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# A Quasi-Boundary Semi-Analytical Approach for Two-Dimensional Backward Advection-Dispersion Equation

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**Abstract:** In this study, we employ a semi-analytical approach to solve a two-dimensional advection-dispersion equation (ADE) for identifying the contamination problems. First, the Fourier series expansion technique is used to calculate the concentration field $C(x,y,t)$ at any time $t < T$. Then, we ponder a direct regularization by adding an extra term $\alpha C(x,\ y,\ 0)$ on the final time data $C(x,y,T)$, to reach a second-kind Fredholm integral equation. The termwise separable property of kernel function allows us obtaining a closed-form solution of the Fourier coefficients. A strategy to choose the regularization parameter is offered. The solver utilized in this work can retrieve the spatial distribution of the groundwater contaminant concentration. Several numerical examples are scrutinized to display that the new method can recover all the past data very well, and is good enough to deal with heterogeneous parameters, even though the final time data are noised seriously.

**Keywords:** Groundwater contaminant distribution, Backward advection-dispersion equation, Fredholm integral equation, Ill-posed problem, Fourier series

## 1 Introduction

Accompanied with the advances of technology, many human activities are polluting the groundwater system. Reliable and quantitative predictions of contaminant movement can be made only if we understand the source characteristics [Mahar and Datta (2001)], such as pollutant concentration, contaminant location, categories of pollution and so on. For the mathematical modeling of the problem, many researchers [Gorelick, Evans and Remson (1983); Wagner (1992); Atmadja (2001); Atmadja and Bagtzoglou (2001a, 2001b, 2003); Liu, Chang and Chang (2010)]

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have employed the backward advection-dispersion equation (BADE) to govern this problem. By accurately identifying those groundwater pollution source properties, one can deal with the problem effectively.

Let us consider the two-dimensional BADE:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[D\frac{\partial C}{\partial x}\right] + \frac{\partial}{\partial y}\left[D\frac{\partial C}{\partial y}\right] - u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial y}, \tag{1}$$

$$C(0,y,t) = C(a,y,t) = C(x,0,t) = C(x,b,\ t) = 0,\ 0 \le t \le T, \tag{2}$$

$$C(x,y,T) = C_T(x,y),\ 0 \le x \le a\ ,\ 0 \le y \le b\ , \tag{3}$$

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

One way to tackle an ill-posed problem is by a perturbation of 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 utilized by Denche and Bessila (2005), and an optimal regularization proposed by Boussetila and Rebbani (2006). Showalter (1983) first regularized this sort inverse problem by considering a quasi-boundary-value approximation to the final value problem, that is, to replace Eq. (3) by

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

The problems (1), (2) and (4) can be presented to be well-posed for each $\alpha > 0$.

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

In this article, we utilize a direct regularization technique to transform the BADE into a second-kind Fredholm integral equation by using the quasi-boundary method. By employing 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 algorithm, whose accuracy is much better than the MJBBE method proposed by Atmadja and Bagtzoglou (2001b). Especially, the proposed method is time-saving and easy to implement. A similar second-kind Fredholm integral equation regularization scheme was first employed by Liu (2007a) to tackle a direct problem of elastic torsion of a bar with arbitrary cross-section, where it was called a meshless regularized integral equation approach. Liu (2007b, 2007c) extended it to solve the Laplace direct problem in arbitrary plane domains. Resorting on the basis of those good results and experiences, Liu (2009a, 2009b) utilized this new algorithm to treat the inverse Robin coefficient problem of Laplace equation and backward heat conduction problems. Besides, Chang, Liu and Chang (2010a, 2010b) employed the quasi-boundary idea to resolve the one-dimensional (1-D) and two-dimensional (2-D) backward heat conduction problem, respectively, and Liu (2010) also used a similar method to tackle the 1-D backward wave propagation problem.

The present paper is organized as follows. We derive the second-kind Fredholm integral equation by a direct regularization in Section 2. In Section 3, we derive a closed-form solution of the second-kind Fredholm integral equation. Section 4 provides a selection principle of the regularization parameter and gives some numerical experiments to demonstrate and validate the proposed scheme. Finally, some conclusions are drawn in Section 5.

## 2 The Fredholm integral equation

By employing the technique for separation of variables, we are easy to write a series expansion of $C(x, y, t)$ satisfying Eqs. (1) and (2):

$$C(x,\ y,\ t) = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} d_{kj}$$
$$\exp\{(ux+vy)/2D - [(u^2+v^2)/4D^2 + (k\pi/a)^2 + (j\pi/b)^2]Dt\}$$
$$\times \sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}, \quad (5)$$

where $d_{kj}$ are coefficients to be determined. By imposing the two-point boundary condition (4) on the above equation, we attain

$$C(x,\ y,\ T) = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} d_{kj}$$
$$\exp\{(ux+vy)/2D - [(u^2+v^2)/4D^2 + (k\pi/a)^2 + (j\pi/b)^2]DT\}$$
$$\times \sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b} = C_T(x,\ y) - \alpha C(x,\ y,\ 0). \quad (6)$$

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

$$d_{kj} = \frac{4}{ab}\exp\{[(u^2+v^2)/4D^2+(k\pi/a)^2+(j\pi/b)^2]Dt\}$$
$$\times\int_0^b\int_0^a \exp[-(u\xi+v\varphi)/2D]\sin\frac{k\pi\xi}{a}\sin\frac{j\pi\varphi}{b}C(\xi,\ \varphi,\ t)d\xi d\varphi. \quad (7)$$

Substituting Eq. (7) for $d_{kj}$ into Eq. (6) and supposing that the order of summation and integral can be interchanged, it follows that

$$\begin{aligned}\left(K_{xy}^{T-t}C(\cdot,\ \cdot,\ t)\right)\ (x,\ y) &:= \int_0^b\int_0^a K(x,\ \xi;\ y,\ \varphi;\ T-t)C(\xi,\ \varphi,\ t)d\xi d\varphi \\ &= C_T(x,\ y)-\alpha C(x,\ y,\ 0),\end{aligned} \quad (8)$$

where

$$K(x,\ \xi;\ y,\ \varphi;\ t) =$$
$$\frac{4}{ab}\sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\exp\{(ux+vy)/2D-[(u^2+v^2)/4D^2+(k\pi/a)^2+(j\pi/b)^2]Dt\}$$
$$\times\sin\frac{k\pi x}{a}\sin\frac{k\pi\xi}{a}\sin\frac{j\pi y}{b}\sin\frac{j\pi\varphi}{b} \quad (9)$$

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

To retrieve the initial concentration $C(x, y, 0)$, we have to solve the two-dimensional second-kind Fredholm integral equation:

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

which is acquired from Eq. (8) by taking $t$ = 0. Taking $x=\eta$ and $y=\omega$ in Eq. (10), we can get

$$\alpha C(\eta,\ \omega,\ 0)+\int_0^b\int_0^a K(\eta,\ \xi;\ \omega,\ \varphi;\ T)C(\xi,\ \varphi,\ 0)d\xi d\varphi = C_T(\eta,\ \omega), \quad (11)$$

and applying the operator $\mathbf{K}_{xy}^{t}$ on the above equation and noting that

$$\left(\mathbf{K}_{xy}^{t}C(\cdot,\ \cdot,\ 0)\right)\ (x,\ y) = \int_0^b\int_0^a K(x,\eta;\ y,\omega;\ t)C(\eta,\ \omega,\ 0)d\eta d\omega = C(x,\ y,\ t),$$
$$\left(\mathbf{K}_{xy}^{t}\mathbf{K}_{\eta\omega}^{\mathrm{T}}C(\cdot,\ \cdot,\ 0)\right)\ (x,\ y) = \left(\mathbf{K}_{xy}^{\mathrm{T}}\mathbf{K}_{\eta\omega}^{t}C(\cdot,\ \cdot,\ 0)\right)\ (x,\ y),$$

we have

$$\alpha C(x,\ y,\ t)+\int_0^b\int_0^a K(x,\ \xi;\ y,\ \varphi;\ T)C(\xi,\ \varphi,\ t)d\xi d\varphi = F(x,\ y,\ t)$$
$$=\int_0^b\int_0^a K(x,\ \xi;\ y,\ \varphi;\ t)C_T(\xi,\ \varphi)d\xi d\varphi. \quad (12)$$

## 3 A closed-form regularization solution

Furthermore, we start from Eq. (10) by a different method, instead of Eq. (12), since Eq. (10) is simpler than Eq. (12). We presume that the kernel function in Eq. (10) can be approximated by $m$ and $n$ terms with

$$K(x,\ \xi;\ y,\ \varphi;\ T)=\frac{4}{ab}$$
$$\sum_{j=1}^{n}\sum_{k=1}^{m}\exp\{\ [u(x-\xi)+v(y-\varphi)]/2D-[(u^2+v^2)/4D^2+(k\pi/a)^2+(j\pi/b)^2]DT\}$$
$$\times\sin\frac{k\pi x}{a}\sin\frac{k\pi\xi}{a}\sin\frac{j\pi y}{b}\sin\frac{j\pi\varphi}{b} \quad (13)$$

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

By inspection of Eq. (13), we can get

$$K(x,\ \xi;\ y,\ \varphi;\ T)=\mathbf{P}(x,\ y;\ T)\cdot\mathbf{Q}(\xi,\varphi), \quad (14)$$

where **P** and **Q** are *nm*-vectors given by

$$\mathbf{P} := \frac{4e^{(ux+vy)/2D}}{ab}\begin{bmatrix} \exp\{-[(u^2+v^2)/4D^2+\rho_{11}^2]DT\}\sin\frac{\pi x}{a}\sin\frac{\pi y}{b} \\ \exp\{-[(u^2+v^2)/4D^2+\rho_{21}^2]DT\}\sin\frac{2\pi x}{a}\sin\frac{\pi y}{b} \\ \vdots \\ \exp\{-[(u^2+v^2)/4D^2+\rho_{m1}^2]DT\}\sin\frac{m\pi x}{a}\sin\frac{\pi y}{b} \\ \exp\{-[(u^2+v^2)/4D^2+\rho_{12}^2]DT\}\sin\frac{\pi x}{a}\sin\frac{2\pi y}{b} \\ \exp\{-[(u^2+v^2)/4D^2+\rho_{22}^2]DT\}\sin\frac{2\pi x}{a}\sin\frac{2\pi y}{b} \\ \vdots \\ \exp\{-[(u^2+v^2)/4D^2+\rho_{m2}^2]DT\}\sin\frac{m\pi x}{a}\sin\frac{2\pi y}{b} \\ \vdots \\ \exp\{-[(u^2+v^2)/4D^2+\rho_{1n}^2]DT\}\sin\frac{\pi x}{a}\sin\frac{n\pi y}{b} \\ \exp\{-[(u^2+v^2)/4D^2+\rho_{2n}^2]DT\}\sin\frac{2\pi x}{a}\sin\frac{n\pi y}{b} \\ \vdots \\ \exp\{-[(u^2+v^2)/4D^2+\rho_{mn}^2]DT\}\sin\frac{m\pi x}{a}\sin\frac{n\pi y}{b} \end{bmatrix},$$

$$\mathbf{Q} := e^{-(u\xi+v\varphi)/2D}\begin{bmatrix} \sin\frac{\pi\xi}{a}\sin\frac{\pi\varphi}{b} \\ \sin\frac{2\pi\xi}{a}\sin\frac{\pi\varphi}{b} \\ \vdots \\ \sin\frac{m\pi\xi}{a}\sin\frac{\pi\varphi}{b} \\ \sin\frac{\pi\xi}{a}\sin\frac{2\pi\varphi}{b} \\ \sin\frac{2\pi\xi}{a}\sin\frac{2\pi\varphi}{b} \\ \vdots \\ \sin\frac{m\pi\xi}{a}\sin\frac{2\pi\varphi}{b} \\ \vdots \\ \sin\frac{\pi\xi}{a}\sin\frac{n\pi\varphi}{b} \\ \sin\frac{2\pi\xi}{a}\sin\frac{n\pi\varphi}{b} \\ \vdots \\ \sin\frac{m\pi\xi}{a}\sin\frac{n\pi\varphi}{b} \end{bmatrix}, \tag{15}$$

where $\rho_{kj}^2 = k^2/a^2 + j^2/b^2$, $k = 1,2,\ldots,m$, $j = 1,2,\ldots,n$ and the dot between **P** and **Q** denotes the inner product, which is sometimes written as $\mathbf{P}^{\mathrm{T}}\mathbf{Q}$, where the superscript T signifies the transpose. With the aid of Eq. (14), Eq. (10) can be written as

$$\alpha C(x,\ y,\ 0) + \int_0^b\int_0^a \mathbf{P}^{\mathrm{T}}(x,\ y)\mathbf{Q}(\xi,\ \varphi)C(\xi,\ \varphi,\ 0)d\xi d\varphi = C_T(x,\ y), \tag{16}$$

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

$$\mathbf{c} := \int_0^b \int_0^a \mathbf{Q}(\xi,\ \varphi) C(\xi,\ \varphi,\ 0) d\xi d\varphi \tag{17}$$

to be an unknown vector with dimensions $mn$.
Multiplying Eq. (16) by $\mathbf{Q}(x, y)$, and integrating it, we can obtain

$$\alpha \int_0^b \int_0^a \mathbf{Q}(x,\ y) C(x,\ y,\ 0) dxdy + \int_0^b \int_0^a \mathbf{Q}(x,\ y) \mathbf{P}^{\mathrm{T}}(x,\ y) dxdy \\ \times \int_0^b \int_0^a \mathbf{Q}(\xi,\ \varphi) C(\xi,\ \varphi,\ 0) d\xi d\varphi = \int_0^b \int_0^a C_T(x,\ y) \mathbf{Q}(x,\ y) dxdy. \tag{18}$$

By definition (17) we thus have

$$\left(\alpha \mathbf{I}_{nm} + \int_0^b \int_0^a \mathbf{Q}(\xi,\ \varphi) \mathbf{P}^{\mathrm{T}}(\xi,\ \varphi) d\xi d\varphi\right) c := \int_0^b \int_0^a C_T(\xi,\ \varphi) \mathbf{Q}(\xi,\ \varphi) d\xi d\varphi, \tag{19}$$

where $\mathbf{I}_{nm}$ means an identity matrix of order $mn$. Solving Eq. (19) one has

$$\mathbf{c} = \left(\alpha \mathbf{I}_{nm} + \int_0^b \int_0^a \mathbf{Q}(\xi,\ \varphi) \mathbf{P}^{\mathrm{T}}(\xi,\ \varphi) d\xi d\varphi\right)^{-1} \int_0^b \int_0^a C_T(\xi,\ \varphi) \mathbf{Q}(\xi,\ \varphi) d\xi d\varphi. \tag{20}$$

On the other hand, from Eq. (16) we obtain

$$\alpha C(x,\ y,\ 0) = C_T(x,\ y) - \mathbf{P}(x,\ y) \cdot c. \tag{21}$$

Inserting Eq. (20) into the above equation, we get

$$\alpha C(x,\ y,\ 0) = C_T(x,\ y) - \mathbf{P}(x,\ y) \cdot \left(\alpha \mathbf{I}_{nm} + \int_0^b \int_0^a \mathbf{Q}(\xi,\ \varphi) \mathbf{P}^{\mathrm{T}}(\xi,\ \varphi) d\xi d\varphi\right)^{-1} \\ \times \int_0^b \int_0^a C_T(\xi,\ \varphi) \mathbf{Q}(\xi,\ \varphi) d\xi d\varphi. \tag{22}$$

Owing to the orthogonality of

$$\int_0^b \int_0^a \sin\frac{j\pi\xi}{a} \sin\frac{k\pi\xi}{a} \sin\frac{m\pi\varphi}{b} \sin\frac{n\pi\varphi}{b} d\xi d\varphi = \frac{ab}{4} \delta_{jk} \delta_{mn}, \tag{23}$$

where $\delta_{jk}$ and $\delta_{mn}$ are the Kronecker delta, the $nm \times nm$ matrix can be written as

$$\begin{aligned}
&\int_0^b \int_0^a \mathbf{Q}(\xi,\ \varphi)\mathbf{P}^{\mathrm{T}}(\xi,\ \varphi)d\xi d\varphi = \\
&diag\{\exp\{-[(u^2+v^2)/4D^2+\rho_{11}^2]DT\},\exp\{-[(u^2+v^2)/4D^2+\rho_{21}^2]DT\}, \\
&\ \ldots,\exp\{-[(u^2+v^2)/4D^2+\rho_{m1}^2]DT\},\exp\{-[(u^2+v^2)/4D^2+\rho_{12}^2]DT\}, \\
&\ \exp\{-[(u^2+v^2)/4D^2+\rho_{22}^2]DT\},\ldots,\exp\{-[(u^2+v^2)/4D^2+\rho_{m2}^2]DT\},\ldots, \\
&\ \exp\{-[(u^2+v^2)/4D^2+\rho_{1n}^2]DT\},\exp\{-[(u^2+v^2)/4D^2+\rho_{2n}^2]DT\},\ldots, \\
&\ \exp\{-[(u^2+v^2)/4D^2+\rho_{mn}^2]DT\},
\end{aligned} \tag{24}$$

in which, diag denotes that the matrix is a diagonal matrix. Inserting Eq. (24) into Eq. (22), we hence acquire

$$\begin{aligned}
&C(x,\ y,\ 0) = \frac{1}{\alpha}C_T(x,\ y) - \frac{1}{\alpha}P^{\mathrm{T}}(x,\ y) \\
&diag\left[\frac{1}{\alpha+\exp\{-[(u^2+v^2)/4D^2+\rho_{11}^2]DT\}},\right. \\
&\frac{1}{\alpha+\exp\{-[(u^2+v^2)/4D^2+\rho_{21}^2]DT\}},\ldots, \\
&\frac{1}{\alpha+\exp\{-[(u^2+v^2)/4D^2+\rho_{m1}^2]DT\}}, \\
&\frac{1}{\alpha+\exp\{-[(u^2+v^2)/4D^2+\rho_{12}^2]DT\}}, \\
&\frac{1}{\alpha+\exp\{-[(u^2+v^2)/4D^2+\rho_{22}^2]DT\}},\ldots, \\
&\frac{1}{\alpha+\exp\{-[(u^2+v^2)/4D^2+\rho_{m2}^2]DT\}},\ldots, \\
&\frac{1}{\alpha+\exp\{-[(u^2+v^2)/4D^2+\rho_{1n}^2]DT\}}, \\
&\frac{1}{\alpha+\exp\{-[(u^2+v^2)/4D^2+\rho_{2n}^2]DT\}},\ldots, \\
&\left.\frac{1}{\alpha+\exp\{-[(u^2+v^2)/4D^2+\rho_{mn}^2]DT\}}\right] \int_0^b \int_0^a C_T(\xi,\ \varphi)Q(\xi,\ \varphi)d\xi d\varphi.
\end{aligned} \tag{25}$$

Using Eq. (15) for **P** and **Q**, we can obtain

$$C(x,\ y,\ 0) = \frac{1}{\alpha} C_T(x,\ y)$$

$$-\frac{4}{\alpha ab} \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \frac{\exp\{-[(u^2+v^2)/4D^2 + (k\pi/a)^2 + (j\pi/b)^2]DT\}}{\alpha + \exp\{-[(u^2+v^2)/4D^2 + (k\pi/a)^2 + (j\pi/b)^2]DT\}}$$

$$\times \int_0^b \int_0^a \sin\frac{k\pi x}{a} \sin\frac{k\pi\xi}{a} \sin\frac{j\pi y}{b} \sin\frac{j\pi\varphi}{b}$$
$$\exp\{[u(x-\xi) + v(y-\varphi)]/2D\} C_T(\xi,\ \varphi) d\xi d\varphi, \quad (26)$$

where the summation upper bound $m$ and $n$ can be replaced by $\infty$ since our argument is independent of $m$ and $n$. For a given $C_T(x,\ y)$, through some integrals one may use the above equation to calculate $C(x, y, 0)$.

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

$$C^{\alpha}(x,\ y,\ t) = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} d_{kj}^{\alpha}$$
$$\exp\{(ux+vy)/2D) - [(u^2+v^2)/4D^2 + (k\pi/a)^2 + (j\pi/b)^2]Dt\}$$
$$\times \sin\frac{k\pi x}{a} \sin\frac{j\pi y}{b}, \quad (27)$$

where

$$d_{kj}^{\alpha} = \frac{4}{ab} \int_0^b \int_0^a \exp[-(u\xi + v\varphi)/2D] \sin\frac{k\pi\xi}{a} \sin\frac{j\pi\varphi}{b} C(\xi,\ \varphi,\ 0) d\xi d\varphi. \quad (28)$$

Inserting Eq. (26) into the above equation and using the orthogonality equation (23), one has

$$d_{kj}^{\alpha} = \frac{4}{ab\{\alpha + \exp\{-[(u^2+v^2)/4D^2 + (k\pi/a)^2 + (j\pi/b)^2]DT\}\}}$$

$$\times \int_0^b \int_0^a \exp[(ux+vy)/2D] \sin\frac{k\pi\xi}{a} \sin\frac{j\pi\varphi}{b} C_T(\xi,\ \varphi) d\xi d\varphi. \quad (29)$$

Eqs. (27) and (29) compose an analytical solution of the two-dimensional BADE. To tell it from the exact solution $C(x, y, t)$, we have used the symbol $C^{\alpha}(x,\ y,\ t)$ for reminding it to be a regularization solution.

## 4 Selection of the regularization parameter $\alpha$ and numerical examples

Up to this point, we have not yet clarified how to determine the regularization parameter $\alpha$. Assume that $C_T$ has the following Fourier sine series expansion:

$$C_T(x,\ y) = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} d_{kj}^{*} \sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}, \tag{30}$$

where

$$d_{kj}^{*} = \frac{4}{ab}\int_0^b\int_0^a \sin\frac{k\pi\xi}{a}\sin\frac{j\pi\varphi}{b} C_T(\xi,\ \varphi)d\xi d\varphi \tag{31}$$

Substituting Eq. (30) into Eq. (26), we acquire

$$C^{\alpha}(x,\ y,\ 0) = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} \frac{\exp\{-[(u^2+v^2)/4D^2+(k\pi/a)^2+(j\pi/b)^2]DT\}}{\alpha+\exp\{-[(u^2+v^2)/4D^2+(k\pi/a)^2+(j\pi/b)^2]DT\}} d_{kj}^{*} \times \sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}, \tag{32}$$

where we indicate that

$$\frac{\exp\{-[(u^2+v^2)/4D^2+(k\pi/a)^2+(j\pi/b)^2]DT\}}{\alpha+\exp\{-[(u^2+v^2)/4D^2+(k\pi/a)^2+(j\pi/b)^2]DT\}} = \frac{1}{1+\alpha\exp\{[(u^2+v^2)/4D^2+(k\pi/a)^2+(j\pi/b)^2]DT\}}.$$

In a practical calculation, we can only perform a finite sum in Eq. (32) to $k = m$ and $j = n$.

For a better numerical solution, we require to set

$$\alpha\exp\{[(u^2+v^2)/4D^2+(m\pi/a)^2+(n\pi/b)^2]DT\} = \alpha_0 \le 1.$$

On the other hand, the term

$$\exp\{-[(u^2+v^2)/4D^2+(m\pi/a)^2+(n\pi/b)^2]DT\} /(\alpha+\exp\{-[\ (u^2+v^2)/4D^2+(m\pi/a)^2+(n\pi/b)^2]DT\})$$

in Eq. (32) will be very small when $a$, $b$, $m$, $n$ and/or $T$ are large, which may result in a large numerical error. Hence, we have a criterion to choose $m$ and $n$ when $\alpha$ and $\alpha_0$ are clarified:

$$m = \frac{a}{\pi}\sqrt{\frac{1}{DT}\log\left(\frac{\alpha_0}{\alpha}\right) - \frac{u^2+v^2}{4D^2} - \left(\frac{n\pi}{b}\right)^2},$$
$$n = \frac{b}{\pi}\sqrt{\frac{1}{DT}\log\left(\frac{\alpha_0}{\alpha}\right) - \frac{u^2+v^2}{4D^2} - \left(\frac{m\pi}{a}\right)^2}.$$

On the other hand, once $m$, $n$ and $\alpha_0$ are given, we can employ the following criterion to select $\alpha$:

$$\alpha = \frac{\alpha_0}{\exp\{[(u^2+v^2)/4D^2+(m\pi/a)^2+(n\pi/b)^2]DT\}}. \tag{33}$$

We now apply the quasi-boundary approach to the calculations of BADE through numerical examples. When the input final measured data are contaminated by random noise, we can appraise the stability of our approach by imposing the different levels of random noise on the final data:

$$\hat{C}_T(x_i,y_j) = C_T(x_i,y_j) + sR(i,j), \tag{34}$$

where $C_T(x_i,y_j)$ are the exact data. The noisy data $R(i,\ j)$ are random numbers in [-1, 1], and $s$ means the level of noise. Then, the noisy data $\hat{C}_T(x_i,y_j)$ are used in the calculations. Usually, when the exact data are small, we utilize relative random noise to represent noise

$$s_r = \frac{s}{|C_T^{max}|} \times 100\%, \tag{35}$$

where $C_T^{max}$ is the maximum datum.

### *4.1 Numerical method for the homogeneous ADE*

Let us consider the Fourier sine series expansion of the initial condition

$$C(x,\ y,\ 0) = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} d_{kj}\exp\{(ux+vy)/2D\}\sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}, \tag{36}$$

Substituting the above equation into Eq. (28), we acquire

$$\begin{aligned} d_{kj} &= \frac{4}{ab}\int_0^b\int_0^a \exp[-(u\xi+v\varphi)/2D]C(\xi,\ \varphi,\ 0)\sin\frac{k\pi\xi}{a}\sin\frac{j\pi\varphi}{b}d\xi d\varphi \\ &= \frac{4}{ab}\int_0^{28}\int_{13.5}^{14.5} C_1\exp[-(u\xi+v\varphi)/2D]\sin\frac{k\pi\xi}{a}\sin\frac{j\pi\varphi}{b}d\xi d\varphi \\ &= \frac{4}{ab}\left[\frac{e^{-14.5s}(-s\sin 14.5g - g\cos 14.5g) + e^{-13.5s}(s\sin 13.5g + g\cos 13.5g)}{s^2+g^2}\right] \\ &\times \left[\frac{e^{-28f}(-f\sin 28h - h\cos 28h) + h}{f^2+h^2}\right], \end{aligned} \tag{37}$$

where

$$g = \frac{k\pi}{a},\ h = \frac{j\pi}{b},\ s = \frac{u}{2D},\ f = \frac{v}{2D}. \tag{38}$$

Then, the data to be recovered are given by

$$C(x,\ y,\ t) = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} d_{kj}$$
$$\exp\{(ux+vy)/2D - [(u^2+v^2)/4D^2 + (k\pi/a)^2 + (j\pi/b)^2]Dt\}$$
$$\times \sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}, \tag{39}$$

Hence, by Eqs. (27) and (29) we obtain a regularized solution:

$$C^{\alpha}(x,\ y,\ t) = \frac{1}{1+\alpha\exp\{-[(u^2+v^2)/4D^2 + (k\pi/a)^2 + (j\pi/b)^2]DT\}}$$
$$\times \sum_{j=1}^{\infty}\sum_{k=1}^{\infty} d_{kj}\exp\{(ux+vy)/2D - [(u^2+v^2)/4D^2 + (k\pi/a)^2 + (j\pi/b)^2]Dt\}$$
$$\times \sin\frac{k\pi x}{a}\sin\frac{j\pi y}{b}. \tag{40}$$

For this example with $T$ = 2, the comparisons of exact solutions and regularized solutions under $D$ = 2.8, $u$ = 1, and $v$ = 0 were plotted in Fig. 1. Fig. 2 compares the exact solution with the regularized solution under $D$ = 2.8, $u$ = 1, $v$ = 0, $\alpha_0 = 10^{-6}, \Delta x = \Delta y = 28/100$, $k = 50$ and $t = 4.8$. After viewing the output data, we find that the corresponding mass and concentration peak errors are, respectively about $\varepsilon_M$ = 0% and $\varepsilon_P$ = 0% for $t$ = 1.8 (Fig. 1), and $\varepsilon_M$ = 0% and $\varepsilon_P$ = 0% for $t$ = 4.8 (Fig. 2), i.e., Fig. 2 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

$$\varepsilon_M = \frac{Mass^e - Mass^n}{Mass^e} \times 100\%; \tag{41}$$

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

$$\varepsilon_P = \frac{\max(C^e) - \max(C^n)}{\max(C^e)} \times 100\%, \tag{42}$$

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.

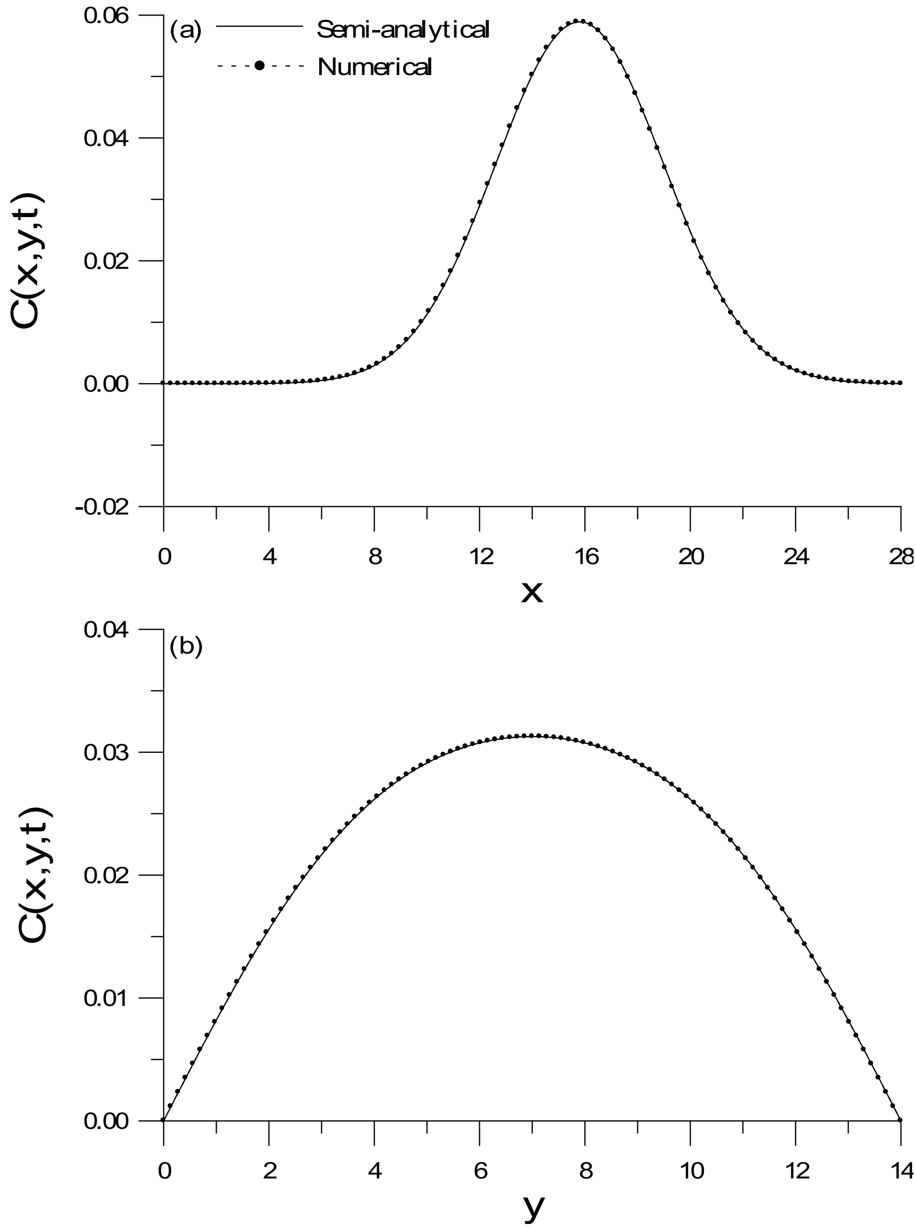


Figure 1: Comparisons of semi-analytical solutions and numerical solutions for homogeneous BADE problem with data at the time $t = 1.8$ been retrieved.

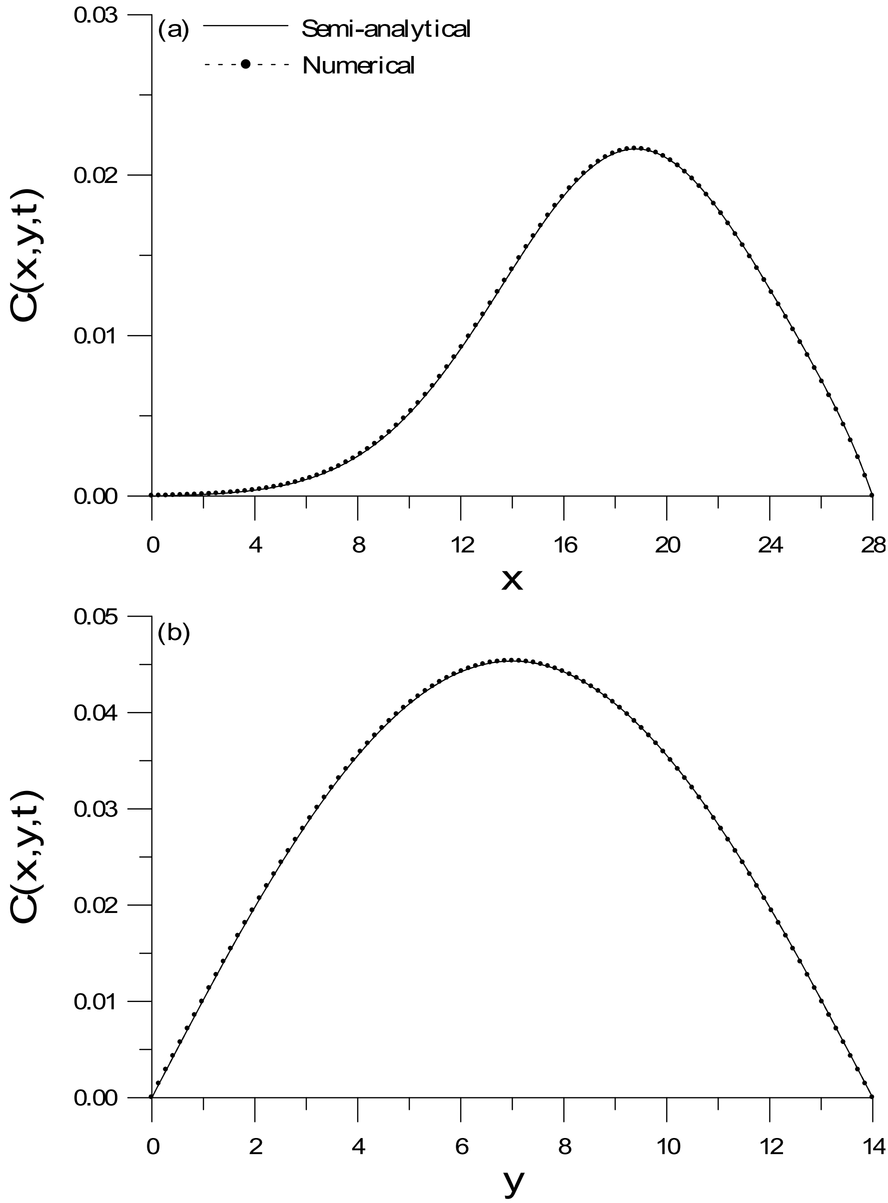


Figure 2: Comparisons of semi-analytical solutions and numerical solutions for homogeneous BADE problem with data at the time $t = 4.8$ been retrieved.

### *4.2 Numerical method for the heterogeneous ADE*

Two cases involving heterogeneity in the dispersion coefficient $D$ are to be analyzed. In all the heterogeneous parameter cases, the $x$-direction velocity is fixed to one, but the $y$-direction velocity is fixed to zero. The heterogeneity configurations are presented in Table 1. Two different zones, each with a distinct value of $D$, are employed. For configuration 1 the two zones are (1) outer zones for $0 \le x < 13$ and $15 < x \le 28$, and (2) inner zone for $13 < x \le 15$. Both configurations 1 and 2 use the same longitudinal range $0 \le y \le 14$. The results in Figs. 3 and 4 are all calculated by the new numerical approach with $\Delta x = \Delta y = 28/100$, $\alpha_0 = 10^{-6}$ and $k =$ 50, where accurate results are acquired. The mass and concentration peak errors of Figs. 1 to 4 induced by our scheme for the heterogeneous and homogeneous cases at $t$ = 1.8 and $t$ = 4.8 are very small near to zero.

Table 1: Dispersion coefficient configurations for two-dimensional heterogeneous BADE.

| Configuration | $D_O$ | $D_i$ | Inner zone width |
|---|---|---|---|
| 1 | 2.2 | 2.4 | 2 |
| 2 | 3.0 | 2.7 | 6 |

In configuration 2, when the input final measured data are contaminated by random noise, we are concerned with the stability of our method, which is investigated by adding the relative random noise on the final data. The numerical results with $T$ = 2 were compared with those without considering random noise in Fig. 5. Note that the relative random noise $s_r$ = 5% disturbs the numerical solutions deviating from the exact solution very small. The exact solutions and numerical solutions are plotted in Figs. 6(a)-(c) sequentially. Even under the noise, the numerical solution displayed in Fig. 6(c) is a good approximation to the exact initial data as shown in Fig. 6(a). However, to the authors' best knowledge, there has been no report that numerical schemes can calculate this ill-posed 2-D BADE very well as of our method.

## 5 Conclusions

In this paper, we have transformed the two-dimensional BADE into a second-kind two-dimensional Fredholm integral equation through a direct regularization technique and a quasi-boundary concept. By utilizing the Fourier series expansion technique and a termwise separable property of kernel function, a semi-analytical solution of the regularized type for approximating the exact solution is represented. The influence of regularization parameter on the perturbed solution is specified.

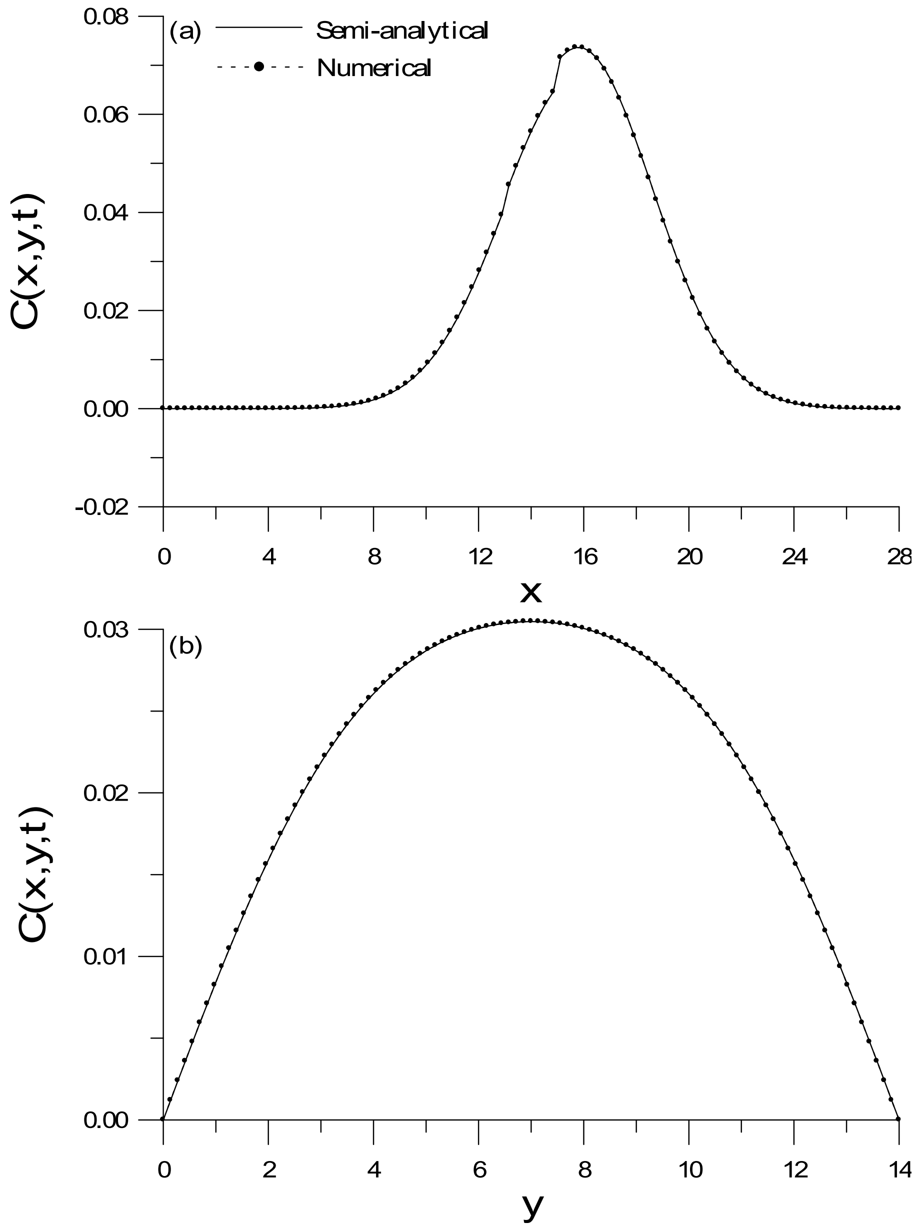


Figure 3: Comparisons of semi-analytical solutions and numerical solutions for configuration 1 with data at the time $t = 1.8$ been retrieved.

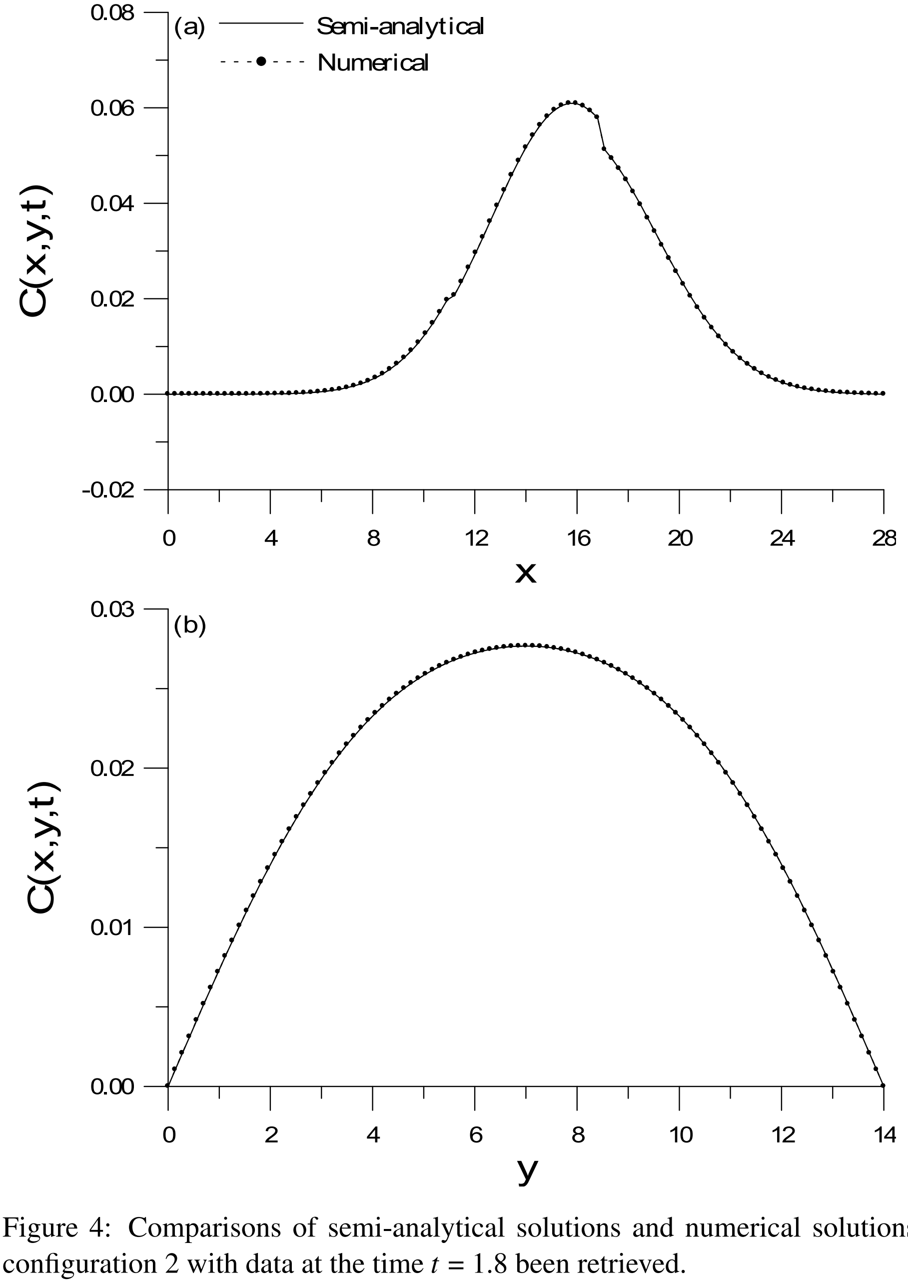


Figure 4: Comparisons of semi-analytical solutions and numerical solutions for configuration 2 with data at the time $t = 1.8$ been retrieved.

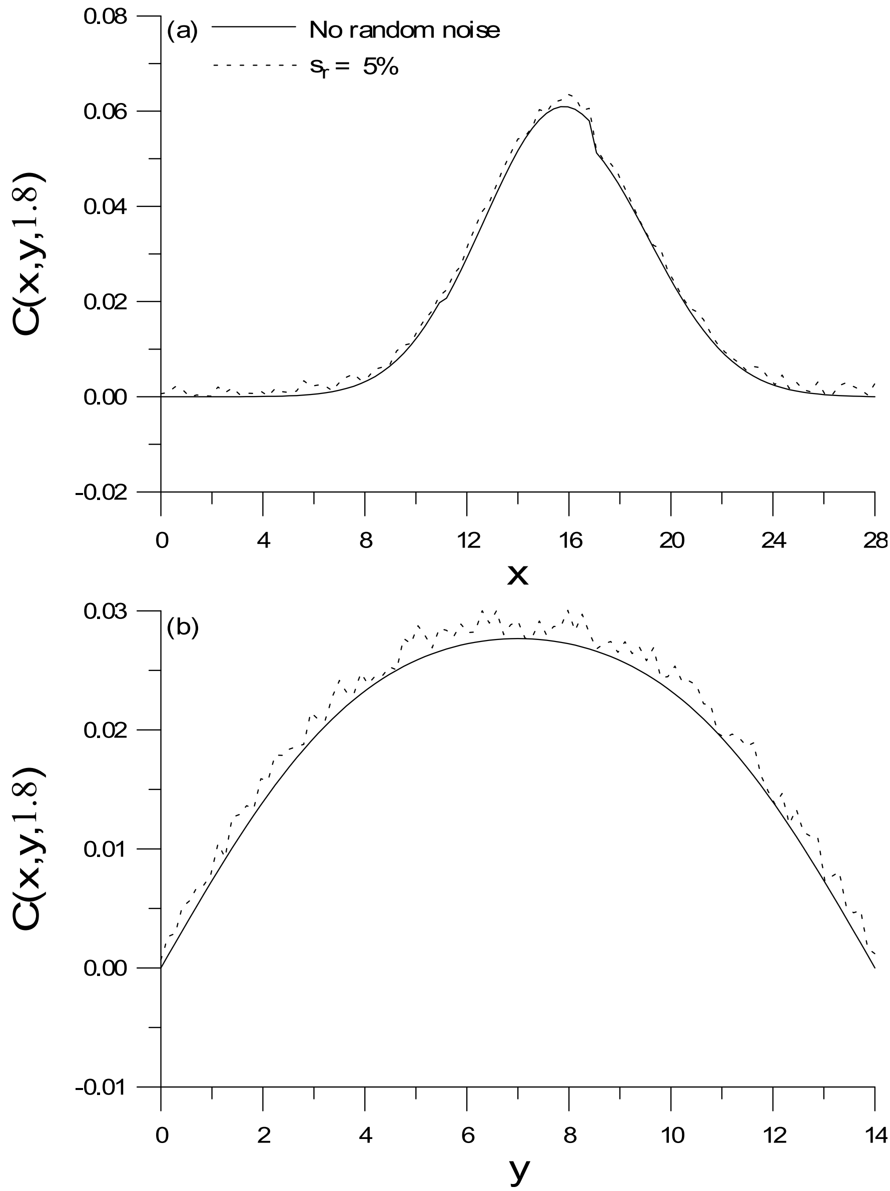


Figure 5: Comparisons of BADE solutions with and without random noise effect for Example 2 are plotted in (a) with respect to $x$ at fixed $y = 12$, and in (b) with respect to $y$ at fixed $x = 21$.

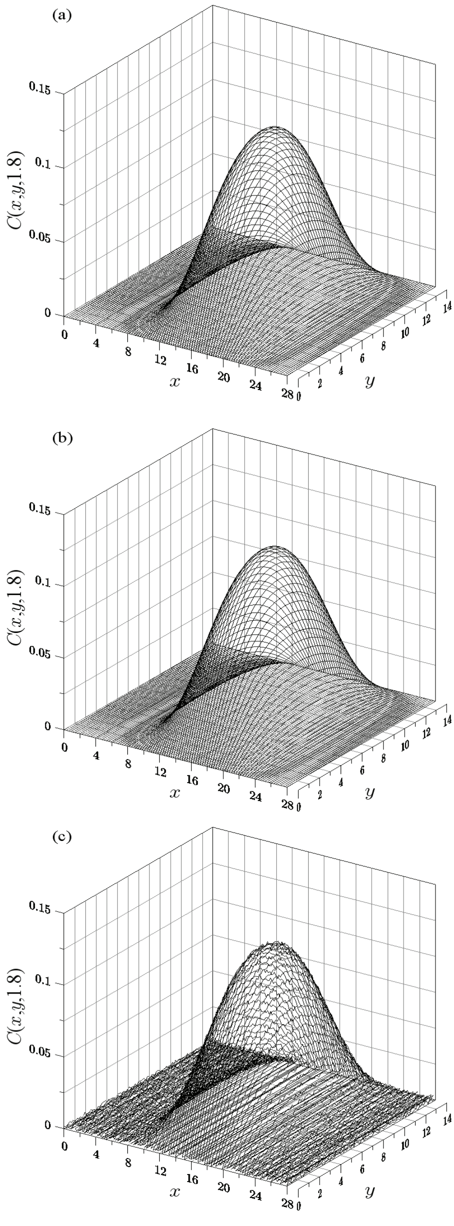


Figure 6: The semi-analytical solution for Example 2 of two-dimensional BADE are plotted in (a), in (b) the BADE solution without random noise effect, and in (c) the BADE solution with random noise.

Several numerical experiments have shown that the proposed method can recover all initial data very well, even though the final data are very small or noised by a large disturbance, and the initial data to be retrieved are not smooth. Thus, the current scheme is recommended to cope with the two-dimensional BADE.

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