf{P} := \frac{2e^{vx/2D}}{l} \begin{bmatrix} e^{-[(v/2D)^2+(\pi/l)^2]DT} \sin \frac{\pi x}{l} \\ e^{-[(v/2D)^2+(2\pi/l)^2]DT} \sin \frac{2\pi x}{l} \\ \vdots \\ e^{-[(v/2D)^2+(m\pi/l)^2]DT} \sin \frac{m\pi x}{l} \end{bmatrix}, \quad \mathbf{Q} := e^{-v\xi/2D} \begin{bmatrix} \sin \frac{\pi \xi}{l} \\ \sin \frac{2\pi \xi}{l} \\ \vdots \\ \sin \frac{m\pi \xi}{l} \end{bmatrix}, \tag{13}$$

and the dot between  $\mathbf{P}$  and  $\mathbf{Q}$  denotes the inner product, which is sometime written as  $\mathbf{P}^T \mathbf{Q}$ , where the superscript  $T$  signifies the transpose.

With the aid of Eq. (12), Eq. (10) can be decomposed as

$$\alpha C(x, 0) + \int_0^x \mathbf{P}^T(x) \mathbf{Q}(\xi) C(\xi, 0) d\xi + \int_x^l \mathbf{P}^T(x) \mathbf{Q}(\xi) C(\xi, 0) d\xi = C_T(x), \tag{14}$$

where we omit the parameter  $T$  in  $\mathbf{P}$  for clarity. Let us define

$$\begin{aligned} \mathbf{c}_1(x) &:= \int_0^x \mathbf{Q}(\xi) C(\xi, 0) d\xi, \\ \mathbf{c}_2(x) &:= \int_l^x \mathbf{Q}(\xi) C(\xi, 0) d\xi, \end{aligned} \tag{15}$$

and Eq. (14) can be expressed as

$$\alpha C(x, 0) + \mathbf{P}^T(x) [\mathbf{c}_1(x) - \mathbf{c}_2(x)] = C_T(x). \tag{16}$$

If  $\mathbf{c}_1$  and  $\mathbf{c}_2$  can be solved, we can calculate  $C(x, 0)$ .

Using the Leibniz rule and taking the differential of Eq. (15) with respect to  $x$ , we obtain

$$\mathbf{c}'_1(x) = \mathbf{Q}(x) C(x, 0), \quad \mathbf{c}'_2(x) = \mathbf{Q}(x) C(x, 0). \tag{17}$$

From Eqs. (14)-(16), we obtain

$$\alpha \mathbf{c}'_1(x) = Q(x) \mathbf{P}^T(x) [\mathbf{c}_2(x) - \mathbf{c}_1(x)] + C_T(x) Q(x), \mathbf{c}_1(0) = 0, \tag{18}$$

$$\alpha \mathbf{c}'_2(x) = Q(x) \mathbf{P}^T(x) [\mathbf{c}_2(x) - \mathbf{c}_1(x)] + C_T(x) Q(x), \mathbf{c}_2(l) = 0. \tag{19}$$

Thus, the above two equations constitute a two-point boundary value problem.

### 5 A closed-form solution

In this section, we will find a closed-form solution of  $C(x, 0)$ . From Eq. (17) we observe that  $\mathbf{c}'_1 = \mathbf{c}'_2$ , which means that

$$\mathbf{c}_1 = \mathbf{c}_2 + \mathbf{d}, \tag{20}$$

where  $\mathbf{d}$  is a constant vector to be determined. By using the right-boundary condition in Eq. (19), we find that

$$\mathbf{c}_1(l) = \mathbf{c}_2(l) + \mathbf{d} = \mathbf{d}. \tag{21}$$

Substituting Eq. (20) into (18), we have

$$\alpha \mathbf{c}'_1(x) = -Q(x) \mathbf{P}^\top(x) \mathbf{d} + C_T(x) \mathbf{Q}(x), \mathbf{c}_1(0) = 0. \tag{22}$$

Integrating and using the left-boundary condition, it follows that

$$\mathbf{c}_1(x) = \frac{-1}{\alpha} \int_0^x \mathbf{Q}(\xi) \mathbf{P}^\top(\xi) d\xi \mathbf{d} + \frac{1}{\alpha} \int_0^x C_T(\xi) \mathbf{Q}(\xi) d\xi. \tag{23}$$

Taking  $x = l$  in the above equation and imposing condition (21), one obtains a governing equation for  $\mathbf{d}$ :

$$\left( \alpha I_m + \int_0^l \mathbf{Q}(\xi) \mathbf{P}^\top(\xi) d\xi \right) \mathbf{d} = \int_0^l C_T(\xi) \mathbf{Q}(\xi) d\xi. \tag{24}$$

It is straightforward to write

$$\mathbf{d} = \left( \alpha I_m + \int_0^l \mathbf{Q}(\xi) \mathbf{P}^\top(\xi) d\xi \right)^{-1} \int_0^l C_T(\xi) \mathbf{Q}(\xi) d\xi. \tag{25}$$

On the other hand, from Eqs. (16) and (20) we have

$$\alpha C(x, 0) = C_T(x) - \mathbf{P}(x) \cdot \mathbf{d}. \tag{26}$$

Inserting Eq. (25) into the above equation, we obtain

$$\alpha C(x, 0) = C_T(x) - \mathbf{P}(x) \cdot \left( \alpha I_m + \int_0^l \mathbf{Q}(\xi) \mathbf{P}^\top(\xi) d\xi \right)^{-1} \int_0^l C_T(\xi) \mathbf{Q}(\xi) d\xi. \tag{27}$$

Due to the orthogonality of

$$\int_0^l \sin \frac{j\pi\xi}{l} \sin \frac{k\pi\xi}{l} d\xi = \frac{l}{2} \delta_{jk}, \tag{28}$$

where  $\delta_{jk}$  is the Kronecker delta, the  $m \times m$  matrix can be explicitly written as

$$\int_0^l \mathbf{Q}(\xi) \mathbf{P}^\top(\xi) d\xi = \text{diag} \left[ e^{-[(v/2D)^2 + (\pi/l)^2]DT}, e^{-[(v/2D)^2 + (2\pi/l)^2]DT}, \dots, e^{-[(v/2D)^2 + (m\pi/l)^2]DT} \right], \quad (29)$$

where  $\text{diag}$  means that the matrix is a diagonal matrix.

Inserting Eq. (29) into Eq. (27), we therefore obtain

$$C(x, 0) = \frac{1}{\alpha} C_T(x) - \frac{1}{\alpha} \mathbf{P}^\top(x) \text{diag} \left[ \frac{1}{\alpha + e^{-[(v/2D)^2 + (\pi/l)^2]DT}}, \frac{1}{\alpha + e^{-[(v/2D)^2 + (2\pi/l)^2]DT}}, \dots, \frac{1}{\alpha + e^{-[(v/2D)^2 + (m\pi/l)^2]DT}} \right] \int_0^l C_T(\xi) \mathbf{Q}(\xi) d\xi. \quad (30)$$

While we use Eq. (13) for  $\mathbf{P}$  and  $\mathbf{Q}$ , we can get

$$C(x, 0) = \frac{1}{\alpha} C_T(x) - \frac{2}{\alpha l} \sum_{k=1}^{\infty} \frac{e^{-[(v/2D)^2 + (k\pi/l)^2]DT}}{\alpha + e^{-[(v/2D)^2 + (k\pi/l)^2]DT}} \int_0^l \sin \frac{k\pi x}{l} \sin \frac{k\pi \xi}{l} e^{v(x-\xi)/2D} C_T(\xi) d\xi, \quad (31)$$

where the summation upper bound  $m$  has been replaced by  $\infty$  because our argument is independent of  $m$  and  $m$  denotes a number of the finite terms in the numerical example. For a given  $C_T(x)$ , through some integrals one may employ the above equation to calculate  $C(x, 0)$ .

If  $C(x, 0)$  is available, we can calculate  $C(x, t)$  at any time  $t < T$  by

$$C^\alpha(x, t) = \sum_{k=1}^{\infty} a_k^\alpha e^{-[(v/2D)^2 + (k\pi/l)^2]Dt} e^{vx/2D} \sin \frac{k\pi x}{l}, \quad (32)$$

where

$$a_k^\alpha = \frac{2}{l} \int_0^l e^{-v\xi/2D} \sin \frac{k\pi \xi}{l} C(\xi, 0) d\xi. \quad (33)$$

Inserting Eq. (31) into the above equation and utilizing the orthogonality equation (29) again, it is verified that

$$a_k^\alpha = \frac{2}{l[\alpha + e^{-[(v/2D)^2 + (k\pi/l)^2]DT}]} \int_0^l e^{-v\xi/2D} \sin \frac{k\pi \xi}{l} C_T(\xi) d\xi. \quad (34)$$

Eqs. (32) and (34) constitute an analytical solution of the ADE. In order to distinguish it from the exact solution  $C(x, t)$ , we have used the symbol  $C^\alpha(x, t)$  to denote the regularized solution.



**6 Selection of the regularization parameter  $\alpha$  and numerical examples**

Up to this point, however, we have not yet specified how to select a suitable regularization parameter  $\alpha$ . Suppose that  $C_T(x) \in L^2(0, l)$  satisfying condition (A1) and that  $C_T(x)$  having a Fourier sine series expansion:

$$C_T(x) = \sum_{k=1}^{\infty} a_k^* e^{vx/2D} \sin \frac{k\pi x}{l}, \tag{35}$$

where

$$a_k^* = \frac{2}{l} \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi. \tag{36}$$

Substituting Eq. (35) into Eq. (31) and utilizing the orthogonality equation (29) again, we obtain

$$C^\alpha(x, 0) = \sum_{k=1}^{\infty} \frac{e^{-[(v/2D)^2+(k\pi/l)^2]DT}}{\alpha + e^{-[(v/2D)^2+(k\pi/l)^2]DT}} a_k^* \sin \frac{k\pi x}{l}, \tag{37}$$

where we note that

$$\frac{e^{-[(v/2D)^2+(k\pi/l)^2]DT}}{\alpha + e^{-[(v/2D)^2+(k\pi/l)^2]DT}} = \frac{1}{1 + \alpha e^{[(v/2D)^2+(k\pi/l)^2]DT}}.$$

In a practical calculation, we can only perform a finite sum in Eq. (37) and let  $k = m$  be the upper bound.

For a better numerical solution, we require that

$$\alpha e^{[(v/2D)^2+(m\pi/l)^2]DT} = \alpha_0 \ll 1.$$

Otherwise, the term  $e^{-[(v/2D)^2+(m\pi/l)^2]DT} / (\alpha + e^{-[(v/2D)^2+(m\pi/l)^2]DT})$  in Eq. (37) would be very small when  $v, D, T$  and  $l$  are finite and  $m$  is very large, which may lead to a large numerical error. Therefore, we have a criterion to select  $m$  when  $\alpha$  and  $\alpha_0$  are specified:

$$m = \frac{l}{\pi} \sqrt{\frac{1}{DT} \log \left( \frac{\alpha_0}{\alpha} \right) - \left( \frac{v}{2D} \right)^2}.$$

On the other hand, when  $m$  and  $\alpha_0$  are given, we can use the following criterion to choose  $\alpha$ :

$$\alpha = \frac{\alpha_0}{e^{[(v/2D)^2+(m\pi/l)^2]DT}}. \tag{38}$$

### 6.1 Numerical Method for the Homogeneous ADE

Now, let us take into account the one-dimensional ADE:

$$C_t = DC_{xx} - vC_x, \quad 0 \leq x \leq l, \quad 0 < t < T, \quad (39)$$

$$C(0,t) = C(l,t) = 0, \quad 0 \leq t \leq T, \quad (40)$$

$$C(x,0) = 0, \quad \forall 0 < x < 13.5 \text{ and } 14.5 < x < 28, \quad (41)$$

$$C(x,0) = \mathbf{c}_1 = 1 \quad 13.5 \leq x \leq 14.5, \quad (42)$$

where  $l = 28$  and we first consider the Fourier sine series expansion of the initial condition

$$C(x,0) = \sum_{k=1}^{\infty} a_k e^{vx/2D} \sin \frac{k\pi x}{l}. \quad (43)$$

Substituting the above equation into Eq. (33), we obtain

$$\begin{aligned} a_k &= \frac{2}{l} \int_0^l e^{-v\xi/2D} C(\xi,0) \sin \frac{k\pi\xi}{l} d\xi \\ &= \frac{2}{l} \int_{13.5}^{14.5} \mathbf{c}_1 e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} d\xi \\ &= \frac{2}{l} \left[ \frac{e^{-14.5s}(-s \sin 14.5b - b \cos 14.5b) + e^{-13.5s}(s \sin 13.5b + b \cos 13.5b)}{s^2 + b^2} \right], \end{aligned} \quad (44)$$

where

$$b = \frac{k\pi}{l}, \quad s = \frac{v}{2D}. \quad (45)$$

Then, the data to be retrieved is given by

$$C(x,t) = \sum_{k=1}^{\infty} a_k e^{vx/2D - [(v/2D)^2 + (k\pi/l)^2]Dt} \sin \frac{k\pi x}{l}. \quad (46)$$

Therefore, by Eqs. (32) and (34) we obtain a regularized solution:

$$C^\alpha(x,t) = \frac{1}{1 + \alpha e^{[(v/2D)^2 + (k\pi/l)^2]Dt}} \sum_{k=1}^{\infty} a_k e^{vx/2D - [(v/2D)^2 + (k\pi/l)^2]Dt} \sin \frac{k\pi x}{l}. \quad (47)$$

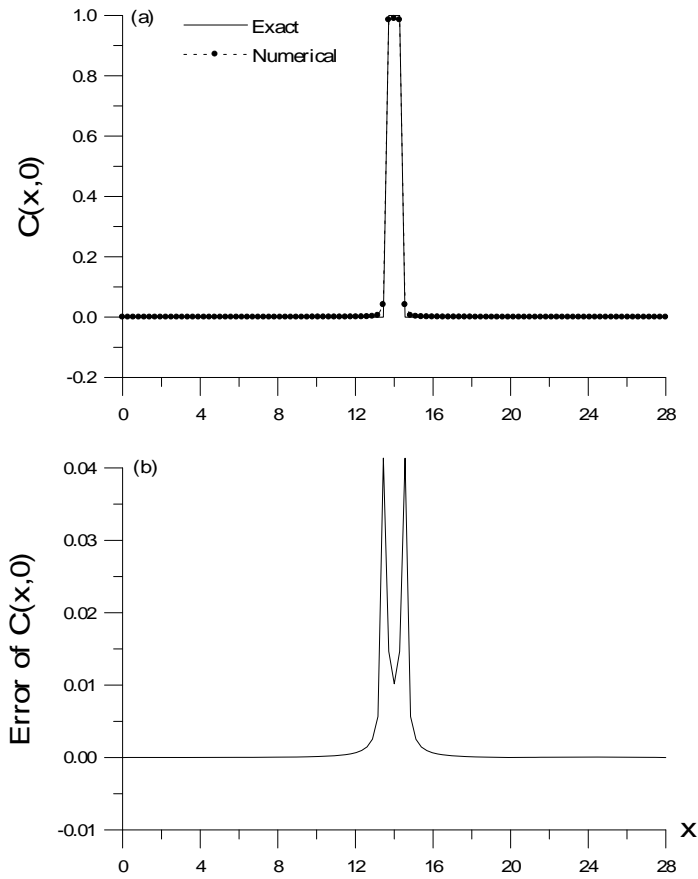


Figure 1: For homogeneous ADE problem we compare numerical and exact data at  $t = 0$  retrieved from final time  $T = 2$  in (a), and in (b) plotting the numerical errors.

Table 1: Comparing the mass and concentration peak errors of the present method and MJBBE of homogeneous ADE problem.

Time	$\varepsilon_M(\%)$		$\varepsilon_P(\%)$	
	MJBBE	Present	MJBBE	Present
$T = 2 \quad t = 1.8$	-0.024	1.0E-8	0.41	1.0E-8
$T = 2 \quad t = 1.1$	-0.11	1.0E-8	2.61	1.0E-8
$T = 5 \quad t = 4.8$		1.0E-8		1.0E-8
$T = 5 \quad t = 4.1$		1.0E-8		1.0E-8

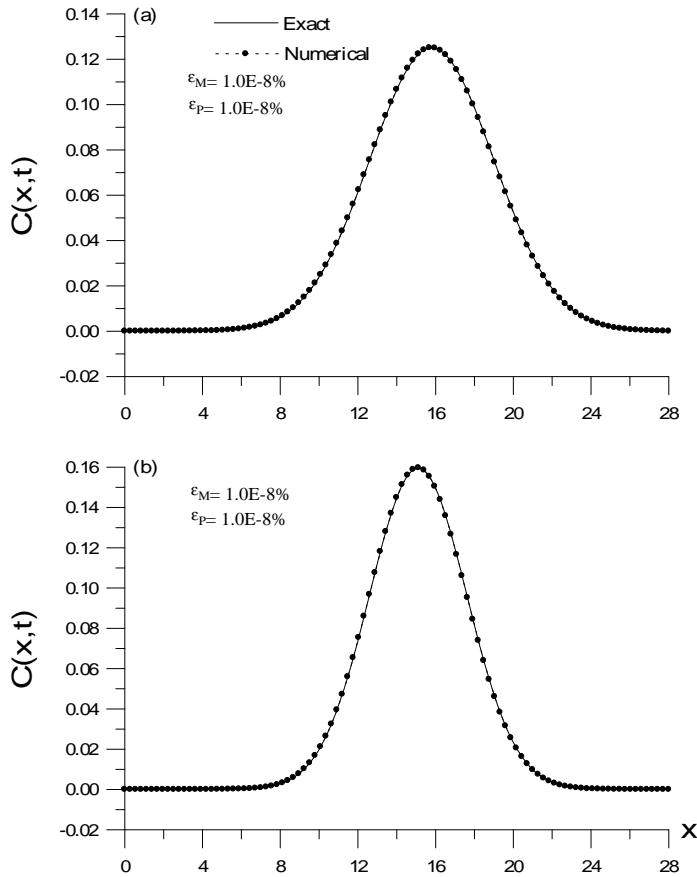


Figure 2: Comparisons of exact solutions and numerical solutions for homogeneous ADE problem with data at different times retrieved: (a)  $t = 1.8$ , (b)  $t = 1.1$ .

For this example with  $T = 2$ , comparisons of exact solutions and regularized solutions under  $D = 2.8$  and  $\nu = 1$  were plotted in Fig. 1(a), and the corresponding errors of  $C(x,0)$  were plotted in Fig. 1(b). In Fig. 2, we present the numerical results and numerical errors for the final time of  $T = 2$ . Figs. 2(a) and 2(b) compare the exact solution with the regularized solution under  $D = 2.8$ ,  $\nu = 1$ ,  $\alpha_0 = 10^{-10}$ ,  $\Delta x = 28/100$ ,  $k = 50$  and  $t = 1.8, 1.1$ . Upon compared with the numerical results computed by Atmadja and Bagtzoglou (2001b) with the MJBBE method (see Fig. 5 of the above cited paper), and Wang and Zabaras (2006) with a hierarchical Bayesian computation method (see Figs. 1 and 2 of the above cited paper), we can say that the present method is much more accurate than the MJBBE method and the

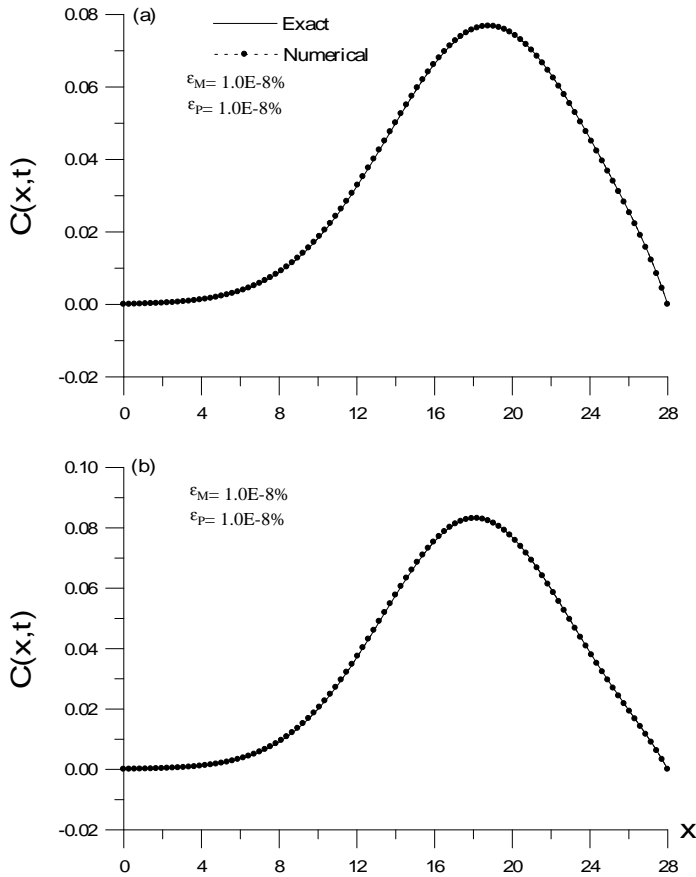


Figure 3: For homogeneous ADE practical problem we compare numerical and exact data at  $t = 0$  retrieved from final time  $T = 5$  in (a), and in (b) plotting the numerical errors.

Bayesian method. After viewing the output data, which are summarized in Table 1, we find that the corresponding mass and concentration peak errors are, respectively about  $\epsilon_M = 1.0E-8\%$  and  $\epsilon_P = 1.0E-8\%$  for  $t = 1.8$ ,  $\epsilon_M = 1.0E-8\%$  and  $\epsilon_P = 1.0E-8\%$  for  $t = 1.1$  (Figs. 2a and 2b),  $\epsilon_M = 1.0E-8\%$  and  $\epsilon_P = 1.0E-8\%$  for  $t = 4.8$ , and  $\epsilon_M = 1.0E-8\%$  and  $\epsilon_P = 1.0E-8\%$  for  $t = 4.1$  (Figs. 3a and 3b), i.e., Fig. 3 shows that the plume traveling a distance is much larger than its initial spread, where the mass error and the concentration peak error are defined as

[1] mass error, normalized by the exact mass

$$\varepsilon_M = \frac{Mass^e - Mass^n}{Mass^e} \times 100\%; \quad (48)$$

[2] concentration peak error, normalized by the exact peak concentration

$$\varepsilon_P = \frac{\max(C^e) - \max(C^n)}{\max(C^e)} \times 100\%, \quad (49)$$

where  $\max(\ )$  denotes the maximum value of  $(\ )$  for all grid points in the domain, and the superscripts e and n stand for exact and numerical values, respectively.

## 6.2 Group Preserving Scheme (GPS) and Present Method for the Homogeneous ADE

In the previous numerical example, we employed closed-form solutions as the inputs of the final time data. In practice, we cannot easily obtain the closed-form solution of the backward in time ADE when the available data  $C_T(x)$  is not in a closed-form; therefore, many numerical schemes are used to calculate the problem. Instead of directly using Eqs. (32) and (34) as a semi-analytic solution of the backward in time ADE where the data  $C_T(x)$  can be in a discretized form, we apply the trapezoidal rule to perform the integral. Here, the final data of the above example is calculated by GPS [Liu (2001)] with a time increment  $\Delta t = 5 \times 10^{-5}$ :

$$C(x, T) = C_T(x), \quad 0 \leq t < T, \quad (50)$$

Let  $l = 28$ , and substitute Eq. (50) for  $C_T(x)$  into Eq. (34) to obtain

$$a_k^\alpha = \frac{2}{l[\alpha + e^{-[(v/2D)^2 + (k\pi/l)^2]DT}]} \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi. \quad (51)$$

Substituting Eq. (51) into Eq. (32), we have

$$C^\alpha(x, t) = \sum_{m=1}^{\infty} a_k^\alpha e^{-[(v/2D)^2 + (m\pi/l)^2]Dt} e^{vx/2D} \sin \frac{m\pi x}{l}, \quad (52)$$

which gives

$$C^\alpha(x, 0) = \sum_{m=1}^{\infty} a_k^\alpha e^{vx/2D} \sin \frac{m\pi x}{l}, \quad (53)$$

We display the exact solutions and regularized solutions for a fixed  $T = 5$  with  $\alpha = 10^{-9}$  in Fig. 4(a), and the corresponding errors of  $C(x, 0)$  are plotted in Fig. 4(b). In Fig. 4(a), it is evident that the Gibbs phenomenon inevitably appears in the numerical evaluation of a finitely-truncated Fourier series near a point of discontinuity.

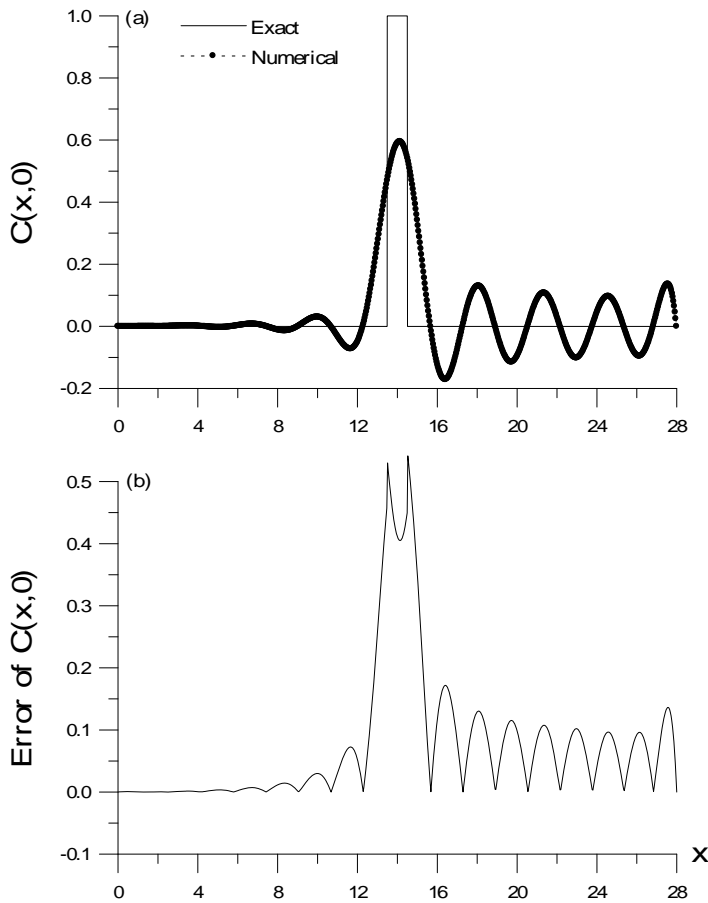


Figure 4: Comparisons of exact solutions and numerical solutions for homogeneous ADE problem with data at different times retrieved: (a)  $t = 4.8$ , (b)  $t = 4.1$ .

### 6.3 Numerical Method for the Heterogeneous ADE

Three cases involving heterogeneity in the dispersion coefficient  $D$  are to be analyzed. In all the heterogeneous parameter cases the velocity is fixed to be one. The heterogeneity configurations are shown in Table 2. Two different zones, each with a distinct value of  $D$ , are used. For configuration 1 the two zones are (1) outer zones for  $0 \leq x < 13$  and  $15 < x \leq 28$ , and (2) inner zone for  $13 < x \leq 15$ . Both configurations 2 and 3 use (1) outer zones for  $0 \leq x < 11$  and  $17 < x \leq 28$ , and (2) inner zone for  $11 < x \leq 17$ . The results in Figs. 5 to 8 are all calculated by the new numerical method with  $\Delta x = 28/100$ ,  $\alpha_0 = 10^{-10}$  and  $k = 50$ , where accurate

results are obtained.

Table 2: Dispersion coefficient configurations for heterogeneous ADE.

Configuration	$D_O$	$D_i$	Inner zone width
1	2.8	3.0	2
2	3.5	2.7	6
3	3.0	2.7	6

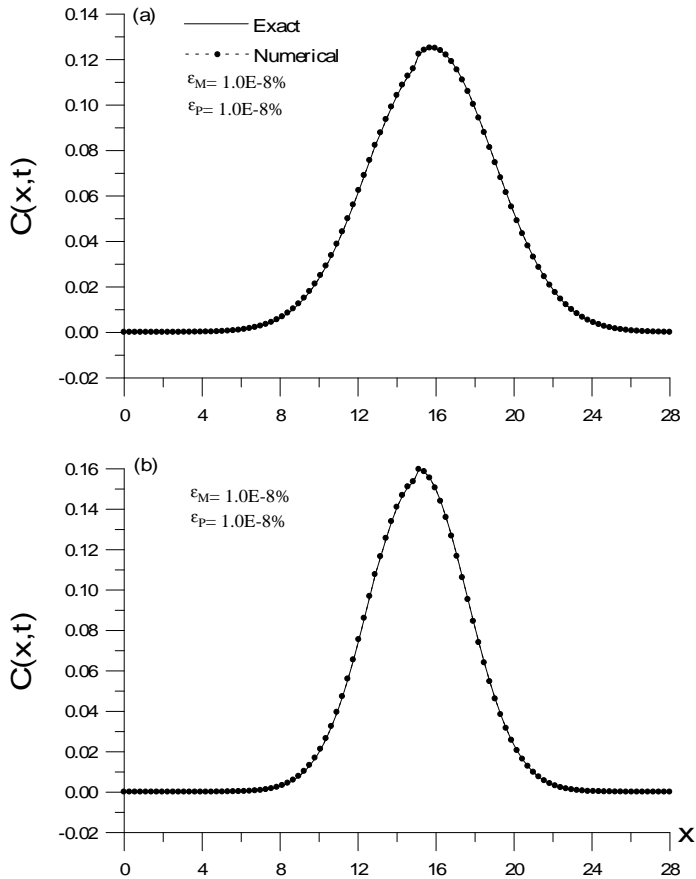


Figure 5: Comparisons of exact solutions and numerical solutions for configuration 1 with data at different times retrieved: (a)  $t = 1.8$ , (b)  $t = 1.1$ .

In configuration 3, when the input final measured data are contaminated by random noise, we are concerned with the stability of our method, which is investigated by



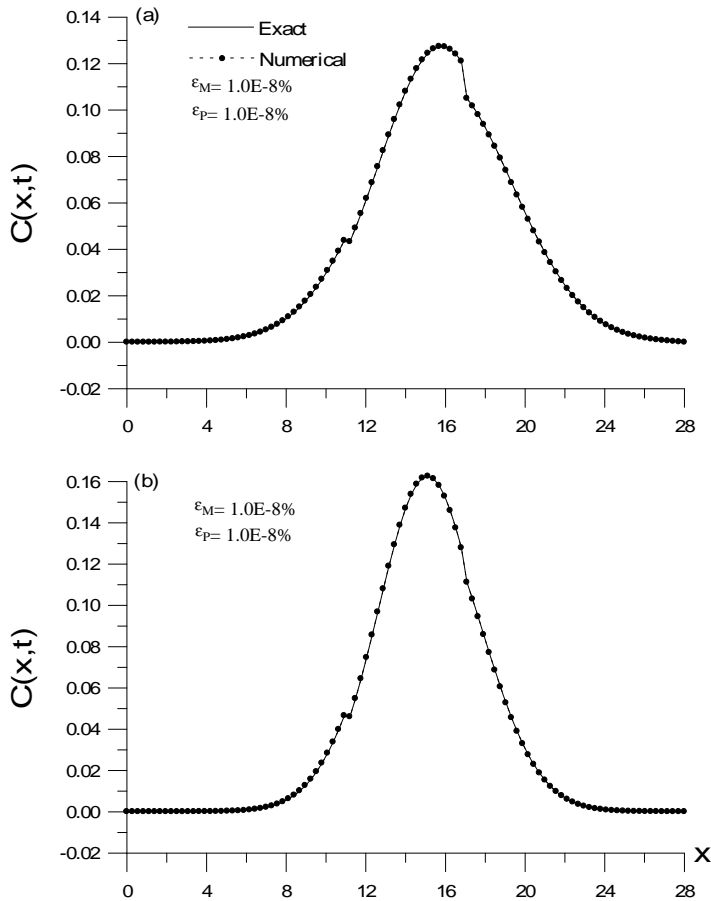


Figure 6: Comparisons of exact solutions and numerical solutions for configuration 2 with data at different times retrieved: (a)  $t = 1.8$ , (b)  $t = 1.1$ .

adding the different levels of random noise on the final data. We use the function `RANDOM_NUMBER` given in Fortran to generate the noisy data  $R(i)$ , where  $R(i)$  are random numbers in  $[0, 1]$ . The numerical results with  $T = 2$  were compared with those without considering random noise in Figs. 7 and 8. The noise is obtained by multiplying  $R(i)$  by a factor  $s$ . It can be seen that the noise level with  $s = 0.003$  disturb the numerical solutions deviating from the exact solution very small. Upon compared with the numerical results computed by Atmadja and Bagtzoglou (2001b) with the MJBBE method (see Fig. 8, Fig. 10 and Fig. 11 of the above cited paper), we can say that the proposed method is much more accurate than the MJBBE method. The mass errors of Figs. 3 to 8 induced by our method for the het-

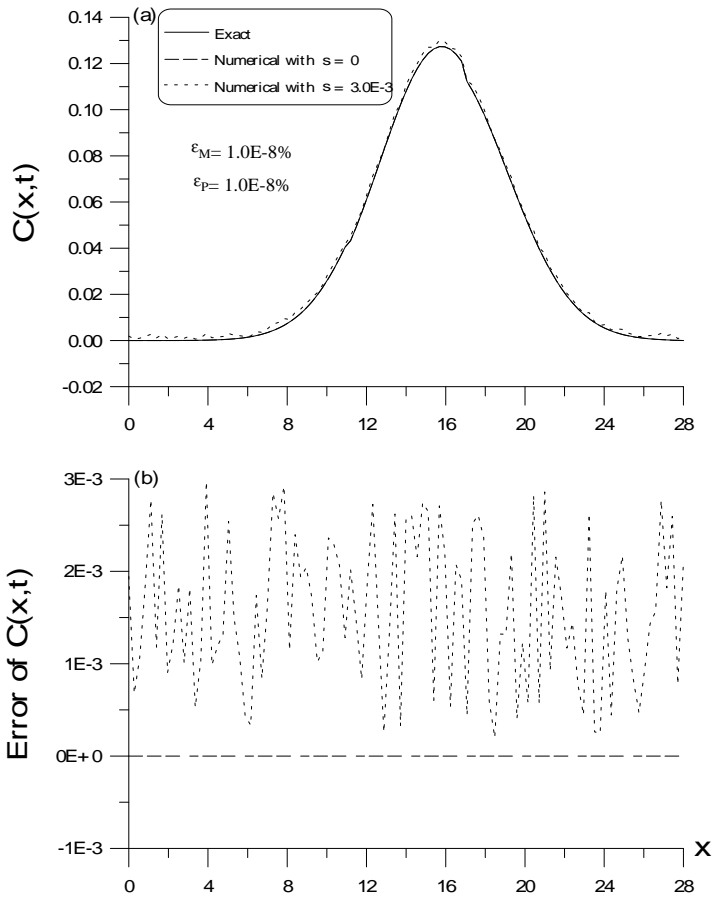


Figure 7: Comparisons of exact solutions and numerical solutions for configuration 3 with data at  $t = 1.8$  retrieved and made in (a) with different noise levels  $s = 0$ , 0.003, and (b) the corresponding numerical errors.

erogeneous and homogeneous cases at  $t = 1.8$ ,  $t = 1.1$ ,  $t = 4.8$  and  $t = 4.1$  are equal to 1.0E-8%. A summary of the mass and peak errors for different heterogeneity configurations can be found in Table 3. Obviously, our results are much better than those obtained by Atmadja and Bagtzoglou (2001b).

## 7 Conclusions

In this article, we have transformed the 1D backward in time ADE into a second kind Fredholm integral equation through a direct regularization technique and a

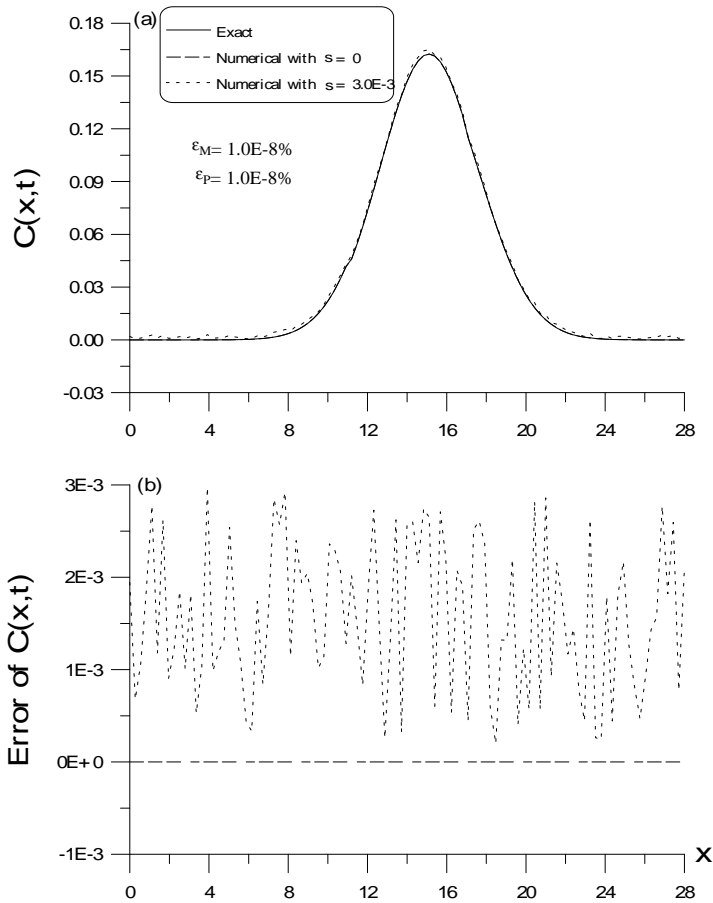


Figure 8: Comparisons of exact solutions and numerical solutions for configuration 3 with data at  $t = 1.1$  retrieved and made in (a) with different noise levels  $s = 0$ , 0.003, and (b) the corresponding numerical errors.

quasi-boundary idea. By utilizing the Fourier series expansion technique and a termwise separable property of kernel function, a series solution for approximating the exact solution is presented. The effect of regularized parameter on the perturbed solution is clear, which brings well about a better choice of the regularized parameter to avoid for causing a large numerical error. The uniform convergence and error estimate of the regularized solution are provided. We demonstrate that the new regularized technique is applicable to the groundwater contamination problems. Several numerical examples have shown that the new approach can retrieve all the initial data very well, even though the final data are very small or noised by

Table 3: Summary of mass and concentration peak errors of the present method and MJBBE for the heterogeneous ADE cases.

configuration	Time	$\varepsilon_M(\%)$		$\varepsilon_P(\%)$	
		MJBBE	Present	MJBBE	Present
1	$T = 2 \quad t = 1.8$	-0.24	1.0E-8	-0.21	1.0E-8
	$T = 2 \quad t = 1.1$	-1.10	1.0E-8	-0.87	1.0E-8
2	$T = 2 \quad t = 1.8$	1.47	1.0E-8	1.78	1.0E-8
	$T = 2 \quad t = 1.1$	6.79	1.0E-8	8.54	1.0E-8
3	$T = 2 \quad t = 1.8$	0.63	1.0E-8	0.83	1.0E-8
	$T = 2 \quad t = 1.1$	2.82	1.0E-8	4.08	1.0E-8

a large disturbance, and the initial data to be recovered are not smooth. Our method has no numerical errors, which can be extended to 2D and 3D problems and is expected to yield good results. However, the computational procedures of the MJBBE method are very complex and the numerical errors of the MJBBE method are only in the order of  $O(10^{-2})$ - $(10^{-3})$ . Thus, it is highly recommended to exploit the new approach in the numerical computations of ADE.

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### Appendix: Error estimation

In Section 5, we have derived a regularized solution  $C^\alpha(x, t)$  of Eqs. (1)-(3) under the regularized approximation (4) with a regularized parameter  $\alpha > 0$ . We can prove the following main results.

**Theorem 1:** Suppose that the final data  $C_T \in L^2(0, l)$ . Then a sufficient and necessary condition that the inverse problem (1)-(3) has a solution is that

$$\sum_{k=1}^{\infty} e^{2[(v/2D)^2 + (k\pi/l)^2]DT} \left( \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi \right)^2 < \infty. \quad (\text{A.1})$$

**Proof:** Taking  $\alpha = 0$  in Eq. (34) and inserting it into Eq. (32), we have a formal exact solution of Eqs. (1)-(3):

$$C(x, t) = \sum_{k=1}^{\infty} a_k^* e^{-[(v/2D)^2 + (k\pi/l)^2]D(t-T)} e^{vx/2D} \sin \frac{k\pi x}{l}, \quad (\text{A.2})$$

where

$$a_k^* = \frac{2}{l} \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi. \tag{A.3}$$

Eq. (A1) is available by applying the Parseval equality on the Fourier sine series of  $C(x, 0) \in L^2(0, l)$ :

$$C(x, 0) = \sum_{k=1}^{\infty} a_k^* e^{[(v/2D)^2 + (k\pi/l)^2]Dt} e^{vx/2D} \sin \frac{k\pi x}{l}, \tag{A.4}$$

which is obtained from Eq. (A2) by inserting  $t = 0$ . This ends the proof.

**Theorem 2:** If the final data  $C_T(x)$  is bounded in the interval  $x \in [0, l]$ , then for any  $\alpha > 0$  and  $t_0 > 0$ , the regularized solution series (32) converges uniformly for all  $t \geq t_0$  and  $x \in [0, l]$ .

**Proof:** Since  $\alpha > 0$ , and  $C_T(x)$  is bounded, say  $|C_T(x)| \leq E^*, x \in [0, l]$ , for some  $E^* > 0$ , from Eq. (34) we have

$$\begin{aligned} |a_k| &= \frac{2}{l[\alpha + e^{-[(v/2D)^2 + (k\pi/l)^2]Dt}]} \left| \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi \right| \\ &\leq \frac{2}{l\alpha} \int_0^l |C_T(\xi)| d\xi \leq \frac{2E^*}{\alpha} =: E, \end{aligned} \tag{A.5}$$

where  $E$  is a positive constant. Thus, for any  $t \geq t_0 > 0$  we have

$$\left| a_k e^{-[(v/2D)^2 + (k\pi/l)^2]Dt} \sin \frac{k\pi x}{l} \right| \leq E e^{-[(v/2D)^2 + (k\pi/l)^2]Dt_0}. \tag{A.6}$$

Through the ratio test, it is obvious that the series  $\sum_{k=1}^{\infty} e^{-[(v/2D)^2 + (k\pi/l)^2]Dt_0}$  converges. Therefore, by the Weierstrass M-test [Apostol (1974)], the series in Eq. (32) converges uniformly with respect to  $x$  and  $t$  whenever  $t \geq t_0$  and  $x \in [0, l]$ . This ends the proof.

**Theorem 3:** If the final data  $C_T(x)$  satisfies condition (A1) and there exists an  $\varepsilon \in (0, 1)$ , such that

$$\frac{2}{l} \sum_{k=1}^{\infty} e^{2[(v/2D)^2 + (k\pi/l)^2]D(1+\varepsilon)T} \left( \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi \right)^2 := M^2(\varepsilon) < \infty, \tag{A.7}$$

then for any  $\alpha > 0$ , and  $t \geq 0$  the regularized solution  $C^\alpha(x, t)$  satisfies the following error estimation:

$$\|C^\alpha(\cdot, t) - C(\cdot, t)\|_{L^2(0, l)} \leq \alpha^\varepsilon M(\varepsilon). \tag{A.8}$$

**Proof:** From Eqs. (28), (32), (34), (A2) and (A3) it follows that

$$C(x, t) - C^\alpha(x, t) = \sum_{k=1}^{\infty} b_k e^{[(v/2D)^2 + (k\pi/l)^2]D(T-t)} \sin \frac{k\pi x}{l}, \quad (\text{A.9})$$

where

$$b_k = \frac{2\alpha}{l[\alpha + e^{-[(v/2D)^2 + (k\pi/l)^2]DT}]} \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi. \quad (\text{A.10})$$

By using the Parseval's identity on Eq. (A9), we obtain

$$\|C(x, t) - C^\alpha(x, t)\|_{L^2(0, l)}^2 = \frac{2}{l} \sum_{k=1}^{\infty} b_k^2 e^{2[(v/2D)^2 + (k\pi/l)^2]D(T-t)}. \quad (\text{A.11})$$

Substituting Eq. (A10) for into Eq. (A11) leads to

$$\begin{aligned} \|C(x, t) - C^\alpha(x, t)\|_{L^2(0, l)}^2 &= \sum_{k=1}^{\infty} \frac{2\alpha^2}{l[\alpha + e^{-[(v/2D)^2 + (k\pi/l)^2]DT}]^2} e^{2[(v/2D)^2 + (k\pi/l)^2]D(T-t)} \\ &\quad \times \left( \int_0^l \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi \right)^2. \end{aligned}$$

Thus, for any  $\varepsilon \in (0, 1)$  we have the following estimation:

$$\begin{aligned} &\|C(x, t) - C^\alpha(x, t)\|_{L^2(0, l)}^2 \\ &= \frac{2\alpha^2}{l} \sum_{k=1}^{\infty} e^{2[(v/2D)^2 + (k\pi/l)^2]D(T-t)} \\ &\quad [(\alpha + e^{-[(v/2D)^2 + (k\pi/l)^2]DT})^\varepsilon (\alpha + e^{-[(v/2D)^2 + (k\pi/l)^2]DT})^{1-\varepsilon}]^{-2} \\ &\quad \times \left( \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi \right)^2 \\ &\leq \frac{2\alpha^2}{l} \sum_{k=1}^{\infty} e^{2[(v/2D)^2 + (k\pi/l)^2]D(T-t)} [e^{2[(v/2D)^2 + (k\pi/l)^2]DT}]^\varepsilon [\alpha^{1-\varepsilon}]^{-2} \\ &\quad \left( \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi \right)^2 \\ &= \frac{2\alpha^{2\varepsilon}}{l} \sum_{k=1}^{\infty} e^{2[(v/2D)^2 + (k\pi/l)^2]D((1+\varepsilon)T-t)} \left( \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi \right)^2 \\ &\leq \frac{2\alpha^{2\varepsilon}}{l} \sum_{k=1}^{\infty} e^{2[(v/2D)^2 + (k\pi/l)^2]D(1+\varepsilon)T} \left( \int_0^l e^{-v\xi/2D} \sin \frac{k\pi\xi}{l} C_T(\xi) d\xi \right)^2 \\ &= \alpha^{2\varepsilon} M^2(\varepsilon). \end{aligned} \quad (\text{A.12})$$

Therefore, we complete the proof.

The above three theorems are important to guarantee that the proposed regularization is workable. Although the problem we consider is ill-posed, we have assumed that the exact solution is existent to cast the error estimation in a manner that is typical in the partial differential equation approximations.

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