

A Regularized Integral Equation Scheme for Three-Dimensional Groundwater Pollution Source Identification Problems

Chih-Wen Chang¹

Abstract: We utilize a regularized integral equation scheme to resolve the three-dimensional backward advection-dispersion equation (BADE) for identifying the groundwater pollution source identification problems in this research. First, the Fourier series expansion method is employed to estimate the concentration field $C(x, y, z, t)$ at any time $t < T$. Second, we contemplate a direct regularization by adding an extra term $\alpha(x, y, z, 0)$ to transform a second-kind Fredholm integral equation for $C(x, y, z, 0)$. The termwise separable property of the kernel function permits us to acquire a closed-form regularized solution. In addition, a tactic to determine the regularization parameter is recommended. We find that the proposed method is robust and applicable to the three-dimensional BADE when several numerical experiments with the large heterogeneous parameters and the noisy final time data are examined.

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

1 Introduction

The advection-dispersion equation (ADE) is generally employed to delineate the movement of the pollution in porous media. The advection process in ADE describes the solute movement with the average fluid flow, whereas the dispersion process interprets the velocity variations resulted in the solute spreading. These reliable and quantitative predictions of pollution movement can be made merely if we realize the source characteristics [Mahar and Datta (2001)], such as contaminant concentration, categories of pollution and so forth. For the mathematical model-

¹ Computing Technology Integration Division, National Center for High-Performance Computing, Taichung 40763, Taiwan. Tel.: +886-4-24620202#860. Fax.: +886-4-24627373. *E-mail address:* 0903040@nchc.narl.org.tw

ing of the issue, a lot of scholars [Gorelick, Evans and Remson (1983); Wagner (1992); Atmadja (2001); Atmadja and Bagtzoglou (2001a); Atmadja and Bagtzoglou (2001b); Atmadja and Bagtzoglou (2003); Liu, Chang and Chang (2009); Liu, Chang and Chang (2010); Chang and Liu (2011)] have utilized the backward advection-dispersion equation (BADE) to govern this groundwater pollution source problem. One can tackle the problem effectively by accurately identifying those groundwater contamination source properties.

The current paper is organized the following sections. Section 2 represents the BADE and its final time condition and boundary conditions. We derive the second-kind Fredholm integral equation by a direct regularization in Section 3. In Section 4, we derive a closed-form solution of the second-kind Fredholm integral equation. Section 5 offers a determination principle of the regularization parameter and presents some numerical instances to manifest and verifies the proposed approach. Some concluding remarks are drawn in Section 6.

2 Groundwater pollution source identification problems

Let us consider the following three-dimensional BADE:

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

$$\begin{aligned} C(0, y, z, t) = C(a, y, z, t) = C(x, 0, z, t) = C(x, b, z, t) = C(x, y, z, 0) \\ = C(x, y, c, t) = 0, \quad 0 \leq t \leq T, \end{aligned} \quad (2)$$

$$C(x, y, z, T) = C_T(x, y, z), \quad 0 \leq x \leq a, \quad 0 \leq y \leq b, \quad 0 \leq z \leq c. \quad (3)$$

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, w is the transport velocity in the z direction, and $C_T(x, y, z)$ is the observed plume's spatial distribution at a time T . The spatial domain is presumed to be sufficiently huge that the plume does not arrive at the boundary.

One way to deal with an ill-posed problem is by a disturbance of it into a well-posed one. Many perturbing techniques have been employed, including a biharmonic regularization proposed by Lattés and Lions (1969), a pseudo-parabolic regularization developed by Showalter and Ting (1970), a stabilized quasi-reversibility used by Miller (1973), the method of quasi-reversibility utilized by Mel'nikova (1992), a hyperbolic regularization proposed by Ames and Cobb (1997), the Gajewski and Zacharias quasi-reversibility employed 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 pondering a quasi-boundary-value approximation to the final value problem, that is, to substitute Eq. (3) by

$$\alpha C(x, y, z, 0) + C(x, y, z, T) = C_T(x, y, z). \quad (4)$$

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

In our previous paper, Chang, Liu and Chang (2007) have coped with the above quasi-boundary two-point boundary value problem for the case of $D = 1$ and $u = v = w = 0$ by an extension of the Lie-group shooting approach, which was originally proposed by Liu (2006) to tackle the second-order boundary value issues.

In this study, we propose a direct regularization technique to transform the BADE into a second-kind Fredholm integral equation by utilizing the regularized integral equation scheme. By using the eigenfunctions expansion techniques and separating kernel function, we can derive a closed-form solution of the second-kind Fredholm integral equation, which is the foremost contribution of this paper. Another one is the application of the Fredholm integral equation to develop an effective numerical scheme. In particular, the presented approach is easy to implement and time-saving. A similar second-kind Fredholm integral equation regularization algorithm was first used by Liu (2007a) to deal with a direct problem of elastic torsion of a bar with arbitrary cross-section, where it was named a meshless regularized integral equation scheme. Liu (2007b, 2007c) extended it to resolve the Laplace direct problem in arbitrary plane domains. Resorting on the basis of those excellent experiences and results, Liu (2009a, 2009b) employed this new method to address the inverse Robin coefficient problem of Laplace equation and backward heat conduction problems. In addition, Chang, Liu and Chang (2010a, 2010b) and Chang (2011) used the quasi-boundary concept to resolve the one-dimensional (1-D), two-dimensional (2-D) and three-dimensional (3-D) backward heat conduction problems, respectively, and Liu (2010) also utilized a similar approach to cope with the 1-D backward wave propagation issue.

3 The Fredholm integral equation

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

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

where d_{ijk} are coefficients to be chosen. By imposing the boundary condition (4) on the above equation, we acquire

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

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

$$d_{ijk} = \frac{8 \exp\{[(u^2 + v^2 + w^2)/4D^2 + (i\pi/a)^2 + (j\pi/b)^2 + (k\pi/c)^2]Dt\}}{abc} \times \int_0^c \int_0^b \int_0^a \exp[-(u\xi + v\varphi + w\rho)/2D] \sin \frac{i\pi\xi}{a} \sin \frac{j\pi\varphi}{b} \sin \frac{k\pi\rho}{c} C(\xi, \varphi, \rho, t) qd\xi d\varphi d\rho. \quad (7)$$

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

$$\begin{aligned} & (\mathbf{K}_{xyz}^{T-t} C(\cdot, \cdot, \cdot, t))(x, y, z) \\ & := \int_0^c \int_0^b \int_0^a K(x, \xi; y, \varphi; z, \rho; T-t) C(\xi, \varphi, \rho, t) d\xi d\varphi d\rho \\ & = C_T(x, y, z) - \alpha C(x, y, z, 0), \quad (8) \end{aligned}$$

where

$$K(x, \xi; y, \varphi; z, \rho; t) = \frac{8}{abc} \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} \exp\{(ux + vy + wz)/2D - [(u^2 + v^2 + w^2)/4D^2 + (i\pi/a)^2 + (j\pi/b)^2 + (k\pi/c)^2]Dt\} \times \sin \frac{i\pi x}{a} \sin \frac{i\pi\xi}{a} \sin \frac{j\pi y}{b} \sin \frac{j\pi\varphi}{b} \sin \frac{k\pi z}{c} \sin \frac{k\pi\rho}{c} \quad (9)$$

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

To recover the initial temperature $C(x, y, z, 0)$, we have to resolve the three-dimensional second-kind Fredholm integral equation:

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

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

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

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

$$\begin{aligned} & (\mathbf{K}_{xyz}^t C(\cdot, \cdot, \cdot, 0)) (x, y, z) \\ &= \int_0^c \int_0^b \int_0^a K(x, \eta; y, \omega; z, \tau; t) C(\eta, \omega, \tau, 0) d\eta d\omega d\tau \\ &= C_T(x, y, z, t), \end{aligned}$$

$$(\mathbf{K}_{xyz}^t \mathbf{K}_{\eta\omega\tau}^T C(\cdot, \cdot, \cdot, 0)) (x, y, z) = (\mathbf{K}_{xyz}^T \mathbf{K}_{\eta\omega\tau}^t C(\cdot, \cdot, \cdot, 0)) (x, y, z),$$

we have

$$\begin{aligned} \alpha C(x, y, z, t) + \int_0^c \int_0^b \int_0^a K(x, \xi; y, \varphi; z, \rho; T) C(\xi, \varphi, \rho, t) d\xi d\varphi d\rho \\ = F(x, y, z, t) \\ = \int_0^c \int_0^b \int_0^a K(x, \xi; y, \varphi; z, \rho; t) C_T(\xi, \varphi, \rho) d\xi d\varphi d\rho. \end{aligned} \quad (12)$$

4 A closed-form solution

However, we start from Eq. (10) by a different approach, rather than Eq. (12), because Eq. (10) is simpler than Eq. (12). We presume that the kernel function in Eq. (10) can be approximated by q, n and m terms with

$$\begin{aligned} K(x, \xi; y, \varphi; z, \rho; T) = \frac{8}{abc} \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} d_{ijk} \exp\{[u(x-\xi) + v(y-\varphi) + w(z-\rho)]/2D \\ - [(u^2 + v^2 + w^2)/4D^2 + (i\pi/a)^2 + (j\pi/b)^2 + (k\pi/c)^2]DT\} \\ \times \sin \frac{i\pi x}{a} \sin \frac{i\pi \xi}{a} \sin \frac{j\pi y}{b} \sin \frac{j\pi \varphi}{b} \sin \frac{k\pi z}{c} \sin \frac{k\pi \rho}{c} \end{aligned} \quad (13)$$

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

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

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

$$\mathbf{P} := \frac{8e^{(ux+vy+wz)/2D}}{abc} \begin{bmatrix} \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{111}^2\}DT\} \sin \frac{\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{211}^2\}DT\} \sin \frac{2\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{\pi z}{c} \\ \vdots \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{q11}^2\}DT\} \sin \frac{q\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{121}^2\}DT\} \sin \frac{\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{221}^2\}DT\} \sin \frac{2\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{\pi z}{c} \\ \vdots \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{q21}^2\}DT\} \sin \frac{q\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{\pi z}{c} \\ \vdots \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{1n1}^2\}DT\} \sin \frac{\pi x}{a} \sin \frac{n\pi y}{b} \sin \frac{\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{2n1}^2\}DT\} \sin \frac{2\pi x}{a} \sin \frac{n\pi y}{b} \sin \frac{\pi z}{c} \\ \vdots \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{qn1}^2\}DT\} \sin \frac{q\pi x}{a} \sin \frac{n\pi y}{b} \sin \frac{\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{112}^2\}DT\} \sin \frac{\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{2\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{212}^2\}DT\} \sin \frac{2\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{2\pi z}{c} \\ \vdots \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{q12}^2\}DT\} \sin \frac{q\pi x}{a} \sin \frac{\pi y}{b} \sin \frac{2\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{122}^2\}DT\} \sin \frac{\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{2\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{222}^2\}DT\} \sin \frac{2\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{2\pi z}{c} \\ \vdots \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{q22}^2\}DT\} \sin \frac{q\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{2\pi z}{c} \\ \vdots \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{12m}^2\}DT\} \sin \frac{\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{m\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{22m}^2\}DT\} \sin \frac{2\pi x}{a} \sin \frac{2\pi y}{b} \sin \frac{m\pi z}{c} \\ \exp\{-(u^2+v^2+w^2)/4D^2+\rho_{qnm}^2\}DT\} \sin \frac{q\pi x}{a} \sin \frac{n\pi y}{b} \sin \frac{m\pi z}{c} \end{bmatrix},$$

$$\mathbf{Q} := \begin{bmatrix} \sin \frac{\pi \xi}{a} \sin \frac{\pi \varphi}{b} \sin \frac{\pi \rho}{c} \\ \sin \frac{2\pi \xi}{a} \sin \frac{\pi \varphi}{b} \sin \frac{\pi \rho}{c} \\ \vdots \\ \sin \frac{q\pi \xi}{a} \sin \frac{\pi \varphi}{b} \sin \frac{\pi \rho}{c} \\ \sin \frac{\pi \xi}{a} \sin \frac{2\pi \varphi}{b} \sin \frac{\pi \rho}{c} \\ \sin \frac{2\pi \xi}{a} \sin \frac{2\pi \varphi}{b} \sin \frac{\pi \rho}{c} \\ \vdots \\ \sin \frac{q\pi \xi}{a} \sin \frac{2\pi \varphi}{b} \sin \frac{\pi \rho}{c} \\ \vdots \\ \sin \frac{\pi \xi}{a} \sin \frac{n\pi \varphi}{b} \sin \frac{\pi \rho}{c} \\ \sin \frac{2\pi \xi}{a} \sin \frac{n\pi \varphi}{b} \sin \frac{\pi \rho}{c} \\ \vdots \\ \sin \frac{q\pi \xi}{a} \sin \frac{n\pi \varphi}{b} \sin \frac{\pi \rho}{c} \\ \sin \frac{\pi \xi}{a} \sin \frac{\pi \varphi}{b} \sin \frac{2\pi \rho}{c} \\ \sin \frac{2\pi \xi}{a} \sin \frac{\pi \varphi}{b} \sin \frac{2\pi \rho}{c} \\ \vdots \\ \sin \frac{q\pi \xi}{a} \sin \frac{\pi \varphi}{b} \sin \frac{2\pi \rho}{c} \\ \sin \frac{\pi \xi}{a} \sin \frac{2\pi \varphi}{b} \sin \frac{2\pi \rho}{c} \\ \sin \frac{2\pi \xi}{a} \sin \frac{2\pi \varphi}{b} \sin \frac{2\pi \rho}{c} \\ \vdots \\ \sin \frac{q\pi \xi}{a} \sin \frac{2\pi \varphi}{b} \sin \frac{2\pi \rho}{c} \\ \vdots \\ \sin \frac{\pi \xi}{a} \sin \frac{2\pi \varphi}{b} \sin \frac{m\pi \rho}{c} \\ \sin \frac{2\pi \xi}{a} \sin \frac{2\pi \varphi}{b} \sin \frac{m\pi \rho}{c} \\ \sin \frac{q\pi \xi}{a} \sin \frac{n\pi \varphi}{b} \sin \frac{m\pi \rho}{c} \end{bmatrix}, \tag{15}$$

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

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

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

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

to be an unknown vector with dimensions qnm .

Multiplying Eq. (16) by $\mathbf{Q}(x, y, z)$, and integrating it, we can acquire

$$\begin{aligned} & \alpha \int_0^c \int_0^b \int_0^a \mathbf{Q}(x, y, z) C(x, y, z, 0) dx dy dz \\ & + \int_0^c \int_0^b \int_0^a \mathbf{Q}(x, y, z) \mathbf{P}^T(x, y, z) dx dy dz \\ & \times \int_0^c \int_0^b \int_0^a \mathbf{Q}(\xi, \varphi, \rho) C(\xi, \varphi, \rho, 0) d\xi d\varphi d\rho \\ & = \int_0^c \int_0^b \int_0^a C_T(x, y, z) \mathbf{Q}(x, y, z) dx dy dz. \end{aligned} \quad (18)$$

By definition (17) we therefore have

$$\begin{aligned} & \left(\alpha \mathbf{I}_{mnq} + \int_0^c \int_0^b \int_0^a \mathbf{Q}(\xi, \varphi, \rho) \mathbf{P}^T(\xi, \varphi, \rho) d\xi d\varphi d\rho \right) \mathbf{c} \\ & := \int_0^c \int_0^b \int_0^a C_T(\xi, \varphi, \rho) \mathbf{Q}(\xi, \varphi, \rho) d\xi d\varphi d\rho, \end{aligned} \quad (19)$$

where \mathbf{I}_{mnq} denotes an identity matrix of order qnm . Solving Eq. (19) one has

$$\begin{aligned} \mathbf{c} = & \left(\alpha \mathbf{I}_{mnq} + \int_0^c \int_0^b \int_0^a \mathbf{Q}(\xi, \varphi, \rho) \mathbf{P}^T(\xi, \varphi, \rho) d\xi d\varphi d\rho \right)^{-1} \\ & \int_0^c \int_0^b \int_0^a C_T(\xi, \varphi, \rho) \mathbf{Q}(\xi, \varphi, \rho) d\xi d\varphi d\rho. \end{aligned} \quad (20)$$

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

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

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

$$\begin{aligned} & \alpha C(x, y, z, 0) = C_T(x, y, z) \\ & - \mathbf{P}(x, y, z) \cdot \left(\alpha \mathbf{I}_{mnq} + \int_0^c \int_0^b \int_0^a \mathbf{Q}(\xi, \varphi, \rho) \mathbf{P}^T(\xi, \varphi, \rho) d\xi d\varphi d\rho \right)^{-1} \\ & \quad \times \int_0^c \int_0^b \int_0^a C_T(\xi, \varphi, \rho) \mathbf{Q}(\xi, \varphi, \rho) d\xi d\varphi d\rho. \end{aligned} \quad (22)$$

Owing to the orthogonality of

$$\int_0^c \int_0^b \int_0^a \sin \frac{i\pi\xi}{a} \sin \frac{j\pi\xi}{a} \sin \frac{k\pi\xi}{a} \sin \frac{q\pi\varphi}{b} \sin \frac{m\pi\varphi}{b} \sin \frac{n\pi\varphi}{b} \sin \frac{r\pi\rho}{c} \sin \frac{s\pi\rho}{c} \sin \frac{w\pi\rho}{c} d\xi d\varphi d\rho = \frac{abc}{8} \delta_{ijk} \delta_{rsw}, \quad (23)$$

where δ_{ijk} , δ_{qmn} and δ_{rsw} are the Kronecker delta, the $qnm \times qnm$ matrix can be written as

$$\begin{aligned} & \int_0^c \int_0^b \int_0^a \mathbf{Q}(\xi, \varphi, \rho) \mathbf{P}^T(\xi, \varphi, \rho) d\xi d\varphi d\rho \\ = & \text{diag} \{ \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{111}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{211}^2]DT \}, \dots, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{q11}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{121}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{221}^2]DT \}, \dots, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{q21}^2]DT \}, \dots, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{1n1}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{2n1}^2]DT \}, \dots, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{qn1}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{112}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{212}^2]DT \}, \dots, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{q12}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{122}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{222}^2]DT \}, \dots, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{q22}^2]DT \}, \dots, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{12m}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{22m}^2]DT \}, \\ & \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{qnm}^2]DT \}, \end{aligned} \quad (24)$$

where diag means that the matrix is a diagonal matrix. Inserting Eq. (24) into Eq. (22), we thus acquire

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

$$\begin{aligned}
& -\frac{1}{\alpha} \mathbf{P}^T(x, y, z) \text{diag} \left[\frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{111}^2]DT \}} \right], \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{211}^2]DT \}}, \dots, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{q11}^2]DT \}}, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{121}^2]DT \}}, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{221}^2]DT \}}, \dots, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{q21}^2]DT \}}, \dots, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{1n1}^2]DT \}}, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{2n1}^2]DT \}}, \dots, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{qn1}^2]DT \}}, \dots, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{112}^2]DT \}}, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{212}^2]DT \}}, \dots, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{q12}^2]DT \}}, \dots, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{122}^2]DT \}}, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{222}^2]DT \}}, \dots, \\
& \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{q22}^2]DT \}}, \dots,
\end{aligned}$$

$$\left. \begin{aligned} & \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{12m}^2]DT \}} \\ & \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{22m}^2]DT \}} \\ & \frac{1}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + \rho_{qnm}^2]DT \}} \end{aligned} \right] \int_0^c \int_0^b \int_0^a C_T(\xi, \varphi, \rho) \mathbf{Q}(\xi, \varphi, \rho) d\xi d\varphi d\rho. \quad (25)$$

Using Eq. (15) for \mathbf{P} and \mathbf{Q} , we can attain

$$\begin{aligned} C(x, y, z, 0) &= \frac{1}{\alpha} C_T(x, y, z) - \frac{8}{\alpha abc} \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} \\ & \frac{\exp\{ -[(u^2 + v^2 + w^2)/4D^2 + (i\pi/a)^2 + (j\pi/b)^2 + (k\pi/c)^2]DT \}}{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + (i\pi/a)^2 + (j\pi/b)^2 + (k\pi/c)^2]DT \}} \\ & \times \int_0^c \int_0^b \int_0^a \sin \frac{i\pi x}{a} \sin \frac{i\pi \xi}{a} \sin \frac{j\pi y}{b} \sin \frac{j\pi \varphi}{b} \sin \frac{k\pi z}{c} \sin \frac{k\pi \rho}{c} \\ & \exp\{ [u(x - \xi) + v(y - \varphi) + w(z - \rho)]/2D \} C_T(\xi, \varphi, \rho) d\xi d\varphi d\rho, \end{aligned} \quad (26)$$

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

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

$$\begin{aligned} C^\alpha(x, y, z, t) &= \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} d_{ijk}^\alpha \\ & \exp\{ (ux + vy + wz)/2D - [(u^2 + v^2 + w^2)/4D^2 + (i\pi/a)^2 + (j\pi/b)^2 + (k\pi/c)^2]Dt \} \\ & \times \sin \frac{i\pi x}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c}, \end{aligned} \quad (27)$$

where

$$\begin{aligned} d_{ijk}^\alpha &= \frac{8}{abc} \int_0^c \int_0^b \int_0^a \exp[-(u\xi + v\varphi + w\rho)/2D] \\ & \sin \frac{i\pi \xi}{a} \sin \frac{j\pi \varphi}{b} \sin \frac{k\pi \rho}{c} C(\xi, \varphi, \rho, 0) d\xi d\varphi d\rho. \end{aligned} \quad (28)$$

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

$$d_{ijk}^\alpha =$$

8

$$abc\{\alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + (i\pi/a)^2 + (j\pi/b)^2 + (k\pi/c)^2]DT\}\} \\ \times \int_0^c \int_0^b \int_0^a \exp[(ux + vy + wz)/2D] \\ \sin \frac{i\pi\xi}{a} \sin \frac{j\pi\varphi}{b} \sin \frac{k\pi\rho}{c} C_T(\xi, \varphi, \rho) d\xi d\varphi d\rho. \quad (29)$$

Eqs. (27) and (29) compose an analytical solution of the three-dimensional BHCP. To discriminate it from the exact solution $C(x, y, z, t)$, we have utilized the symbol $C^\alpha(x, y, z, t)$ to denote that it is a regularization solution.

5 Selection of the regularization parameter α and numerical examples

Up to this point, we have not yet specified how to determine the regularization parameter α . Presume that f has the following Fourier sine series expansion:

$$C_T(x, y, z) = \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} d_{ijk}^* \sin \frac{i\pi x}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c}, \quad (30)$$

where

$$d_{ijk}^* = \frac{8}{abc} \int_0^c \int_0^b \int_0^a \sin \frac{i\pi\xi}{a} \sin \frac{j\pi\varphi}{b} \sin \frac{k\pi\rho}{c} C_T(\xi, \varphi, \rho) d\xi d\varphi d\rho \quad (31)$$

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

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

where we indicate that

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

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

For a better numerical solution, we require to set

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

On the other hand, the term $\exp\{ -[(u^2 + v^2 + w^2)/4D^2 + (q\pi/a)^2 + (n\pi/b)^2 + (m\pi/c)^2]DT\} / \{ \alpha + \exp\{ -[(u^2 + v^2 + w^2)/4D^2 + (q\pi/a)^2 + (n\pi/b)^2 + (m\pi/c)^2]DT\} \}$ in Eq. (32) will be very small when a, b, c, q, m, n and/or T are large, which may result in a large numerical error. Hence, we have a criterion to choose q, m and n when α and α_0 are clarified:

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

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

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

On the other hand, once q, m, n and α_0 are given, we can employ the following criterion to select α :

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

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:

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

where $C_T(x_i, y_j, z_k)$ is the exact data. We employ the function RANDOM_NUMBER given in Fortran to generate the noisy data $R(i, j, k)$, which are random numbers in $[-1, 1]$, and s denotes the level of noise. Then, the noisy data $\hat{C}_T(x_i, y_j, z_k)$ are used in the calculations. Usually, when the exact data are small, we utilize relative random noise to represent noise

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

where C_T^{max} is the maximum datum.

5.1 Example 1

Let us deliberate the first numerical experiment of three-dimensional BHCP:

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

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

$$\begin{aligned} & d_{ijk} \\ &= \frac{8}{abc} \int_0^c \int_0^b \int_0^a \exp[-(u\xi + v\varphi + w\rho)/2D] C(\xi, \varphi, \rho, 0) \\ & \quad \sin \frac{i\pi\xi}{a} \sin \frac{j\pi\varphi}{b} \sin \frac{k\pi\rho}{c} d\xi d\varphi d\rho \\ &= \frac{8}{abc} \int_0^{15} \int_0^{20} \int_{13.5}^{14.5} C_1 \exp[-(u\xi + v\varphi + w\rho)/2D] \\ & \quad \sin \frac{i\pi\xi}{a} \sin \frac{j\pi\varphi}{b} \sin \frac{k\pi\rho}{c} d\xi d\varphi d\rho \\ &= \frac{8}{abc} \left[\frac{e^{-14.5s}(-s \sin 14.5g - g \cos 14.5g) + e^{-13.5s}(s \sin 13.5g + g \cos 13.5g)}{s^2 + g^2} \right] \\ & \quad \times \left[\frac{e^{-20f}(-f \sin 20h - h \cos 20h) + h}{f^2 + h^2} \right] \times \left[\frac{e^{-15p}(-p \sin 15r - r \cos 15r) + r}{p^2 + r^2} \right], \quad (37) \end{aligned}$$

where

$$g = \frac{i\pi}{a}, h = \frac{j\pi}{b}, s = \frac{u}{2D}, f = \frac{v}{2D}, r = \frac{k\pi}{c}, p = \frac{w}{2D}. \quad (38)$$

Then, the data to be recovered are given by

$$\begin{aligned} & C(x, y, z, t) = \\ & \sum_{k=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} d_{ijk} \exp\{(ux + vy + wz)/2D - [(u^2 + v^2 + w^2)/4D^2 + (i\pi/a)^2 + (j\pi/b)^2] \end{aligned}$$

$$+(k\pi/c)^2]Dt\} \times \sin \frac{i\pi x}{a} \sin \frac{j\pi y}{b} \sin \frac{k\pi z}{c}, \quad (39)$$

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

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

For this example with $T = 2$, the comparisons of semi-analytical solutions and regularized solutions under $D = 2.8$, $u = 1$, and $v = 0$ were plotted in Fig. 1. Fig. 2 compares the semi-analytical solution with the regularized solution under $T = 100.5$, $D = 2.8$, $u = 1$, $v = 0$, $w = 0$, $\alpha_0 = 10^{-16}$, $\Delta x = 25/100$, $\Delta y = 20/100$, $\Delta z = 15/100$, $k = 50$ and $t = 0.5$. After viewing the output data, we discover that the corresponding mass and concentration peak errors are, respectively about $\epsilon_M = 0\%$ and $\epsilon_P = 0\%$ for $t = 1.8$ (Fig. 1), and $\epsilon_M = 0\%$ and $\epsilon_P = 0\%$ for $t = 0.5$ (Fig. 2), i.e., Fig. 2 displays 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

$$\epsilon_M = \frac{Mass^e - Mass^n}{Mass^e} \times 100\%; \quad (41)$$

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

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

where $\max(\)$ denotes the maximum value of $(\)$ for all grid points in the domain, and the superscript e and n stand for exact and numerical values, respectively. Besides, we employ this approach to estimate the stringent example with three velocities ($u = 1$, $v = 2$ and $w = 3$) of different directions and $T = 100.5$. From the output information of Fig. 3, we reveal that $\epsilon_M = 0\%$ and $\epsilon_P = 0\%$ for $t = 0.5$.

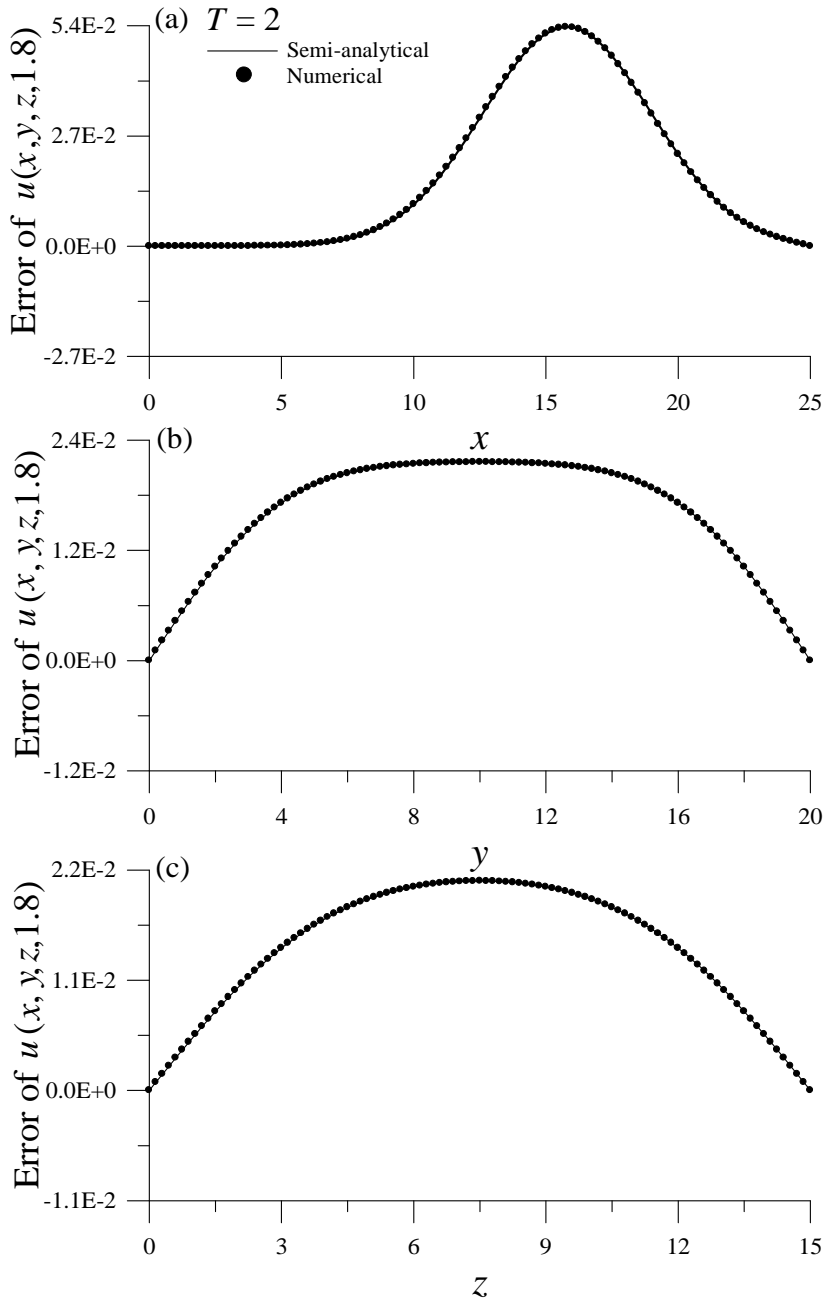


Figure 1: Comparisons of semi-analytical solutions and numerical solutions for homogeneous BADE problem with data at the time $t = 1.8$ been retrieved.

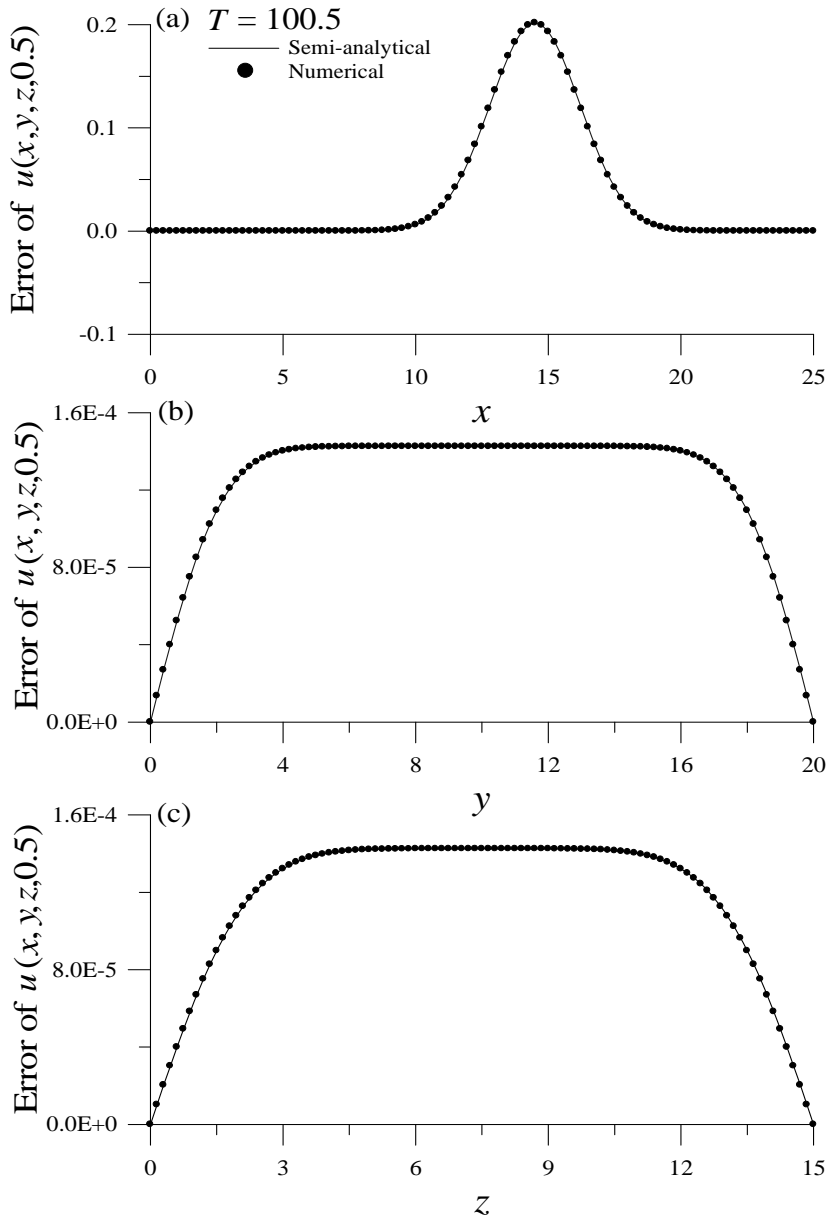


Figure 2: Comparisons of semi-analytical solutions and numerical solutions for homogeneous BADE problem with data at the time $t = 0.5$ been retrieved.

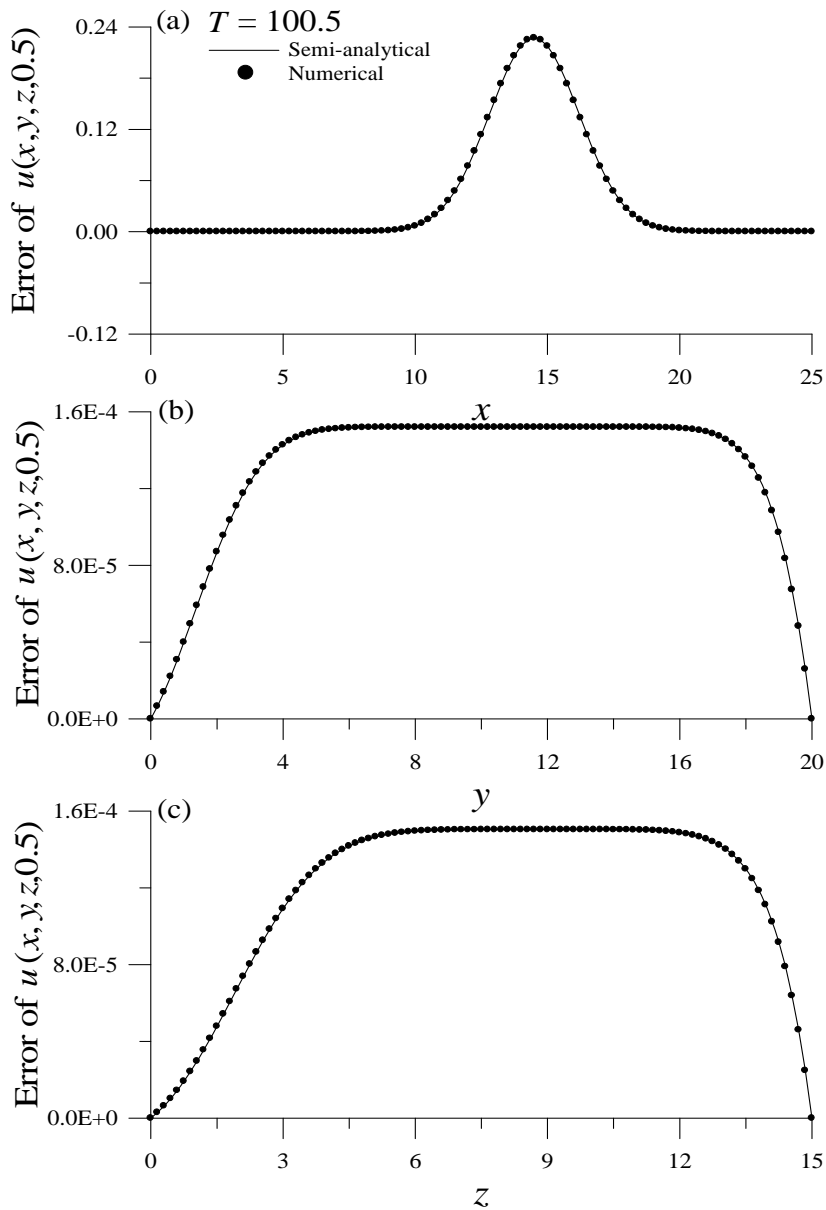


Figure 3: Comparisons of three different transport velocities of semi-analytical solutions and numerical solutions for homogeneous BADE problem with data at the time $t = 0.5$ been retrieved.

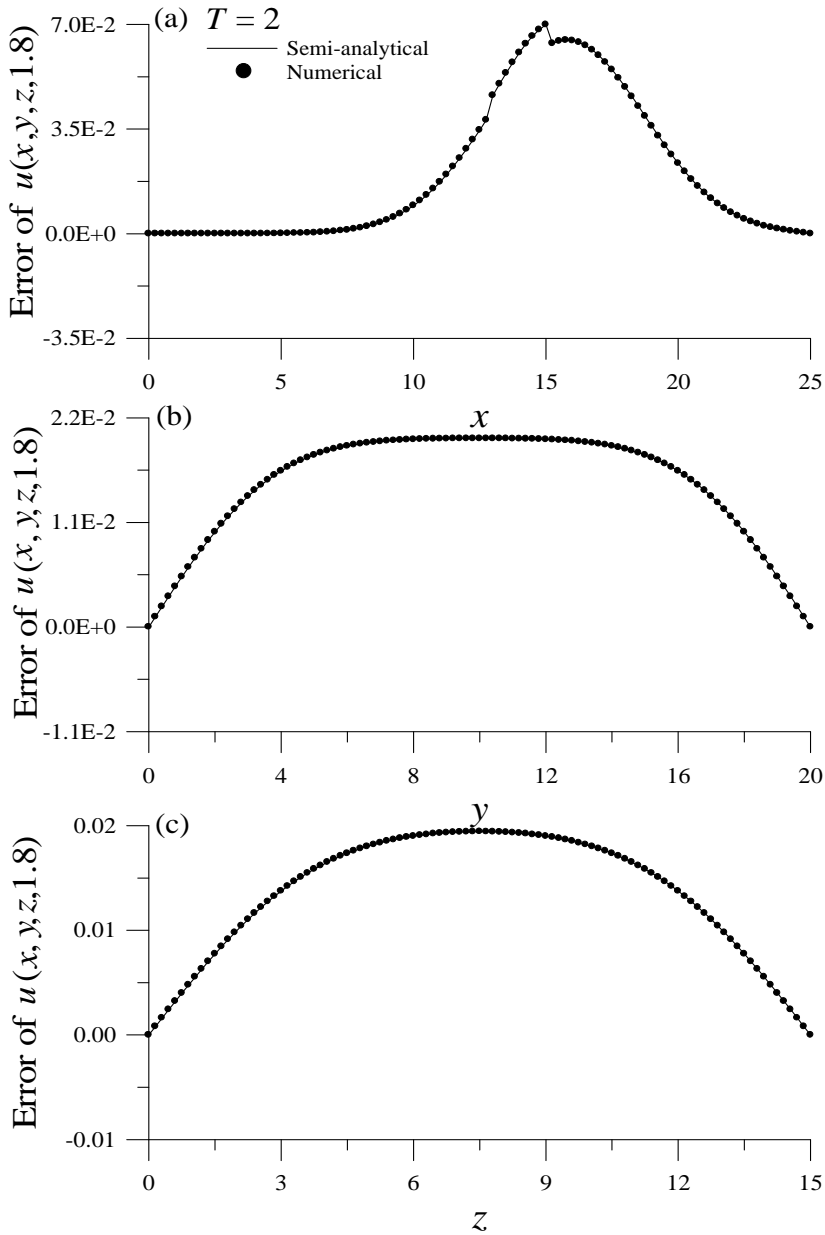


Figure 4: Comparisons of semi-analytical solutions and numerical solutions for configuration 1 with data at the time $t = 1.8$ been retrieved.

5.2 Numerical method for the heterogeneous ADE

Two situations involving heterogeneity in the dispersion coefficient D are to be analyzed. In configuration 1, the heterogeneous parameter case: the x -direction velocity is fixed to one, but the y -direction velocity and z -direction velocity are fixed to zero. Two different zones, each with a distinct value of D , are employed. For configuration 1, the two zones are (1) outer zones for $0 \leq x < 13$ and $15 < x \leq 25$, and (2) inner zone for $13 < x \leq 15$. Both configurations 1 and 2 use the same longitudinal range $0 \leq y \leq 20$ and the same vertical range $0 \leq z \leq 15$. The results in Fig. 4 are calculated by the new numerical approach with $T = 2$, $D_O = 2.4$, $D_i = 2.2$, $u = 1$, $v = 0$, $w = 0$, $\alpha_0 = 10^{-16}$, $\Delta x = 25/100$, $\Delta y = 20/100$, $\Delta z = 15/100$, $k = 50$ and $t = 1.8$, where accurate results are acquired. In Fig 5, the results are estimated by the new numerical scheme with $T = 100.5$, $D_O = 9.4$, $D_i = 1.2$, $u = 1$, $v = 2$, $w = 3$ and $t = 0.5$, where accurate results are obtained.

In configuration 2, the two zones are (1) outer zones for $0 \leq x < 7$ and $20 < x \leq 25$, and (2) inner zone for $7 < x \leq 20$. The results in Fig. 6 are estimated by the new numerical scheme with $T = 2$, $D_O = 2.4$, $D_i = 2.2$, $u = 1$, $v = 0$, $w = 0$, $\alpha_0 = 10^{-16}$, $\Delta x = 25/100$, $\Delta y = 20/100$, $\Delta z = 15/100$ and $t = 1.8$, where accurate results are attained. In Fig 7, the results are calculated by the new numerical approach with $T = 100.5$, $D_O = 9.4$, $D_i = 1.2$, $u = 1$, $v = 2$, $w = 3$ and $t = 0.5$, where accurate results are obtained. The mass and concentration peak errors of Figs. 1 to 7 induced by our scheme for the heterogeneous and homogeneous cases at $t = 1.8$ and $t = 0.5$ are very small near to zero. In addition, when the input final measured data are contaminated by random noise, we are interested in the stability of our method, which is investigated by adding the relative random noise on the final data. The numerical results with $T = 100.5$ were compared with those without considering random noise in Fig. 8(a)-(c) sequentially. Note that these different relative random noises s_r disturb the numerical solutions deviating from the semi-analytical solution very small. Furthermore, to the author's best knowledge, there has been no report that numerical approaches can calculate this ill-posed 3-D BADE very well as of our algorithm.

6 Conclusions

In this article, we have transformed the three-dimensional BADE into a second-kind three-dimensional Fredholm integral equation through a direct regularization concept and a quasi-boundary idea. By employing the Fourier series expansion technique and a termwise separable property of kernel function, a numerical solution of the regularized type for approximating the semi-analytical solution is illustrated. The influence of regularization parameter on the disturbed solution is

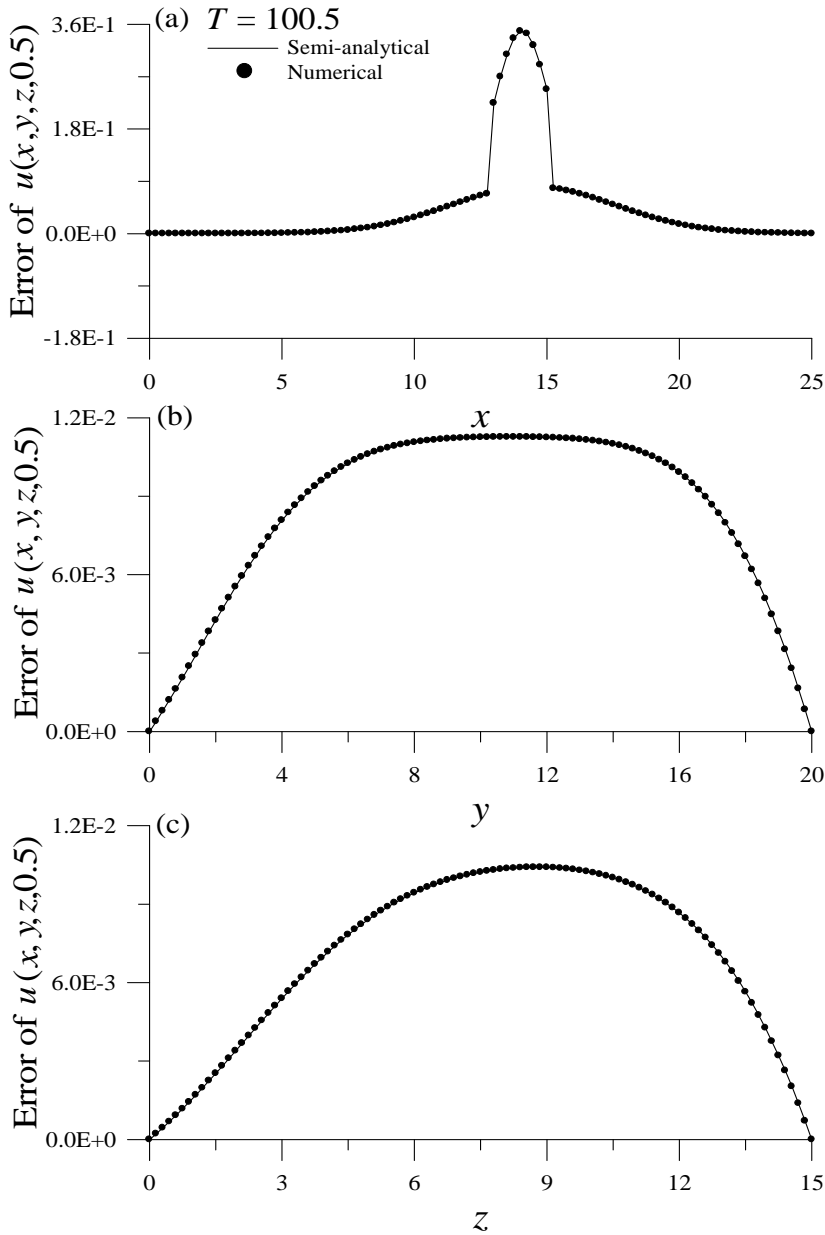


Figure 5: Comparisons of three different transport velocities of semi-analytical solutions and numerical solutions for configuration 1 with data at the time $t = 0.5$ been retrieved.

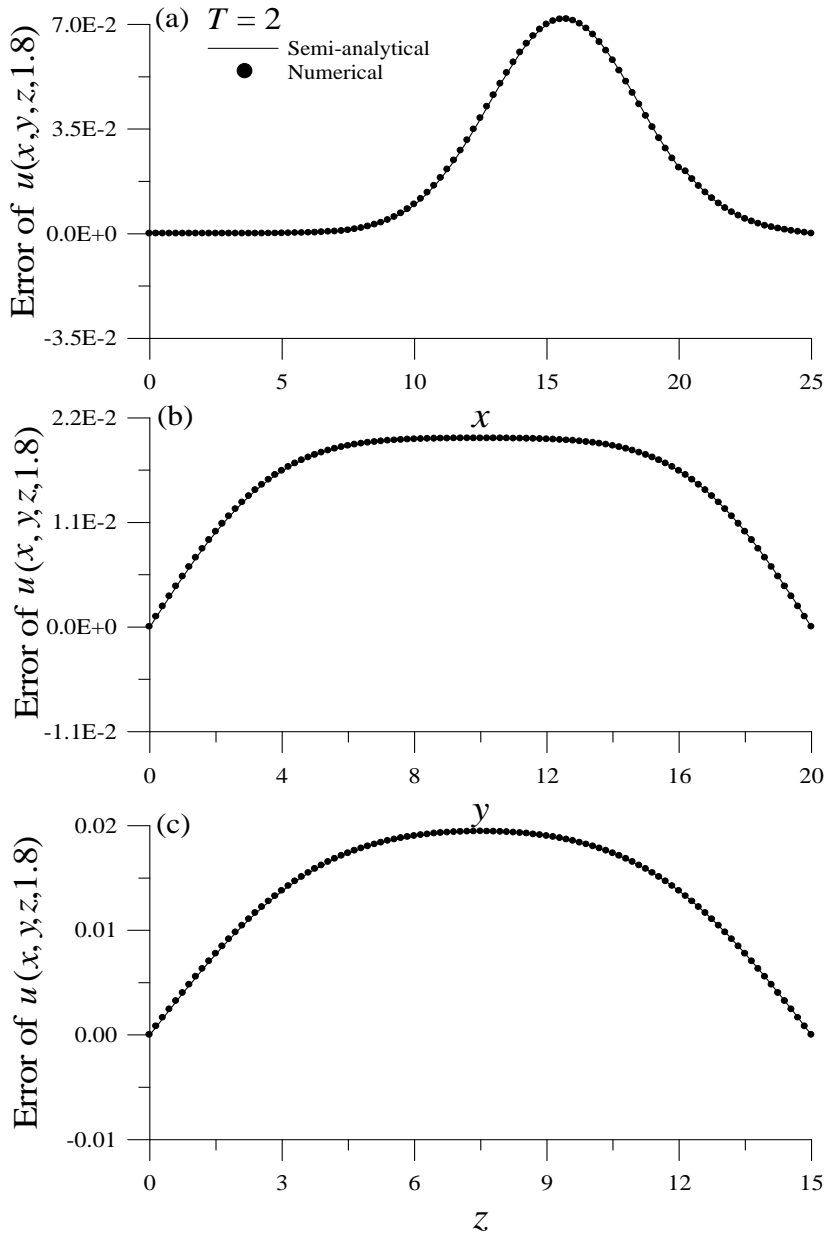


Figure 6: Comparisons of semi-analytical solutions and numerical solutions for configuration 2 with data at the time $t = 1.8$ been retrieved.

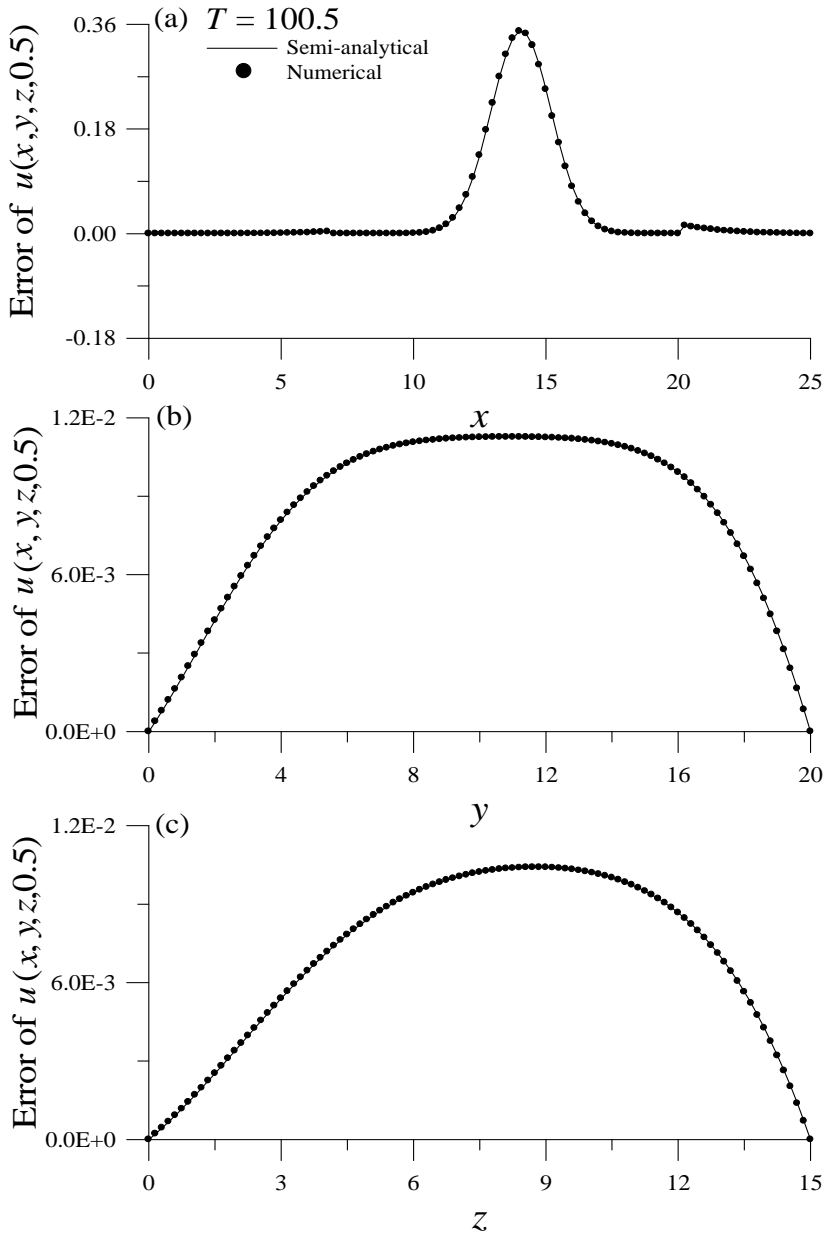


Figure 7: Comparisons of three different transport velocities of semi-analytical solutions and numerical solutions for configuration 2 with data at the time $t = 0.5$ been retrieved.

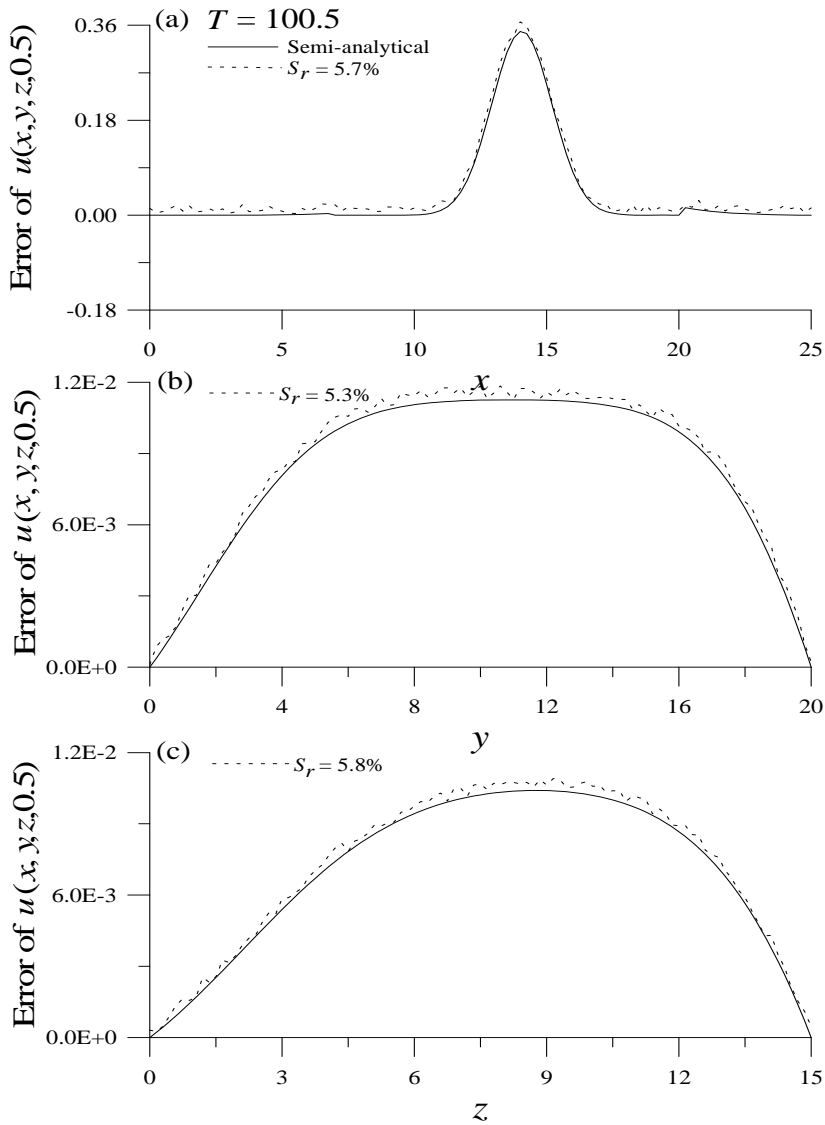


Figure 8: Comparisons of BADE solutions with and without random noise effect for configuration 2 are plotted in (a) with respect to x at fixed $y = 17$ and $z = 12$, and in (b) with respect to y at fixed $x = 21$ and $z = 12$, and in (c) with respect to z at fixed $x = 21$ and $y = 17$.

shown. Several numerical experiments have represented that the proposed scheme can retrieve all initial data very well, even though the final data are very small or noised by a large disturbance. Therefore, the present approach is advocated to deal with the three-dimensional BADE.

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