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A coefficient identification problem for a system of advection-reaction equations in water quality modeling ☆

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ABSTRACT

A coefficient identification problem (CIP) for a system of one-dimensional advection-reaction equations using boundary data is considered. The advection-reaction equations are used to describe the transportation of pollutants in rivers or streams. Stability for the considered CIP is proved using global Carleman estimates. The CIP is solved using the least-squares approach accompanied with the adjoint equation technique for computing the Fréchet derivatives of the objective functional. Lipschitz-type error estimates of the reconstructed coefficients are proved. Numerical tests are presented to illustrate the performance of the proposed algorithm.

1. Introduction

Several mathematical models have been developed for simulating water quality in rivers, streams, lakes, and estuaries [1]. In water quality management, these models can be used for policy making and enforcement. For example, in the planning phase of an economical development, water quality models can be used for simulating the effect of a new wastewater system on a local water system. The simulation enables policy makers to set water quality standards for the new wastewater system. In policy enforcement, these models may be used in the determination of pollution sources [2].

Dissolved oxygen (DO) and biochemical oxygen demand (BOD) are among the most important water quality indicating factors. DO is the amount of oxygen present in a unit volume of water. Maintaining a sufficient level of DO is critical for the preservation of the aquatic ecosystem in rivers and lakes. DO in water is affected by several biological and chemical processes. While photosynthesis and oxygen diffusion from air (superficial reaeration) increases the DO in water, organic waste is the primary factor which reduces the DO in water. The term BOD is used to quantitatively describe the amount of DO per unit volume required to decompose organic waste [2–4,1]. That is, the BOD can be used as an indicator of water pollution.

One of the earliest water quality model was developed by Streeter and Phelps for the Ohio River in 1925 [5]. They proposed a one-dimensional (1-d) steady-state model which describes the DO and BOD along a river section. The model was later extended to include the time-dependent DO and BOD, see, e.g., [6,7,1,8]. More complex models, such as QUAL2E [9] or WASP [10], include more state variables such as ammonia, nitrites, nitrates, organic nitrogen, organic phosphorus, and orthophosphates.

The extended non-dispersive Streeter-Phelps model is described by the following advection-reaction equations [2,1,8]

$$\frac{\partial b(x,t)}{\partial t} + v(x,t)\frac{\partial b(x,t)}{\partial x} = -k_d(x)b(x,t) + s(x,t), \tag{1}$$

$$\frac{\partial d(x,t)}{\partial t} + v(x,t)\frac{\partial d(x,t)}{\partial x} = k_d(x)b(x,t) - k_r(x)d(x,t), \tag{2}$$

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for $(x,t) \in Q := (0,L) \times (0,T)$, where $b(x,t)$ and $d(x,t)$ are the BOD and DO, respectively; $v(x,t)$ is the water velocity; $k_d(x)$ and $k_r(x)$ are the deoxygenation and reaeration coefficients, respectively; and $s(x,t)$ represents the sources of BOD, i.e., pollution sources. We note that although equation (1) is independent of (2), it describes the relation between the pollution source, represented by $s(x,t)$, and DO data. In this paper, we assume that the coefficients k_d and k_r vary in space but are independent of time. In addition, the water is assumed to flow in only one direction, that means, the velocity $v(x,t)$ does not change sign in Q. Without loss of generality, we assume that $v(x,t) > 0$ for all $(x,t) \in Q$. The above equations are coupled with the following initial and boundary conditions:

$$b(x,0) = f_b(x); \quad d(x,0) = f_d(x), \tag{3}$$

$$b(0,t) = g_b(t); \quad d(0,t) = g_d(t), \tag{4}$$

where f_b, f_d, g_b, and g_d are given functions.

We note that the above model neglects the dispersion of DO and BOD. Some analyses concerning the validity of this non-dispersive model have been carried out in the literature, see e.g., [11,1,12]. The common qualitative conclusion from these analyses is that the dispersion is negligible if the water velocity is large enough, which is usually the case for rivers and streams. In contrast, the dispersion may dominate the advection of pollution in lakes and estuaries subject to tidal action [13].

The biggest challenge in using water quality models in practice is that their parameters may vary greatly from one river to another. Even for a river, these parameters may depend on weather and hydraulic conditions. As a result, using these models requires a time-consuming parameter selection procedure. For model (1)–(4), while the velocity v is usually computed using hydraulic model described by the so-called Saint-Venant equation [2,1], the space-dependent coefficients $k_d(x)$ and $k_r(x)$ are much harder to model or choose. Although there are some empirical formulas for the coefficient k_r proposed in the literature (see, e.g., [14], chapter 10), a systematic approach for estimating k_d and k_r from in-situ measurements has not been considered. Therefore, in this work we propose a method for automatically estimating the parameters $k_d(x)$ and $k_r(x)$ from DO and BOD data measured at the downstream boundary $x = L$. Let $k_d^*(x)$ and $k_r^*(x)$ be the exact coefficients to be determined and $(b^*(x,t), d^*(x,t))$ be the corresponding solution of the forward problem. Suggested by the stability estimates for the coefficients k_d and k_r (see Theorem 3.2 below), we assume that we know two functions $\theta_b(t)$ and $\theta_d(t)$ such that

$$\|\theta_b(t) - \frac{\partial b^*(L,t)}{\partial t}\|_{L^2(0,T)} \le \delta, \quad \|\theta_d(t) - \frac{\partial d^*(L,t)}{\partial t}\|_{L^2(0,T)} \le \delta, \tag{5}$$

where δ is a positive constant representing the measurement error.

The CIP of determining the coefficients k_d and k_r from the above boundary BOD and DO data is stated as follows.

Problem 1. Assume that the functions v, s, f_b, f_d, g_b, and g_d are given. Determine $k_d(x)$ and $k_r(x)$ in model (1)–(4) given the functions θ_b and θ_d.

If noisy measurements of $b^*(L,t)$ and $d^*(L,t)$ are given instead of the above data, numerical differentiation methods can be used to approximate $\frac{\partial b^*(L,t)}{\partial t}$ and $\frac{\partial d^*(L,t)}{\partial t}$. However, error bounds of the form (5) can only be proved under additional conditions on the smoothness of the functions b^* and d^*. We do not discuss this issue in this paper.

Contributions of this paper are as follows. First, we prove stability estimates for the coefficients k_d and k_r using a global Carleman estimate. For similar CIPs for first-order scalar hyperbolic equations, stability results have been obtained in [15–18] and a uniqueness result was proved in [19]. We note that if the velocity $v(x,t)$ does not depend on time, stability estimates for k_d and k_r from boundary data of both b and d can be obtained by converting (1) and (2) into Volterra integral equations of second kind (see more details in Remark 3.4). To the best of our knowledge, stability results for the system of the form (1)–(2) with velocity varying with space and time have not been reported in the literature. Second, we prove error estimates of Lipschitz type for the solution of Problem 1 using the least-squares minimization method. The adjoint equation approach is used for computing the gradient of the discretized objective functional. We use the quasi-Newton's method for solving the resulting minimization problem.

The rest of the paper is organized as follows. Section 2 presents some energy estimates for the solution of the forward problem (1)–(2). In Section 3 we state and prove stability estimates for Problem 1. In Section 4 we present the least-squares method for solving the inverse problem, prove error estimates, and derive the gradient of the corresponding objective functional. In Section 5 we show numerical examples to illustrate its performance. Conclusions are drawn in Section 6.

2. Energy estimates for the forward problem

For mathematical analyses, we need the following assumption.

Assumption 1.

1. The velocity function $v(x,t)$ is bounded and continuously differentiable in Q and there are positive constants v_0, v_1 such that $v(x,t) \ge v_0 > 0$ and
$$\max_{(x,t)\in\overline{Q}} \left\{ |v(x,t)|, \left|\frac{\partial v(x,t)}{\partial t}\right|, \left|\frac{\partial v(x,t)}{\partial x}\right| \right\} \le v_1.$$
2. The coefficients $k_d(x)$ and $k_r(x)$ are non-negative and belong to $L^2(0,L) \cap L^\infty[0,L]$.
3. The functions $f_b(x)$, $f_d(x)$ belong to $H^1(0,L)$ and $g_b(t)$, $g_d(t)$ belong to $H^1(0,T)$. Moreover, they are consistent, i.e., $f_b(0) = g_b(0)$ and $f_d(0) = g_d(0)$.

Remark 2.1. Assumption 1 is based on physical reasons. For example, if the river flows in one direction only, the velocity does not change sign. Moreover, if there are no shocks in the water flow, the assumption about the boundedness of the partial derivatives of $v(x,t)$ is also reasonable. The other functions listed in Assumption 1 represent physical quantities, which should be bounded.

To simplify notation, we rewrite model (1)–(4) in the following vector form:

$$\begin{cases} \dfrac{\partial \mathbf{p}}{\partial t} + v(x,t)\dfrac{\partial \mathbf{p}}{\partial x} + K(x)\mathbf{p} = \mathbf{s}(x,t), \ (x,t) \in Q, \\ \mathbf{p}(x,0) = \mathbf{p}_i(x), \quad x \in [0,L], \\ \mathbf{p}(0,t) = \mathbf{p}_0(t), \quad t \in [0,T], \end{cases} \tag{6}$$

where $\mathbf{p} = [b,d]^T$ and the vector-valued functions $\mathbf{p}_i(x) = [f_b(x), f_d(x)]^T$, $\mathbf{p}_0(t) = [g_b(t), g_d(t)]^T$, and $\mathbf{s}(x,t) = [s(x,t), 0]^T$ represent the initial condition, the boundary condition at $x = 0$, and the source term, respectively. The matrix K is given by

$$K(x) = \begin{bmatrix} k_d(x) & 0 \\ -k_d(x) & k_r(x) \end{bmatrix}.$$

We introduce the L^2-norm of $\mathbf{p}$ as

$$\|\mathbf{p}\|_{L^2(Q)} := \left[\|b\|^2_{L^2(Q)} + \|d\|^2_{L^2(Q)}\right]^{1/2}.$$

As in [16], we assume that problem (6) has a solution $\mathbf{p} \in \mathbb{H}^2$, where

$$\mathbb{H} := H^1(0,T;H^1(0,L)) \cap H^2(0,T;L^2(0,L)).$$

Then $\mathbf{p}$ satisfies the following energy estimates.

Lemma 2.1. *Let $\mathbf{p} \in \mathbb{H}^2$ be a solution of (6).*

1. *Assume that $\mathbf{s}$ belongs to $[L^2(Q)]^2$. Then, there exists a constant $C^* > 0$ depending on T, L, v and K only such that*

$$\|\mathbf{p}\|^2_{L^2(Q)} \le C^* \left[\|\mathbf{p}_i\|^2_{L^2(0,L)} + \|\mathbf{p}_0\|^2_{L^2(0,T)} + \|\mathbf{s}\|^2_{L^2(Q)}\right]. \tag{7}$$

2. *Assume that $\frac{\partial \mathbf{s}}{\partial t}$ belongs to $[L^2(Q)]^2$. Then, there exists a constant $C^{**} > 0$ depending on T, L, v and K only such that for all $t \in [0,T]$ we have*

$$\begin{aligned} &\left\|\frac{\partial \mathbf{p}}{\partial t}(\cdot,t)\right\|^2_{L^2(0,L)} \\ &\le C^{**}\left[\|\mathbf{p}_i\|^2_{H^1(0,L)} + \left\|\frac{\partial \mathbf{p}_0}{\partial t}\right\|^2_{L^2(0,L)} + \|\mathbf{s}(\cdot,0)\|^2_{L^2(0,L)} + \left\|\frac{\partial \mathbf{s}}{\partial t}\right\|^2_{L^2(Q)}\right]. \end{aligned} \tag{8}$$

Proof. To prove (7), we multiply $2\mathbf{p}^T$ to both sides of the first equation of (6) and integrate the result over $[0,L]$. We obtain

$$\int_0^L 2\mathbf{p}^T \frac{\partial \mathbf{p}}{\partial t} dx + \int_0^L 2v(x,t)\mathbf{p}^T \frac{\partial \mathbf{p}}{\partial x} dx + \int_0^L 2\mathbf{p}^T K\mathbf{p} dx = \int_0^L 2\mathbf{p}^T \mathbf{s} dx.$$

Since $2\mathbf{p}^T \frac{\partial \mathbf{p}}{\partial t} = \frac{\partial |\mathbf{p}|^2}{\partial t}$ and $2\mathbf{p}^T \frac{\partial \mathbf{p}}{\partial x} = \frac{\partial |\mathbf{p}|^2}{\partial x}$, we have

$$\frac{d}{dt}\int_0^L |\mathbf{p}|^2 dx + \int_0^L v(x,t)\frac{\partial |\mathbf{p}|^2}{\partial x} dx + \int_0^L 2\mathbf{p}^T K\mathbf{p} dx = \int_0^L 2\mathbf{p}^T \mathbf{s} dx.$$

Applying the integration by parts to the second term and the Cauchy-Schwarz inequality to the last term, we have

$$\begin{aligned} \frac{d}{dt}\int_0^L |\mathbf{p}|^2 dx &= -\left[v(L,t)|\mathbf{p}(L,t)|^2 - v(0,t)|\mathbf{p}(0,t)|^2 - \int_0^L \frac{\partial v}{\partial x}(x,t)|\mathbf{p}(x,t)|^2 dx\right] \\ &\quad - \int_0^L 2\mathbf{p}(x,t)^T K(x)\mathbf{p}(x,t) dx + \int_0^L 2\mathbf{p}(x,t)^T \mathbf{s}(x,t) dx. \\ &\le v(0,t)|\mathbf{p}_0(t)|^2 + \int_0^L \frac{\partial v}{\partial x}(x,t)|\mathbf{p}|^2 dx - \int_0^L 2\mathbf{p}(x,t)^T K(x)\mathbf{p}(x,t) dx \\ &\quad + \int_0^L |\mathbf{p}(x,t)|^2 dx + \int_0^L |\mathbf{s}(x,t)|^2 dx. \end{aligned} \tag{9}$$

It follows from Assumption 1 that there exists a constant C depending only on L, v_1, and K such that

$$\int_0^L \frac{\partial v}{\partial x}(x,t)|\mathbf{p}|^2 dx - \int_0^L 2\mathbf{p}^T K\mathbf{p} dx + \int_0^L |\mathbf{p}|^2 dx \le C\int_0^L |\mathbf{p}|^2 dx.$$

Substituting this inequality into (9), we obtain

$$\frac{d}{dt}\int_0^L |\mathbf{p}|^2 dx \le C\int_0^L |\mathbf{p}|^2 dx + v(0,t)|\mathbf{p}_0(t)|^2 + \int_0^L |\mathbf{s}|^2 dx.$$

Using Grönwall's inequality, we have

$$\begin{aligned}&\int_0^L |\mathbf{p}(x,t)|^2 dx\\ &\le e^{Ct}\left\{\int_0^L |\mathbf{p}(x,0)|^2 dx + \int_0^t\left[v(0,\tau)|\mathbf{p}_0(\tau)|^2 + \int_0^L |\mathbf{s}(x,\tau)|^2 dx\right]e^{-C\tau}d\tau\right\}\\ &\le e^{Ct}\left\{\|\mathbf{p}_i\|^2_{L^2(0,L)} + v_1\|\mathbf{p}_0\|^2_{L^2(0,T)} + \|\mathbf{s}\|^2_{L^2(Q)}\right\}.\end{aligned}$$

Integrating both sides over $[0,T]$, we obtain the estimate (7).

To prove (8), we first differentiate both sides of the first equation of (6) (this can be done since $\mathbf{p}\in\mathbb{H}^2$). Then, multiplying $2\frac{\partial \mathbf{p}^T}{\partial t}$ to both sides of the resulting equation, we have

$$\int_0^L 2\frac{\partial \mathbf{p}^T}{\partial t}\frac{\partial^2 \mathbf{p}}{\partial t^2}dx + \int_0^L 2v(x,t)\frac{\partial \mathbf{p}^T}{\partial t}\frac{\partial^2 \mathbf{p}}{\partial t\partial x}dx + \int_0^L 2\frac{\partial \mathbf{p}^T}{\partial t}K\frac{\partial \mathbf{p}}{\partial t}dx = \int_0^L 2\frac{\partial \mathbf{p}^T}{\partial t}\frac{\partial \mathbf{s}}{\partial t}dx.$$

Using similar manipulations as in the proof of the first part, we can show that

$$\|\frac{\partial \mathbf{p}(\cdot,t)}{\partial t}\|^2_{L^2(0,L)} \le e^{Ct}\left\{\|\frac{\partial \mathbf{p}(\cdot,0)}{\partial t}\|^2_{L^2(0,L)} + v_1\|\frac{\partial \mathbf{p}_0}{\partial t}\|^2_{L^2(0,T)} + \|\frac{\partial \mathbf{s}}{\partial t}\|^2_{L^2(Q)}\right\}, \tag{10}$$

where C is the same constant as above. Since $\mathbf{p}\in\mathbb{H}$, $\frac{\partial \mathbf{p}}{\partial t}$ is continuous with respect to t up to $t=0$ due to the Rellich-Kondrachov Theorem (see, e.g., chapter 6 of [20]). Hence, we can take the limit of the first equation of (6) when $t\to 0$ to obtain

$$\frac{\partial \mathbf{p}(x,0)}{\partial t} = -v(x,0)\frac{\partial \mathbf{p}_i(x)}{\partial x} - K(x)\mathbf{p}_i(x) - \mathbf{s}(x,0).$$

Hence,

$$\|\frac{\partial \mathbf{p}(\cdot,0)}{\partial t}\|^2_{L^2(0,L)} \le \tilde{C}\left[\|\mathbf{p}_i\|^2_{H^1(0,L)} + \|\mathbf{s}(\cdot,0)\|^2_{L^2(0,L)}\right], \tag{11}$$

where $\tilde{C}$ is a positive constant depending only on v_1 and K. Inequality (8) follows from (10) and (11). The proof is complete. □

The following energy estimate for the scalar case is also needed in the proof of the stability estimates presented in the next section.

Lemma 2.2. *Let $k(x)$ be a function in the same space as k_d and k_r. Assume that $z(x,t)\in\mathbb{H}$ is a solution of the problem*

$$\begin{cases}\frac{\partial z}{\partial t} + v(x,t)\frac{\partial z}{\partial x} + kz = f(x)r(x,t), & (x,t)\in Q,\\ z(0,t)=0, & t\in[0,T],\\ z(x,0)=0, & x\in[0,L],\end{cases} \tag{12}$$

where $r(x,t)$ satisfies

$$\max_{(x,t)\in\overline{Q}}\left\{\left|\frac{\partial r}{\partial t}(x,t)\right|, |r(x,0)|\right\} \le E,$$

where E is a given constant. Then there exists a constant $\bar{C}>0$ depending only on $T,\ L,\ v,\ k$, and E such that

$$\int_0^L\left(\left|\frac{\partial z}{\partial t}\right|^2 + z^2\right)dx \le \bar{C}\int_0^L |f|^2 dx.$$

Since Lemma 2.2 is a special case of Lemma 2.1, we do not repeat the proof here. Also, see the proof of Lemma 3.4 of [16].

3. Stability analysis for Problem 1 using global Carleman estimates

In this section we state and prove stability estimates for both $k_d(x)$ and $k_r(x)$. These estimates are based on a global Carleman estimate. Using Carleman estimates in analyzing the uniqueness and stability of inverse problems has been extensively discussed in the last few decades, see e.g., [21,22]. The results we obtain here are similar to that of [18]. However, in [18] only a scalar equation was considered. Since in (2) both k_d and k_r are involved, the stability estimate for k_r is more complicated than that of the case considered in [18].

In addition to Assumption 1, we also need the following property in the stability estimates.

Assumption 2. There exists a positive constant ρ such that $f_b(x)\ge\rho$ and $f_d(x)\ge\rho>0$ for all $x\in[0,L]$.

We note that Assumption 2 is commonly used in deriving Carleman estimates, see e.g., [16,18,19].

3.1. Carleman estimate

Let $\sigma,\ \alpha,\ \beta,\ C_0$ be positive constants satisfying the following conditions

$$C_0 - \beta T > 0, \quad \alpha L < \beta T, \quad \alpha v_0 - \beta \geq \sigma. \tag{13}$$

In the following, we define the Carleman weight function $\varphi(x,t)$ as:

$$\varphi(x,t) := \alpha x - \beta t + C_0. \tag{14}$$

Remark 3.1. We note that if T is large enough, the existence of the positive constants $\sigma,\ \alpha,\ \beta,\ C_0$ satisfying conditions (13) holds. Indeed, if T satisfies the condition that $T > L/v_0$, then there exists a constant α satisfying $\beta/v_0 < \alpha < \beta T/L$. In this case, the second inequality in (13) is satisfied. The first and the third inequalities in (13) are satisfied for $0 < \sigma < \alpha v_0 - \beta$ and $C_0 > \beta T$.

From (13), we have $\varphi(x,t) \geq 0$ for all $(x,t) \in Q$. Let $\mathbb{L}$ be the operator defined by $\mathbb{L}z := \dfrac{\partial z}{\partial t} + v(x,t)\dfrac{\partial z}{\partial x}$ for $z \in H^1(Q)$. From condition (13) it follows that

$$\mathbb{L}\varphi = \frac{\partial \varphi}{\partial t} + v(x,t)\frac{\partial \varphi}{\partial x} = -\beta + \alpha v \geq \sigma. \tag{15}$$

Remark 3.2. From here on, in our proofs we will denote generic constants by $C,\ C_r,\ C_1, C_2, \ldots$ which depend only on the known parameters $\alpha, \beta, C_0, T, L, \sigma, v_1, \rho$ and E.

In this section, we need the following Carleman estimate.

Lemma 3.1. *Let $z(x,t)$ be a function in $H^1(Q)$ such that $z(0,t) = 0,\ t \in [0,T]$. Then there exists a constant $C_1 > 0$ such that for $s > 0$ large enough the following inequality holds:*

$$\begin{aligned}
& s^2 \int_0^T \int_0^L e^{2s\varphi(x,t)} z^2 dx dt + s \int_0^L e^{2s\varphi(x,0)} z^2(x,0) dx \\
& \leq C_1 \int_0^T \int_0^L e^{2s\varphi(x,t)} |\mathbb{L}z|^2 dx dt + C_1 s \int_0^T e^{2s\varphi(L,t)} z^2(L,t) dt \\
& \quad + C_1 s \int_0^L e^{2s\varphi(x,T)} z^2(x,T) dx,
\end{aligned} \tag{16}$$

with the Carleman weight function φ defined by (14).

Proof. The Carleman estimate (16) is rather standard and its proof follows the same technique as that used in the literature. For example, see Lemma 1 in [18] for a similar Carleman estimate. However, in (16) the condition on function z is different from that in [18]. Therefore, the proof is slightly different. For the convenience of the reader, we prove (16) here.

Let $w = e^{s\varphi} z$ and $Pw = e^{s\varphi}\mathbb{L}(e^{-s\varphi} w)$, we have

$$Pw = \left(\frac{\partial w}{\partial t} + v\frac{\partial w}{\partial x}\right) - sw\left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right). \tag{17}$$

Therefore,

$$\begin{aligned}
& \int_0^T \int_0^L |Pw|^2 dx dt \\
& = \int_0^T \int_0^L \left(\frac{\partial w}{\partial t} + v\frac{\partial w}{\partial x}\right)^2 dx dt + s^2 \int_0^T \int_0^L w^2 \left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right)^2 dx dt \\
& \quad - 2s \int_0^T \int_0^L \left(\frac{\partial w}{\partial t} + v\frac{\partial w}{\partial x}\right)\left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right) w dx dt \\
& \geq \sigma^2 s^2 \int_0^T \int_0^L w^2 dx dt - 2s \int_0^T \int_0^L \left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right) w \frac{\partial w}{\partial t} dx dt \\
& \quad - 2s \int_0^T \int_0^L v \left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right) w \frac{\partial w}{\partial x} dx dt
\end{aligned}$$

$$\geq \sigma^2 s^2 \int_0^T \int_0^L w^2 dxdt - s \int_0^L \left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right) w^2\Big|_{t=T} dx$$
$$+ s \int_0^L \left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right) w^2\Big|_{t=0} dx - s \int_0^T v \left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right) w^2\Big|_{x=L} dt$$
$$+ s \int_0^T \int_0^L \left[\frac{\partial}{\partial x}\left(v\left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right)\right) + \frac{\partial}{\partial t}\left(\left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right)\right)\right] w^2 dxdt.$$

From Assumptions 1 and 2 and (14), with $s > s_0$ large enough, there exist constants $C_2, C_3 > 0$ such that

$$\int_0^T \int_0^L |Pw|^2 dxdt$$
$$\geq C_2 s^2 \int_0^T \int_0^L w^2 dxdt - s \int_0^L \left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right) w^2\Big|_{t=T} dx$$
$$+ s \int_0^L \left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right) w^2\Big|_{t=0} dx - s \int_0^T v \left(\frac{\partial \varphi}{\partial t} + v\frac{\partial \varphi}{\partial x}\right) w^2\Big|_{x=L} dt$$
$$\geq C_2 s^2 \int_0^T \int_0^L w^2 dxdt - C_3 s \int_0^L w^2(x,T) dx$$
$$+ \sigma s \int_0^L w^2(x,0) dx - C_3 s \int_0^T w^2(L,t) dt.$$

Therefore,

$$C_2 s^2 \int_0^T \int_0^L w^2 dxdt + \sigma s \int_0^L w^2(x,0) dx \leq \int_0^T \int_0^L |Pw|^2 dxdt + C_3 s \int_0^T w^2(L,t) dt$$
$$+ C_3 s \int_0^L w^2(x,T) dx. \tag{18}$$

Hence, the lemma is proved. □

3.2. Stability estimates for $k_d(x)$ and $k_r(x)$

Theorem 3.2. *Assume that Assumptions 1 and 2 are satisfied. Let (b_j, d_j) be the solution of the forward problem (1)–(4) with coefficients $k_d := k_{dj}$ and $k_r := k_{rj}$, $j = 1,2$. Assume that the following condition is satisfied:*

$$\max_{(x,t)\in\overline{Q}} \left\{\left|\frac{\partial b_2}{\partial t}\right|, \left|\frac{\partial d_2}{\partial t}\right|\right\} \leq E, \quad \max_{x\in[0,L]} \{|k_{d1}(x)|, |k_{r1}(x)|\} \leq E. \tag{19}$$

Then there exist positive constants C_d and C_r depending only on the given input functions and constant E such that

$$\int_0^L (k_{d2} - k_{d1})^2 dx \leq C_d \int_0^T \left|\frac{\partial b_1}{\partial t}(L,t) - \frac{\partial b_2}{\partial t}(L,t)\right|^2 dt \tag{20}$$

and

$$\int_0^L (k_{r2} - k_{r1})^2 dx \leq C_r \int_0^T \left|\frac{\partial b_1}{\partial t}(L,t) - \frac{\partial b_2}{\partial t}(L,t)\right|^2 dt$$
$$+ C_r \int_0^T \left|\frac{\partial d_1}{\partial t}(L,t) - \frac{\partial d_2}{\partial t}(L,t)\right|^2 dt. \tag{21}$$

Proof. It is clear that the function $u := b_1 - b_2$ satisfies the following problem:

$$\frac{\partial u}{\partial t} + v(x,t)\frac{\partial u}{\partial x} + k_{d1} u = (k_{d2} - k_{d1}) b_2, \ (x,t) \in Q, \tag{22}$$
$$u(0,t) = 0, \ t \in [0,T], \tag{23}$$
$$u(x,0) = 0, \ x \in [0,L]. \tag{24}$$

Differentiating (22)–(24) with respect to t and setting $z := u_t$, we obtain

$$\frac{\partial z}{\partial t} + v(x,t)\frac{\partial z}{\partial x} + \frac{\partial v(x,t)}{\partial t}\frac{\partial u}{\partial x} + k_{d1} z = (k_{d2} - k_{d1})\frac{\partial b_2}{\partial t}, \ (x,t) \in Q, \tag{25}$$

$$z(0,t) = 0, \ t \in [0,T], \tag{26}$$

$$z(x,0) = (k_{d2} - k_{d1}) f_b(x), \ x \in [0,L]. \tag{27}$$

By Lemma 3.1, there exists a constant C_6 such that

$$\begin{aligned} &s^2 \int_0^T \int_0^L e^{2s\varphi(x,t)} z^2 dxdt + s\int_0^L e^{2s\varphi(x,0)} (k_{d2} - k_{d1})^2 f_b^2(x) dx \\ &\le C_6 \int_0^T \int_0^L e^{2s\varphi(x,t)} |\mathbb{L}z|^2 dxdt + C_6 s \int_0^T e^{2s\varphi(L,t)} z^2(L,t) dt \\ &\quad + C_6 s \int_0^L e^{2s\varphi(x,T)} z^2(x,T) dx. \end{aligned} \tag{28}$$

Since $f_b(x) \ge \rho$ for all $x \in [0,L]$, it implies from (28) that

$$\begin{aligned} &s^2 \int_0^T \int_0^L e^{2s\varphi(x,t)} z^2 dxdt + \rho^2 s\int_0^L e^{2s\varphi(x,0)} (k_{d2} - k_{d1})^2 dx \\ &\le C_6 \int_0^T \int_0^L e^{2s\varphi(x,t)} |\mathbb{L}z|^2 dxdt + C_6 s \int_0^T e^{2s\varphi(L,t)} z^2(L,t) dt \\ &\quad + C_6 s \int_0^L e^{2s\varphi(x,T)} z^2(x,T) dx. \end{aligned} \tag{29}$$

From equation (25), there exists a constant $C_7 > 0$ such that

$$\begin{aligned} |\mathbb{L}z|^2 &= \left| -\frac{\partial v(x,t)}{\partial t}\frac{\partial u}{\partial x} - k_{d1} z + (k_{d2} - k_{d1})\frac{\partial b_2}{\partial t} \right|^2 \\ &\le 3\left| \frac{\partial v(x,t)}{\partial t}\frac{\partial u}{\partial x} \right|^2 + 3k_{d1}^2 z^2 + 3\left| (k_{d2} - k_{d1})\frac{\partial b_2}{\partial t} \right|^2 \\ &\le C_7 \left(\left| \frac{\partial u}{\partial x} \right|^2 + z^2 + (k_{d2} - k_{d1})^2 \right). \end{aligned} \tag{30}$$

Therefore, there exists a constant $C_8 > 0$ such that

$$\begin{aligned} &s^2 \int_0^T \int_0^L e^{2s\varphi(x,t)} z^2 dxdt + \rho^2 s\int_0^L e^{2s\varphi(x,0)} (k_{d2} - k_{d1})^2 dx \\ &\le C_8 \int_0^T \int_0^L e^{2s\varphi(x,t)} z^2 dxdt + C_8 \int_0^T \int_0^L e^{2s\varphi(x,t)} (k_{d2} - k_{d1})^2 dxdt \\ &\quad + C_8 s \int_0^T e^{2s\varphi(L,t)} z^2(L,t) dt + C_8 s \int_0^L e^{2s\varphi(x,T)} z^2(x,T) dx \\ &\quad + C_8 \int_0^T \int_0^L e^{2s\varphi(x,t)} \left| \frac{\partial u}{\partial x} \right|^2 dxdt. \end{aligned} \tag{31}$$

Note that

$$\begin{aligned} &\int_0^T \int_0^L e^{2s\varphi(x,t)} \left| \frac{\partial u}{\partial x} \right|^2 dxdt = \int_0^T \int_0^L e^{2s\varphi(x,t)} \frac{1}{v(x,t)} v(x,t) \left| \frac{\partial u}{\partial x} \right|^2 dxdt \\ &\le \frac{1}{v_0} \int_0^T \int_0^L e^{2s\varphi(x,t)} \left| \frac{\partial u}{\partial x} \right| \left| v(x,t)\frac{\partial u}{\partial x} \right| dxdt \\ &= \frac{1}{v_0} \int_0^T \int_0^L e^{2s\varphi(x,t)} \left| \frac{\partial u}{\partial x} \right| \left| -\frac{\partial u}{\partial t} - k_{d1} u + (k_{d2} - k_{d1}) b_2 \right| dxdt \end{aligned}$$

$$\leq \frac{1}{2v_0}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left[v_0\left|\frac{\partial u}{\partial x}\right|^2+\frac{1}{v_0}\left|-\frac{\partial u}{\partial t}-k_{d1}u+(k_{d2}-k_{d1})b_2\right|^2\right]dxdt$$
$$\leq \frac{1}{2}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left|\frac{\partial u}{\partial x}\right|^2 dxdt + C_9\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(z^2+u^2+(k_{d2}-k_{d1})^2\right)dxdt.$$

Hence,

$$\int_0^T\int_0^L e^{2s\varphi(x,t)}\left|\frac{\partial u}{\partial x}\right|^2 dxdt \leq 2C_9\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(z^2+u^2+(k_{d2}-k_{d1})^2\right)dxdt.$$

Therefore,

$$\begin{aligned}&s^2\int_0^T\int_0^L e^{2s\varphi(x,t)}z^2dxdt+\rho^2 s\int_0^L e^{2s\varphi(x,0)}(k_{d2}-k_{d1})^2dx\\&\leq C_{10}\int_0^T\int_0^L e^{2s\varphi(x,t)}z^2dxdt+C_{10}\int_0^T\int_0^L e^{2s\varphi(x,t)}(k_{d2}-k_{d1})^2dxdt\\&\quad+C_{10}s\int_0^T e^{2s\varphi(L,t)}z^2(L,t)dt+C_{10}s\int_0^L e^{2s\varphi(x,T)}z^2(x,T)dx\\&\quad+C_{10}\int_0^T\int_0^L e^{2s\varphi(x,t)}u^2dxdt.\end{aligned}\tag{32}$$

Since $\varphi(x,t)\leq\varphi(x,0)$ and for $s>s_0$ large enough, we obtain

$$\begin{aligned}&s^2\int_0^T\int_0^L e^{2s\varphi(x,t)}z^2dxdt+\rho^2 s\int_0^L e^{2s\varphi(x,0)}(k_{d2}-k_{d1})^2dx\\&\leq C_{11}s\int_0^T e^{2s\varphi(L,t)}z^2(L,t)dt+C_{11}s\int_0^L e^{2s\varphi(x,T)}z^2(x,T)dx\\&\quad+C_{11}\int_0^T\int_0^L e^{2s\varphi(x,t)}u^2dxdt.\end{aligned}$$

On the other hand

$$\begin{aligned}\frac{\partial}{\partial t}\int_0^L e^{2s\varphi(x,t)}u^2dx&=2s\int_0^L\frac{\partial\varphi(x,t)}{\partial t}e^{2s\varphi(x,t)}u^2dx+2\int_0^L e^{2s\varphi(x,t)}u\frac{\partial u}{\partial t}dx\\&=-2\beta s\int_0^L e^{2s\varphi(x,t)}u^2dx+2\int_0^L e^{2s\varphi(x,t)}u\frac{\partial u}{\partial t}dx\\&\leq\frac{1}{2s\beta}\int_0^L e^{2s\varphi(x,t)}\left|\frac{\partial u}{\partial t}\right|^2dx=\frac{1}{2s\beta}\int_0^L e^{2s\varphi(x,t)}z^2dx.\end{aligned}$$

This inequality implies that

$$\int_0^L e^{2s\varphi(x,t)}u^2dx\leq\frac{1}{2s\beta}\int_0^t\int_0^L e^{2s\varphi(x,t)}z^2dxdt$$

or, equivalently,

$$\int_0^T\int_0^L e^{2s\varphi(x,t)}u^2dx\leq\frac{T}{2s\beta}\int_0^T\int_0^L e^{2s\varphi(x,t)}z^2dxdt.\tag{33}$$

Hence, for $s>s_0$ large enough we have

$$s\int_0^T\int_0^L e^{2s\varphi(x,t)}z^2dxdt+\rho^2\int_0^L e^{2s\varphi(x,0)}(k_{d2}-k_{d1})^2dx$$

$$\le C_{12}\int_0^T e^{2s\varphi(L,t)}z^2(L,t)dt + C_{12}\int_0^L e^{2s\varphi(x,T)}z^2(x,T)dx$$
$$\le C_{12}\int_0^T e^{2s\varphi(L,t)}z^2(L,t)dt + C_{12}e^{2s(\alpha L-\beta T+C_0)}\int_0^L z^2(x,T)dx.$$

Note that $z(x,T)=\frac{\partial u}{\partial t}(x,T)$. By Lemma 2.2 there exists a constant $C_{13}>0$ such that

$$s\int_0^T\int_0^L e^{2s\varphi(x,t)}z^2dxdt + \rho^2\int_0^L e^{2s\varphi(x,0)}(k_{d2}-k_{d1})^2dx$$
$$\le C_{13}\int_0^T e^{2s\varphi(L,t)}z^2(L,t)dt + C_{13}e^{2s(\alpha L-\beta T+C_0)}\int_0^L (k_{d2}-k_{d1})^2dx. \tag{34}$$

Therefore,

$$\rho^2\int_0^L e^{2s\varphi(x,0)}(k_{d2}-k_{d1})^2dx \le C_{13}\int_0^T e^{2s\varphi(L,t)}z^2(L,t)dt$$
$$+ C_{13}e^{2s(\alpha L-\beta T+C_0)}\int_0^L (k_{d2}-k_{d1})^2dx. \tag{35}$$

From (13), we have $\alpha L-\beta T<0$. Thus, for $s>s_0$ large enough we have

$$C_{13}e^{2s(\alpha L-\beta T)} \le \frac{\rho^2}{2}e^{2\alpha sx}. \tag{36}$$

From (35) and (36) we obtain

$$\rho^2\int_0^L e^{2s\varphi(x,0)}(k_{d2}-k_{d1})^2dx$$
$$\le 2C_8\int_0^T e^{2s\varphi(L,t)}z^2(L,t)dt + \frac{\rho^2}{2}\int_0^L e^{2s(\alpha x+C_0)}(k_{d2}-k_{d1})^2dx$$
$$= C_{13}\int_0^T e^{2s\varphi(L,t)}z^2(L,t)dt + \frac{\rho^2}{2}\int_0^L e^{2s\varphi(x,0)}(k_{d2}-k_{d1})^2dx. \tag{37}$$

Therefore, there exists a constant $C_{14}>0$ such that

$$\int_0^L e^{2s\varphi(x,0)}(k_{d2}-k_{d1})^2dx \le C_{14}\int_0^T e^{2s\varphi(L,t)}z^2(L,t)dt.$$

Since $\varphi(x,0)\ge C_0$ and $\varphi(L,t)\le \alpha L+C_0$, let $C_d := C_{14}e^{2L(s_0+1)\alpha}$. It is clear that C_d is independent of s and we obtain

$$\int_0^L (k_{d2}-k_{d1})^2dx \le C_d\int_0^T \left|\frac{\partial u}{\partial t}(L,t)\right|^2 dt$$
$$= C_d\int_0^T \left|\frac{\partial b_1}{\partial t}(L,t)-\frac{\partial b_2}{\partial t}(L,t)\right|^2 dt. \tag{38}$$

Thus, the stability estimate (20) for $k_d(x)$ is proved. To prove the stability estimate (21) for $k_r(x)$, we denote $\widetilde{u} := d_1-d_2$. We have

$$\frac{\partial \widetilde{u}}{\partial t} + v(x,t)\frac{\partial \widetilde{u}}{\partial x} + k_{r1}\widetilde{u} = (k_{r2}-k_{r1})d_2 + k_{d1}u + (k_{d1}-k_{d2})b_2, \tag{39}$$
$$\widetilde{u}(0,t)=0,\ t\in[0,T], \tag{40}$$
$$\widetilde{u}(x,0)=0,\ x\in[0,L], \tag{41}$$

where $u=b_1-b_2$. Setting $w=\widetilde{u}_t$ and differentiating (39)–(41), we obtain

$$\frac{\partial w}{\partial t} + v(x,t)\frac{\partial w}{\partial x} + \frac{\partial v(x,t)}{\partial t}\frac{\partial \widetilde{u}}{\partial x} + k_{r1}w = (k_{r2}-k_{r1})\frac{\partial d_2}{\partial t} + k_{d1}\frac{\partial u}{\partial t} + (k_{d1}-k_{d2})\frac{\partial b_2}{\partial t},$$
$$w(0,t)=0,\ t\in[0,T],$$
$$w(x,0)=(k_{r2}-k_{r1})f_d(x)+(k_{d1}-k_{d2})f_b(x),\ x\in[0,L].$$

By Lemma 3.1, we have

$$
\begin{aligned}
&s^2\int_0^T\int_0^L e^{2s\varphi(x,t)}w^2dxdt+s\int_0^L e^{2s\varphi(x,0)}\left[(k_{r2}-k_{r1})f_d(x)+(k_{d1}-k_{d2})f_b(x)\right]^2dx\\
&\le C_{15}\int_0^T\int_0^L e^{2s\varphi(x,t)}|\mathbb{L}w|^2dxdt+C_{11}s\int_0^T e^{2s\varphi(L,t)}w^2(L,t)dt\\
&\quad+C_{15}s\int_0^L e^{2s\varphi(x,T)}w^2(x,T)dx.
\end{aligned}
$$

Applying the inequality $(a+b)^2\ge\frac{1}{2}a^2-b^2$ for arbitrary real numbers a and b, we have

$$
\begin{aligned}
&s\int_0^L e^{2s\varphi(x,0)}\left[(k_{r2}-k_{r1})f_d(x)+(k_{d1}-k_{d2})f_b(x)\right]^2dx\\
&\ge\frac{s}{2}\int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2f_d^2(x)dx-s\int_0^L e^{2s\varphi(x,0)}(k_{d1}-k_{d2})^2f_b^2(x)dx.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&s^2\int_0^T\int_0^L e^{2s\varphi(x,t)}w^2dxdt+\frac{s}{2}\int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2f_d^2(x)dx\\
&\le C_{15}\int_0^T\int_0^L e^{2s\varphi(x,t)}|\mathbb{L}w|^2dxdt+C_{15}s\int_0^T e^{2s\varphi(L,t)}w^2(L,t)dt\\
&\quad+C_{15}s\int_0^L e^{2s\varphi(x,T)}w^2(x,T)dx+s\int_0^L e^{2s\varphi(x,0)}(k_{d1}-k_{d2})^2f_b^2(x)dx.
\end{aligned}
$$

Furthermore, we have

$$
\begin{aligned}
|\mathbb{L}w|^2&=\left|-\frac{\partial v(x,t)}{\partial t}\frac{\partial\widetilde{u}}{\partial x}-k_{r1}w+(k_{r2}-k_{r1})\frac{\partial d_2}{\partial t}+k_{d1}\frac{\partial u}{\partial t}+(k_{d1}-k_{d2})\frac{\partial b_2}{\partial t}\right|^2\\
&\le 5\left(\left|\frac{\partial v(x,t)}{\partial t}\frac{\partial\widetilde{u}}{\partial x}\right|^2+|k_{r1}w|^2+(k_{r2}-k_{r1})^2\left|\frac{\partial d_2}{\partial t}\right|^2\right.\\
&\qquad\left.+k_{d1}^2\left(\frac{\partial u}{\partial t}\right)^2+(k_{d1}-k_{d2})^2\left|\frac{\partial b_2}{\partial t}\right|^2\right)\\
&\le C_{16}\left(\left|\frac{\partial\widetilde{u}}{\partial x}\right|^2+w^2+(k_{r2}-k_{r1})^2+\left(\frac{\partial u}{\partial t}\right)^2+(k_{d1}-k_{d2})^2\right).
\end{aligned}
\tag{42}
$$

This inequality implies, that there exists a constant $C_{17}>0$ such that

$$
\begin{aligned}
&s^2\int_0^T\int_0^L e^{2s\varphi(x,t)}w^2dxdt+\frac{s}{2}\int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2f_d^2(x)dx\\
&\le C_{17}\int_0^T\int_0^L e^{2s\varphi(x,t)}w^2dxdt+C_{17}\int_0^T\int_0^L e^{2s\varphi(x,t)}(k_{d2}-k_{d1})^2dxdt\\
&\quad+C_{17}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(\frac{\partial u}{\partial t}\right)^2dxdt+C_{17}\int_0^T\int_0^L e^{2s\varphi(x,t)}(k_{r2}-k_{r1})^2dxdt\\
&\quad+C_{17}s\int_0^T e^{2s\varphi(L,t)}w^2(L,t)dt+C_{17}s\int_0^L e^{2s\varphi(x,T)}w^2(x,T)dx\\
&\quad+s\int_0^L e^{2s\varphi(x,0)}(k_{d1}-k_{d2})^2f_b^2(x)dx+C_{17}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(\frac{\partial\widetilde{u}}{\partial x}\right)^2dxdt.
\end{aligned}
\tag{43}
$$

Note that $\varphi(x,t)\le\varphi(x,0)$, with $s>s_0$ large enough then

$$C_{17}\int_0^T\int_0^L e^{2s\varphi(x,t)}(k_{r2}-k_{r1})^2dxdt \le \frac{s}{4}\int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2 f_d^2(x)dx.$$

Therefore,

$$\begin{aligned}
&\frac{s^2}{2}\int_0^T\int_0^L e^{2s\varphi(x,t)}w^2dxdt + \frac{s}{4}\int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2 f_d^2(x)dx\\
&\le C_{17}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(\frac{\partial u}{\partial t}\right)^2dxdt + C_{17}\int_0^T\int_0^L e^{2s\varphi(x,t)}(k_{d2}-k_{d1})^2dxdt\\
&\quad + C_{17}s\int_0^T e^{2s\varphi(L,t)}w^2(L,t)dt + C_{17}s\int_0^L e^{2s\varphi(x,T)}w^2(x,T)dx\\
&\quad + s\int_0^L e^{2s\varphi(x,0)}(k_{d1}-k_{d2})^2 f_b^2(x)dx + C_{17}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(\frac{\partial\widetilde{u}}{\partial x}\right)^2dxdt\\
&\le C_{18}\int_0^T\int_0^L e^{2s\varphi(L,0)}\left(\frac{\partial u}{\partial t}\right)^2dxdt + C_{18}s\int_0^L e^{2s\varphi(L,0)}(k_{d2}-k_{d1})^2dx\\
&\quad + C_{18}s\int_0^T e^{2s\varphi(L,t)}w^2(L,t)dt + C_{18}s\int_0^L e^{2s\varphi(x,T)}w^2(x,T)dx\\
&\quad + C_{18}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(\frac{\partial\widetilde{u}}{\partial x}\right)^2dxdt.
\end{aligned}\tag{44}$$

Since u is the solution of (22)–(24), applying Lemma 2.2 and choosing s large enough, we have

$$C_{18}\int_0^L\left(\frac{\partial u}{\partial t}\right)^2dx \le C_{19}\int_0^L(k_{d2}-k_{d1})^2dx.\tag{45}$$

It follows from (44) and (45) that

$$\begin{aligned}
&2s\int_0^T\int_0^L e^{2s\varphi(x,t)}w^2dxdt + \int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2 f_d^2(x)dx\\
&\le C_{20}e^{2s\varphi(L,0)}\int_0^L(k_{d2}-k_{d1})^2dx + C_{20}\int_0^T e^{2s\varphi(L,t)}w^2(L,t)dt\\
&\quad + C_{20}\int_0^L e^{2s\varphi(x,T)}w^2(x,T)dx + C_{20}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(\frac{\partial\widetilde{u}}{\partial x}\right)^2dxdt\\
&= C_{20}e^{2s\varphi(L,0)}\int_0^L(k_{d2}-k_{d1})^2dx + C_{20}\int_0^T e^{2s\varphi(L,t)}w^2(L,t)dt\\
&\quad + C_{20}\int_0^L e^{2s\varphi(x,T)}\left|\frac{\partial\widetilde{u}}{\partial t}(x,T)\right|^2dx + C_{20}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(\frac{\partial\widetilde{u}}{\partial x}\right)^2dxdt.
\end{aligned}\tag{46}$$

Note that

$$\begin{aligned}
&\int_0^T\int_0^L e^{2s\varphi(x,t)}\left|\frac{\partial\widetilde{u}}{\partial x}\right|^2dxdt = \int_0^T\int_0^L e^{2s\varphi(x,t)}\frac{1}{v(x,t)}v(x,t)\left|\frac{\partial\widetilde{u}}{\partial x}\right|^2dxdt\\
&\le \frac{1}{v_0}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left|\frac{\partial\widetilde{u}}{\partial x}\right|\left|v(x,t)\frac{\partial\widetilde{u}}{\partial x}\right|dxdt\\
&= \frac{1}{v_0}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left|\frac{\partial\widetilde{u}}{\partial x}\right|\left|-\frac{\partial\widetilde{u}}{\partial t} - k_{r1}\widetilde{u} + k_{d1}u + (k_{r2}-k_{r1})d_2\right|dxdt
\end{aligned}$$

$$\le \frac{1}{2}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left|\frac{\partial \widetilde{u}}{\partial x}\right|^2 dxdt$$

$$+\frac{1}{2v_0^2}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left|-\frac{\partial \widetilde{u}}{\partial t} - k_{r1}\widetilde{u} + k_{d1}u + (k_{r2}-k_{r1})b_2\right|^2 dxdt$$

$$\le \frac{1}{2}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left|\frac{\partial \widetilde{u}}{\partial x}\right|^2 dxdt$$

$$+C_{21}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left[w^2+\widetilde{u}^2+u^2+(k_{r2}-k_{r1})^2\right] dxdt.$$

Hence,

$$\int_0^T\int_0^L e^{2s\varphi(x,t)}\left|\frac{\partial \widetilde{u}}{\partial x}\right|^2 dxdt$$

$$\le 2C_{21}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left[w^2+\widetilde{u}^2+u^2+(k_{r2}-k_{r1})^2\right] dxdt.$$

Therefore, for $s > s_0$ large enough there exists a constant $C_{21} > 0$ such that

$$2s\int_0^T\int_0^L e^{2s\varphi(x,t)}w^2 dxdt + \int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2 f_d^2(x)dx$$

$$\le C_{21}e^{2s\varphi(L,0)}\int_0^L (k_{d2}-k_{d1})^2 dx + C_{21}\int_0^T e^{2s\varphi(L,t)}w^2(L,t)dt$$

$$+C_{21}\int_0^L e^{2s\varphi(x,T)}\left|\frac{\partial \widetilde{u}}{\partial t}(x,T)\right|^2 dx + C_{21}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(\widetilde{u}^2+u^2\right)dxdt. \tag{47}$$

Similar to (33), we have

$$\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(\widetilde{u}^2+u^2\right)dxdt \le C_{22}\int_0^T\int_0^L e^{2s\varphi(x,t)}\left(w^2+z^2\right)dxdt. \tag{48}$$

On the other hand,

$$\frac{\partial}{\partial t}\int_0^L \left|\frac{\partial \widetilde{u}}{\partial t}(x,t)\right|^2 dx = -2\int_0^L e^{2s\varphi(x,t)}\frac{\partial \widetilde{u}}{\partial t}\frac{\partial}{\partial t}\Big\{ v(x,t)\frac{\partial \widetilde{u}}{\partial x} + k_{r1}\widetilde{u}$$

$$-(k_{r2}-k_{r1})d_2 - k_{d1}u - (k_{d1}-k_{d2})b_2\Big\}dx$$

$$= -2\int_0^L v\frac{\partial \widetilde{u}}{\partial t}\left(\frac{\partial}{\partial t}\frac{\partial \widetilde{u}}{\partial x}\right)dx - 2\int_0^L k_{r1}\left|\frac{\partial \widetilde{u}}{\partial t}\right|^2 dx$$

$$+2\int_0^L \frac{\partial \widetilde{u}}{\partial t}\Big(-\frac{\partial v(x,t)}{\partial t}\frac{\partial \widetilde{u}}{\partial x} + (k_{r2}-k_{r1})\frac{\partial d_2}{\partial t} + k_{d1}\frac{\partial u}{\partial t} + (k_{d1}-k_{d2})\frac{\partial b_2}{\partial t}\Big)dx$$

$$\le -v(L)\left|\frac{\partial \widetilde{u}}{\partial t}(L,t)\right|^2 + \int_0^L \left|\frac{\partial \widetilde{u}}{\partial t}\right|^2\frac{\partial v}{\partial x}dx - 2\int_0^L k_{r1}\left|\frac{\partial \widetilde{u}}{\partial t}\right|^2 dx + \int_0^L \left|\frac{\partial \widetilde{u}}{\partial t}\right|^2 dx$$

$$+\int_0^L \Big(-\frac{\partial v(x,t)}{\partial t}\frac{\partial \widetilde{u}}{\partial x} + (k_{r2}-k_{r1})\frac{\partial d_2}{\partial t} + k_{d1}\frac{\partial u}{\partial t} + (k_{d1}-k_{d2})\frac{\partial b_2}{\partial t}\Big)^2 dx$$

$$\le C_{23}\int_0^L \left|\frac{\partial \widetilde{u}}{\partial t}\right|^2 dx + 4\int_0^L (k_{r2}-k_{r1})^2\left|\frac{\partial d_2}{\partial t}\right|^2 dx + 4\int_0^L \left|\frac{\partial v(x,t)}{\partial t}\frac{\partial \widetilde{u}}{\partial x}\right|^2 dx$$

$$+4\int_0^L k_{d1}^2\left|\frac{\partial u}{\partial t}\right|^2 dx + 4\int_0^L (k_{d1}-k_{d2})^2\left|\frac{\partial b_2}{\partial t}\right|^2 dx$$

$$\le C_{23}\int_0^L \left|\frac{\partial\widetilde{u}}{\partial t}\right|^2 dx + C_{24}\int_0^L (k_{r2}-k_{r1})^2 dx + C_{24}\int_0^L \left|\frac{\partial\widetilde{u}}{\partial x}\right|^2 dx$$

$$+ C_{24}\int_0^L \left|\frac{\partial u}{\partial t}\right|^2 dx + C_{24}\int_0^L (k_{d1}-k_{d2})^2 dx. \tag{49}$$

From (45) and (49), we obtain

$$\frac{\partial}{\partial t}\int_0^L \left|\frac{\partial\widetilde{u}}{\partial t}(x,t)\right|^2 dx \le C_{25}\int_0^L \left|\frac{\partial\widetilde{u}}{\partial t}\right|^2 dx + C_{25}\int_0^L (k_{r2}-k_{r1})^2 dx$$

$$+ C_{25}\int_0^L (k_{d1}-k_{d2})^2 dx + C_{25}\int_0^L \left|\frac{\partial\widetilde{u}}{\partial x}\right|^2 dx. \tag{50}$$

We have

$$\int_0^L \left|\frac{\partial\widetilde{u}}{\partial x}\right|^2 dx \le \frac{1}{v_0^2}\int_0^L \left|v(x,t)\frac{\partial\widetilde{u}}{\partial x}\right|^2 dx$$

$$= \frac{1}{v_0^2}\int_0^L \left(-\frac{\partial\widetilde{u}}{\partial t} - k_{r1}\widetilde{u} + (k_{r2}-k_{r1})d_2 + k_{d1}u + (k_{d1}-k_{d2})b_2\right)^2 dx$$

$$\le C_{26}\int_0^L \left(\left|\frac{\partial\widetilde{u}}{\partial t}\right|^2 + \widetilde{u}^2 + (k_{r2}-k_{r1})^2 + u^2 + (k_{d1}-k_{d2})^2\right)^2 dx \tag{51}$$

and

$$\frac{\partial}{\partial t}\int_0^L \widetilde{u}^2 dx = 2\int_0^L \widetilde{u}\frac{\partial\widetilde{u}}{\partial t} dx \le \int_0^L \widetilde{u}^2 dx + \int_0^L \left|\frac{\partial\widetilde{u}}{\partial t}\right|^2 dx. \tag{52}$$

From (50)–(52), we have

$$\frac{\partial}{\partial t}\int_0^L \left(\left|\frac{\partial\widetilde{u}}{\partial t}(x,t)\right|^2 + \widetilde{u}^2\right) dx \le C_{27}\int_0^L \left(\left|\frac{\partial\widetilde{u}}{\partial t}(x,t)\right|^2 + \widetilde{u}^2\right) dx$$

$$+ C_{27}\int_0^L (k_{r2}-k_{r1})^2 dx + C_{27}\int_0^L (k_{d1}-k_{d2})^2 dx + C_{27}\int_0^L u^2 dx.$$

From this inequality and the identity $\frac{\partial\widetilde{u}}{\partial t}(x,0) = (k_{d1}-k_{d2})f_b(x) + (k_{r2}-k_{r1})f_d(x)$, with $f_b(x)$ and $f_d(x)$ being bounded functions on $[0,L]$, we obtain

$$\int_0^L \left(\left|\frac{\partial\widetilde{u}}{\partial t}(x,t)\right|^2 + \widetilde{u}^2\right) dx$$

$$\le C_{28}\left(\int_0^t\int_0^L u^2 dx dt + \int_0^L (k_{r2}-k_{r1})^2 dx + \int_0^L (k_{d1}-k_{d2})^2 dx\right) \tag{53}$$

for some positive constant C_{28}. Thus,

$$\int_0^L e^{2s\varphi(x,T)}\left|\frac{\partial\widetilde{u}}{\partial t}(x,T)\right|^2 dx \le e^{2s(\alpha L-\beta T+C_0)}\int_0^L \left|\frac{\partial\widetilde{u}}{\partial t}(x,T)\right|^2 dx \tag{54}$$

$$\le C_{28}e^{2s(\alpha L-\beta T+C_0)}\left(\int_0^T\int_0^L u^2 dx dt + \int_0^L (k_{r2}-k_{r1})^2 dx + \int_0^L (k_{d1}-k_{d2})^2\right) dx.$$

Since $\alpha L - \beta T < 0$, for $s > s_0$ large enough there exists a constant $C_{29} > 0$ such that

$$\int_0^L e^{2s(\alpha L-\beta T+C_0)}(k_{r2}-k_{r1})^2 dx \le \frac{C_{29}}{s}\int_0^L e^{2s(\alpha x+C_0)}(k_{r2}-k_{r1})^2 dx$$

$$= \frac{C_{29}}{s}\int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2 dx. \tag{55}$$

Since $f_d(x) \ge \rho$, from (47), (48), (54) and (55), there exists a constant $C_{30} > 0$ such that

$$\begin{aligned} & s\int_0^T\int_0^L e^{2s\varphi(x,t)} w^2 dxdt + \rho^2 \int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2 dx \\ & \le C_{30} e^{2s\varphi(L,0)} \int_0^L (k_{d2}-k_{d1})^2 dx + C_{30}\int_0^T e^{2s\varphi(L,t)} w^2(L,t)dt \\ & \quad + \frac{C_{30}}{s}\int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2 dx + C_{30}\int_0^T\int_0^L e^{2s\varphi(x,t)} z^2 dxdt \\ & \quad + C_{30} e^{2s(\alpha L-\beta T+C_0)} \int_0^T\int_0^L u^2 dxdt. \end{aligned} \tag{56}$$

From (45), we have

$$\begin{aligned} \frac{\partial}{\partial t}\int_0^L u^2 dx = 2\int_0^L u\frac{\partial u}{\partial t} dx &\le \int_0^L u^2 dx + \int_0^L \left|\frac{\partial u}{\partial t}\right|^2 dx \\ &\le \int_0^L u^2 dx + C_{31}\int_0^L (k_{d2}-k_{d1})^2 dx. \end{aligned}$$

Hence,

$$\int_0^L u^2 dx \le C_{32}\int_0^L (k_{d2}-k_{d1})^2 dx.$$

For $s > s_0$ large enough we have $\frac{C_{30}}{s} \le \frac{\rho^2}{2}$. Therefore,

$$\begin{aligned} & s\int_0^T\int_0^L e^{2s\varphi(x,t)} w^2 dxdt + \frac{\rho^2}{2}\int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2 dx \\ & \le C_{33} e^{2s\varphi(L,0)} \int_0^L (k_{d2}-k_{d1})^2 dx + C_{33}\int_0^T e^{2s\varphi(L,t)} w^2(L,t)dt \\ & \quad + C_{33}\int_0^T\int_0^L e^{2s\varphi(x,t)} z^2 dxdt. \end{aligned}$$

Hence,

$$\begin{aligned} \int_0^L e^{2s\varphi(x,0)}(k_{r2}-k_{r1})^2 dx &\le C_{34} e^{2s\varphi(L,0)} \int_0^L (k_{d2}-k_{d1})^2 dx \\ &\quad + C_{34}\int_0^T e^{2s\varphi(L,t)} w^2(L,t)dt. \end{aligned} \tag{57}$$

Let $C_r = C_{34} e^{2L(s_0+1)\alpha}$. Since $\varphi(x,0) \ge C_0$ and $\varphi(L,t) \le L\alpha + C_0$, we obtain

$$\begin{aligned} \int_0^L (k_{r2}-k_{r1})^2 dx &\le C_r\int_0^T \left|\frac{\partial b_1}{\partial t}(L,t) - \frac{\partial b_2}{\partial t}(L,t)\right|^2 dt \\ &\quad + C_r\int_0^T \left|\frac{\partial d_1}{\partial t}(L,t) - \frac{\partial d_2}{\partial t}(L,t)\right|^2 dt. \end{aligned} \tag{58}$$

The theorem is proved. □

Remark 3.3. Theorem 3.2 provides qualitative estimates of the stability of the CIP. It is worth mentioning that although the constants C_r and C_d only depend on the given functions and constants, it is not easy to obtain quantitative estimates of the upper bounds of these constants. Fortunately, knowledge of these constants is not needed in our numerical computation.

Remark 3.4. If the velocity does not depend on time, i.e., $v(x,t) = v(x) \ge v_0 > 0$, by using the transformation $y := \int_0^x \frac{1}{v(\xi)} d\xi$, the forward problem (1)–(4) is equivalent to the following equations.

$$\frac{\partial \tilde{(}y,t)}{\partial t} + \frac{\partial \tilde{b}(y,t)}{\partial y} = -\tilde{k}_d(y)\tilde{b}(y,t) + \tilde{s}(y,t), \tag{59}$$

$$\frac{\partial \tilde{d}(y,t)}{\partial t} + \frac{\partial \tilde{d}(y,t)}{\partial y} = \tilde{k}_d(y)\tilde{b}(y,t) - \tilde{k}_r(y)\tilde{d}(y,t), \tag{60}$$

$$\tilde{b}(y,0) = \tilde{f}_b(y), \quad \tilde{d}(y,0) = \tilde{f}_d(y), \; y \in [0,\tilde{L}], \tag{61}$$

$$\tilde{b}(0,t) = b_0(t), \quad \tilde{}d(0,t) = d_0(t), \; t \in [0,T], \tag{62}$$

for $(y,t) \in Q := (0,\tilde{L}) \times (0,T)$, where $\tilde{L} = \int_0^L \frac{1}{v(\xi)} d\xi$ and $\tilde{b}(y,t) = b(x,t)$. The other functions in the above equations are defined in the same way.

Using the method of characteristics, we obtain the solution of (59)–(62) as follows.

$$\tilde{b}(y,t) = \begin{cases} \dfrac{\tilde{f}_b(y-t)\mu_1(y-t)}{\mu_1(y)} + \dfrac{1}{\mu_1(y)} \displaystyle\int_{y-t}^{y} \tilde{s}(\xi,\xi+t-y)\mu_1(\xi)d\xi, & t \le y, \\ \dfrac{b_0(t-y)}{\mu_1(y)} + \dfrac{1}{\mu_1(y)} \displaystyle\int_0^y \tilde{s}(\xi,\xi+t-y)\mu_1(\xi)d\xi, & t > y, \end{cases} \tag{63}$$

$$\tilde{d}(y,t) = \begin{cases} \dfrac{\tilde{f}_d(y-t)\mu_2(y-t)}{\mu_2(y)} + \dfrac{1}{\mu_2(y)} \displaystyle\int_{y-t}^{y} \tilde{k}_d(\xi)\tilde{b}(\xi,\xi+t-y)\mu_2(\xi)d\xi, & t \le y, \\ \dfrac{d_0(t-y)}{\mu_2(y)} + \dfrac{1}{\mu_2(y)} \displaystyle\int_0^y \tilde{k}_d(\xi)\tilde{b}(\xi,\xi+t-y)\mu_2(\xi)d\xi, & t > y, \end{cases} \tag{64}$$

where

$$\mu_i(y) = e^{\int_0^y \tilde{k}_i(\xi)d\xi}, \; i = 1,2.$$

If $\tilde{b}(\tilde{L},t) = b(L,t)$ is given, then we have

$$\tilde{b}(\tilde{L},t) = \frac{\tilde{f}_b(\tilde{L}-t)\mu_1(\tilde{L}-t)}{\mu_1(\tilde{L})} + \frac{1}{\mu_1(\tilde{L})} \int_{\tilde{L}-t}^{\tilde{L}} \tilde{s}(\xi,\xi+t-\tilde{L})\mu_1(\xi)d\xi, \quad t \le \tilde{L}.$$

Changing the variable $\tilde{t} := \tilde{L} - t$ and $\tilde{\mu}_1(\tilde{t}) := \mu_1(\tilde{t})/\mu_1(\tilde{L}) = e^{-\int_y^{\tilde{L}} \tilde{k}_d(\xi)d\xi}$ and dividing both sides of the above equation by $\tilde{f}_b(\tilde{t})$ (recall that $\tilde{f}_b(\tilde{t}) \ge \rho > 0$ under Assumption 2), we obtain the following Volterra equation of the second kind for $\tilde{\mu}_1$:

$$\frac{\tilde{b}(\tilde{L},\tilde{t})}{\tilde{f}_b(\tilde{t})} = \tilde{\mu}_1(\tilde{t}) - \int_0^{\tilde{t}} \frac{\tilde{s}(\xi,\xi+t-\tilde{L})}{\tilde{f}_b(\tilde{t})} \tilde{\mu}_1(\xi)d\xi, \quad t \le \tilde{L}. \tag{65}$$

Similarly,

$$\frac{\tilde{d}(\tilde{L},\tilde{t})}{\tilde{f}_d(\tilde{t})} = \tilde{\mu}_2(\tilde{t}) - \int_0^{\tilde{t}} \frac{\tilde{k}_d(\xi)\tilde{b}(\xi,\xi+t-\tilde{L})}{\tilde{f}_d(\tilde{t})} \tilde{\mu}_2(\xi)d\xi, \quad t \le \tilde{L}, \tag{66}$$

for $\tilde{\mu}_2(\tilde{t}) := \mu_2(\tilde{t})/\mu_2(\tilde{L})$. From (65), we can derive a stability estimate for $\tilde{\mu}_1$, and hence $\tilde{k}_d$, using a measurement of $\tilde{b}(\tilde{L},\tilde{t})$. However, since the kernel of (66) depends on the data, it is more difficult to obtain a stability estimate for $\tilde{\mu}_2$.

4. Solving Problem 1 using the least-squares approach

To determine the coefficients $k_d(x)$ and $k_r(x)$ (or equivalently, matrix K), we minimize a least-squares objective functional which measures the misfit between the solution $(b(L,t), d(L,t))$ of the forward problem (1)–(4) and the measured data in an appropriate norm.

Given the data functions θ_b and θ_d in (5), we minimize the following objective functional:

$$J_1(k_d,k_r) := J_1(K) := \frac{1}{2} \int_0^T \left[\left| \frac{\partial b(L,t)}{\partial t} - \theta_b(t) \right|^2 + \left| \frac{\partial d(L,t)}{\partial t} - \theta_d(t) \right|^2 \right] dt. \tag{67}$$

We would like to mention that weight coefficients can be used to account for possible different effects that the two terms in (67) have on the accuracy of the reconstruction of the coefficients k_d and k_r. In some particular practical cases, suitably chosen weight coefficients may improve the efficiency of numerical computation.

To minimize J_1, we use a gradient-based iterative algorithm. Suppose that the noise level δ is known. Then, we stop the iterative process using a Morozov-type discrepancy principle, i.e., we stop the algorithm when a pair of coefficient functions $(\tilde{k}_d, \tilde{k}_r)$ satisfying the following condition is determined:

$$J_1(\tilde{k}_d, \tilde{k}_r) \le \tau\delta^2, \tag{68}$$

where τ is a positive constant larger than one. The existence of the pair $(\tilde{k}_d, \tilde{k}_r)$ satisfying (68) is obvious since the pair (k_1^*, k_2^*) satisfies this condition. We now prove error estimates between $\tilde{k}_d$, $\tilde{k}_r$ and the exact coefficients k_1^* and k_2^*.

4.1. Error estimates for the reconstructed coefficients

Theorem 4.1. *Let k_d^* and k_r^* be the coefficients associated with the noiseless data and the pair $(\tilde{k}_d, \tilde{k}_r)$ satisfies Morozov's discrepancy principle (68). Then the following error estimates holds:*

$$\|\tilde{k}_d - k_d^*\| \le \delta\sqrt{2C_d(1+2\tau)}, \tag{69}$$

$$\|\tilde{k}_r - k_r^*\| \le 2\delta\sqrt{C_r(1+\tau)}, \tag{70}$$

where δ is the noise level defined in (5) and C_d and C_r are the constants in the stability estimates (20) and (21).

Proof. We first prove (69). Let $(\tilde{b}, \tilde{d})$ be the solution of the forward problem associated with the coefficients $\tilde{k}_d$ and $\tilde{k}_r$. Using the stability estimate (20), the Cauchy-Schwarz inequality, we have

$$\begin{aligned}\|\tilde{k}_d - k_d^*\|^2_{L^2(0,L)} &\le C_d \left\| \frac{\partial b^*(L,\cdot)}{\partial t} - \frac{\partial \tilde{b}(L,\cdot)}{\partial t}\right\|^2_{L^2(0,L)} \\ &\le 2C_d\left\{ \left\|\frac{\partial b^*(L,\cdot)}{\partial t} - \theta_b\right\|^2_{L^2(0,L)} + \left\|\theta_b - \frac{\partial \tilde{b}(L,\cdot)}{\partial t}\right\|^2_{L^2(0,L)}\right\}.\end{aligned}$$

It follows from (5) that $\|\frac{\partial b^*(L,\cdot)}{\partial t} - \theta_b\|^2_{L^2(0,L)} \le \delta^2$. On the other hand, from (68) we have that $\|\theta_b - \frac{\partial \tilde{b}(L,\cdot)}{\partial t}\|^2_{L^2(0,L)} = 2J_1(\tilde{k}_d, \tilde{k}_r) \le 2\tau\delta^2$. Hence,

$$\|\tilde{k}_d - k_d^*\|^2_{L^2(0,L)} \le 2C_d(\delta^2 + 2\tau\delta^2).$$

Thus, (69) is proved. Using a similar derivation, we obtain

$$\begin{aligned}\|\tilde{k}_r - k_r^*\|^2_{L^2(0,L)} &\le C_r \left\|\frac{\partial b^*(L,\cdot)}{\partial t} - \frac{\partial \tilde{b}(L,\cdot)}{\partial t}\right\|^2_{L^2(0,L)} + C_r\left\|\frac{\partial d^*(L,\cdot)}{\partial t} - \frac{\partial \tilde{d}(L,\cdot)}{\partial t}\right\|^2_{L^2(0,L)} \\ &\le 2C_r\left\{\left\|\frac{\partial b^*(L,\cdot)}{\partial t} - \theta_b\right\|^2_{L^2(0,L)} + \left\|\frac{\partial d^*(L,\cdot)}{\partial t} - \theta_d\right\|^2_{L^2(0,L)} + 2J_1(\tilde{k}_d, \tilde{k}_r)\right\} \\ &\le 2C_r(2\delta^2 + 2\tau\delta^2).\end{aligned}$$

From this inequality, we obtain (70). The proof is complete. □

4.2. Discretized objective functional and its gradient

To formulate the discretized objective functional, let us first discretize the forward problem (1)–(4). For this purpose, we use a second-order finite difference scheme constructed from the integral form of the forward problem. Consider the uniformly distributed grid points along the x- and t-coordinates:

$$0 = x_0 < x_1 < \cdots < x_{N_x} = L, \quad 0 = t_0 < t_1 < \cdots < t_{N_t} = T. \tag{71}$$

Denote by Δx and Δt the grid sizes in the x- and t-directions. Integrating equation (1) with respect to x over the interval $[x_{i-1}, x_i]$, we obtain

$$\frac{d}{dt}\int_{x_{i-1}}^{x_i} b(x,t)dx + \int_{x_{i-1}}^{x_i} v(x,t)\frac{\partial b(x,t)}{\partial x}dx + \int_{x_{i-1}}^{x_i} k_d(x)b(x,t)dx = \int_{x_{i-1}}^{x_i} s(x,t)dx. \tag{72}$$

To obtain the discrete equation with respect to x, we approximate the second integral in the above equation by

$$\int_{x_{i-1}}^{x_i} v(x,t)\frac{\partial b(x,t)}{\partial x}dx \approx v_{i-1/2}(t)[b_i(t) - b_{i-1}(t)]$$

and the other integrals using the trapezoidal rule. We have

$$\begin{aligned}&\frac{\Delta x}{2}[b'_{i-1}(t) + b'_i(t)] + v_{i-1/2}(t)[b_i(t) - b_{i-1}(t)] + \frac{\Delta x}{2}[k_{di-1}b_{i-1}(t) + k_{di}b_i(t)] \\ &\quad = \frac{\Delta x}{2}[s_{i-1}(t) + s_i(t)].\end{aligned}$$

Dividing both sides by $\frac{\Delta x}{2}$ and approximating the time derivative using the central finite difference, we obtain the following scheme:

$$\begin{aligned}&\frac{b^{n+1}_{i-1} - b^n_{i-1}}{\Delta t} + \frac{b^{n+1}_i - b^n_i}{\Delta t} + \frac{v^n_{i-1/2}[b^n_i - b^n_{i-1}] + v^{n+1}_{i-1/2}[b^{n+1}_i - b^{n+1}_{i-1}]}{\Delta x} \\ &+\frac{1}{2}k_{di-1}[b^n_{i-1} + b^{n+1}_{i-1}] + \frac{1}{2}k_{di}[b^n_i + b^{n+1}_i] = \frac{1}{2}[s^n_{i-1} + s^{n+1}_{i-1} + s^n_i + s^{n+1}_i]\end{aligned} \tag{73}$$

for $i = 1, 2, \ldots, N_x$ and $n = 0, 1, \ldots, N_t - 1$. In this numerical scheme, b^n_i represents an approximation of $b(x_i, t_n)$, $v^n_{i-1/2} := v((x_{i-1} + x_i)/2, t_n)$, $k_{di} := k_d(x_i)$, and $s^n_i := s(x_i, t_n)$. The above numerical scheme is coupled with the following initial and boundary conditions:

$$b^n_0 = g_b(t_n), \; n = 1, 2, \ldots, N_t, \tag{74}$$

$$b^0_i = f_b(x_i), \; i = 0, 1, \ldots, N_x. \tag{75}$$

We can rewrite (73) as follows:

$$\left(1+a_i^{n+1}+\frac{\Delta t}{2}k_{di}\right)b_i^{n+1}+\left(1-a_i^{n+1}+\frac{\Delta t}{2}k_{di-1}\right)b_{i-1}^{n+1}$$
$$-\left(1+a_i^{n}-\frac{\Delta t}{2}k_{di-1}\right)b_{i-1}^{n}-\left(1-a_i^{n}-\frac{\Delta t}{2}k_{di}\right)b_i^{n}$$
$$=\frac{\Delta t}{2}[s_{i-1}^n+s_{i-1}^{n+1}+s_i^n+s_i^{n+1}],\quad i=1,2,\dots,N_x, \tag{76}$$

where $a_i^n := \frac{\Delta t}{\Delta x}v_{i-1/2}^n$. Taking into account the availability of the boundary condition at $i=0$, we can compute b_i^{n+1} sequentially for $i=1,2,\dots,N_x$ at each time step because all the other terms are known.

Similarly, we obtain the following numerical scheme for $d(x,t)$.

$$\left(1+a_i^{n+1}+\frac{\Delta t}{2}k_{ri}\right)d_i^{n+1}+\left(1-a_i^{n+1}+\frac{\Delta t}{2}k_{ri-1}\right)d_{i-1}^{n+1}$$
$$-\left(1+a_i^{n}-\frac{\Delta t}{2}k_{ri-1}\right)d_{i-1}^{n}-\left(1-a_i^{n}-\frac{\Delta t}{2}k_{ri}\right)d_i^{n}$$
$$=\frac{\Delta t}{2}[k_{di-1}b_{i-1}^n+k_{di-1}b_{i-1}^{n+1}+k_{di}b_i^n+k_{di}b_i^{n+1}],\quad i=1,2,\dots,N_x, \tag{77}$$

with the corresponding initial and boundary conditions

$$d_0^n = g_d(t_n),\ n=1,2,\dots,N_t, \tag{78}$$
$$d_i^0 = f_d(x_i),\ i=0,1,\dots,N_x. \tag{79}$$

Remark 4.1. It is possible to prove that the order of approximation of the above numerical scheme is $O(\Delta t^2+\Delta x^2)$, given appropriate smoothness conditions on the input functions.

Concerning the monotonicity and conservativity, we note that it was proved by Godunov in 1959 [23] that monotone schemes are of at most first order. Therefore, the above scheme is not monotone. In addition, it is conservative only if the velocity v is independent of x. Although the monotonicity and conservativity are important in numerical schemes for PDEs with advection, we still obtained an accurate numerical solution for our model since the exact solution is assumed to be smooth.

To simplify the notation, in the discrete problem setting we use k_d and k_r again to denote the discrete parameter vectors, i.e., $k_d := [k_{d0},k_{d1},\dots,k_{dN_x}]^T$ and $k_r := [k_{r0},k_{r1},\dots,k_{rN_x}]^T$. Given the discrete forward problem (74)–(79), we determine k_d and k_r by minimizing the following discrete objective function:

$$\mathcal{F}_1(k_d,k_r) := \frac{\Delta t}{2}\sum_{n=0}^{N_t-1}\left[\frac{b_{N_x}^{n+1}-b_{N_x}^n}{\Delta t}-\theta_b^n\right]^2+\frac{\Delta t}{2}\sum_{n=0}^{N_t-1}\left[\frac{d_{N_x}^{n+1}-d_{N_x}^n}{\Delta t}-\theta_d^n\right]^2$$
$$:= \frac{1}{2\Delta t}\left\{\sum_{n=0}^{N_t-1}\left[\mathcal{M}(b^{n+1}-b^n)-\Delta t\theta_b^n\right]^2+\sum_{n=0}^{N_t-1}\left[\mathcal{M}(d^{n+1}-d^n)-\Delta t\theta_d^n\right]^2\right\}, \tag{80}$$

where $\mathcal{M}=[0,\dots,0,1]$, $\theta_b^n=\dfrac{\theta_b(t_n)+\theta_b(t_{n+1})}{2}$ and $\theta_d^n=\dfrac{\theta_d(t_n)+\theta_d(t_{n+1})}{2}$.

To minimize the objective function $\mathcal{F}_1(k_d,k_r)$, we use gradient-based methods. For this purpose, we use the adjoint equation method for calculating the gradient of $\mathcal{F}_1$. There are two approaches for using the adjoint equation method. The first approach finds the Fréchet derivative of the continuous objective functional, then both the forward problem and the adjoint problem are discretized. The second approach is to formulate the adjoint equation for the discrete forward problem and discrete objective function. Although both approaches provide exact formulas of the gradient of the objective functional, the first approach introduces approximation errors when the objective functional and its gradient are discretized for numerical implementation, whereas the second approach avoids this issue. For this reason, we use the second approach in this paper. It is worth mentioning that due to round-off errors, numerical computation of the gradient of the objective functional may not be exact. However, round-off errors are usually much smaller than approximation errors introduced by the discretization of the continuous objective functional and its gradient in the first approach. Based on our observations with numerical tests, we believe that round-off errors do not have significant effect on the result of the minimization problem.

To simplify the mathematical derivation, we rewrite the discrete forward problem (74)–(79) as follows:

$$b^0=f_b,\quad d^0=f_d, \tag{81}$$
$$A^{n+1}b^{n+1}+B(k_d)(b^n+b^{n+1})-C^nb^n=F_b^n, \tag{82}$$
$$A^{n+1}d^{n+1}+B(k_r)(d^n+d^{n+1})-C^nd^n=B(k_d)(b^n+b^{n+1})+F_d^n, \tag{83}$$
$$\text{for } n=0,1,\dots,N_t-1,$$

where $f_b := [f_b(x_0),f_b(x_1),\dots,f_b(x_{N_x})]^T$, $f_d := [f_d(x_0),f_d(x_1),\dots,f_d(x_{N_x})]^T$. The matrices A^n and C^n are of size $(N_x+1)\times(N_x+1)$ and defined by

$$A^n=\begin{bmatrix}1 & 0 & 0 & \cdots & 0 & 0\\ 1-a_1^n & 1+a_1^n & 0 & \cdots & 0 & 0\\ 0 & 1-a_2^n & 1+a_2^n & \cdots & 0 & 0\\ . & . & . & \cdots & . & .\\ 0 & 0 & 0 & \cdots & 1+a_{N_x-1}^n & 0\\ 0 & 0 & 0 & \cdots & 1-a_{N_x}^n & 1+a_{N_x}^n\end{bmatrix},$$

$$C^n = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 1+a_1^n & 1-a_1^n & 0 & \cdots & 0 & 0 \\ 0 & 1+a_2^n & 1-a_2^n & \cdots & 0 & 0 \\ . & . & . & \cdots & . & . \\ 0 & 0 & 0 & \cdots & 1-a_{N_x-1}^n & 0 \\ 0 & 0 & 0 & \cdots & 1+a_{N_x}^n & 1-a_{N_x}^n \end{bmatrix}.$$

Matrix $B(k_d)$ is also of size $(N_x+1)\times(N_x+1)$ and defined by

$$B(k_d) = \frac{\Delta t}{2}\begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ k_{d0} & k_{d1} & 0 & \cdots & 0 & 0 \\ 0 & k_{d1} & k_{d2} & \cdots & 0 & 0 \\ . & . & . & \cdots & . & . \\ 0 & 0 & 0 & \cdots & k_{dN_x-1} & 0 \\ 0 & 0 & 0 & \cdots & k_{dN_x-1} & k_{dN_x} \end{bmatrix}. \tag{84}$$

Matrix $B(k_r)$ is defined similarly. The vectors b^n and d^n are given by

$$b^n := [b_0^n, b_1^n, \dots, b_{N_x}^n]^T, \quad d^n := [d_0^n, d_1^n, \dots, d_{N_x}^n]^T.$$

Finally, the vectors $F_b^n := [F_{b0}^n, F_{b1}^n, \dots, F_{bN_x}^n]^T$ and $F_d^n := [F_{d0}^n, F_{d1}^n, \dots, F_{dN_x}^n]^T$ are given by

$$F_{b0}^n = g_b(t_{n+1}),\ F_{bi}^n = \frac{\Delta t}{2}[s_{i-1}^n + s_{i-1}^{n+1} + s_i^n + s_i^{n+1}],\ i = 1,\dots,N_x,$$
$$F_{d0}^n = g_d(t_{n+1}),\ F_{di}^n = 0,\ i = 1,\dots,N_x.$$

We remark that it is possible to exclude b_0^n and d_0^n from the above equations by moving them to the right-hand side in (73) and (77) at $i=1$. However, doing so makes the right-hand side vectors depend on the unknown coefficients. This makes the derivation of the gradient of the objective function more complicated.

To obtain the gradient of $\mathcal{F}_1$, consider two pairs of parameter vectors (k_d, k_r) and $(\bar{k}_d, \bar{k}_r)$ and let $(b^0,\dots,b^{N_t}, d^0,\dots,d^{N_t})$ and $(\bar{b}^0,\dots,\bar{b}^{N_t}, \bar{d}^0,\dots,\bar{d}^{N_t})$ be the corresponding solutions of the discrete forward problem associated with these pairs of parameter vectors. We also denote by $\delta k_d = \bar{k}_d - k_d$, $\delta k_r = \bar{k}_r - k_r$, $\delta b^n = \bar{b}^n - b^n$, and $\delta d^n = \bar{d}^n - d^n$. From (80) it follows that

$$\begin{aligned}
\mathcal{F}_1(\bar{k}_d,\bar{k}_r)\ & -\mathcal{F}_1(k_d,k_r) \\
&:= \frac{1}{2\Delta t}\left\{\sum_{n=0}^{N_t-1}\left[\mathcal{M}(\bar{b}^{n+1}-\bar{b}^n) - \Delta t\theta_b^n\right]^2 + \sum_{n=0}^{N_t-1}\left[\mathcal{M}(\bar{d}^{n+1}-\bar{d}^n) - \Delta t\theta_d^n\right]^2\right\}, \\
&-\frac{1}{2\Delta t}\left\{\sum_{n=0}^{N_t-1}\left[\mathcal{M}(b^{n+1}-b^n) - \Delta t\theta_b^n\right]^2 - \sum_{n=0}^{N_t-1}\left[\mathcal{M}(d^{n+1}-d^n) - \Delta t\theta_d^n\right]^2\right\} \\
&= \frac{1}{2\Delta t}\left\{\sum_{n=0}^{N_t-1}\left[\mathcal{M}(\delta b^{n+1}-\delta b^n)\right]^2 + \sum_{n=0}^{N_t-1}\left[\mathcal{M}(\delta d^{n+1}-\delta d^n)\right]^2\right\} \\
&+\frac{1}{\Delta t}\sum_{n=0}^{N_t-1}\left[\mathcal{M}(\delta b^{n+1}-\delta b^n)\right]^T\left[\mathcal{M}(b^{n+1}-b^n) - \Delta t\theta_b^n\right] \\
&+\frac{1}{\Delta t}\sum_{n=0}^{N_t-1}\left[\mathcal{M}(\delta d^{n+1}-\delta d^n)\right]^T\left[\mathcal{M}(d^{n+1}-d^n) - \Delta t\theta_d^n\right], \\
&= \frac{1}{\Delta t}\sum_{n=0}^{N_t-1}(\delta b^{n+1}-\delta b^n)^T\mathcal{M}^T\left[\mathcal{M}(b^{n+1}-b^n) - \Delta t\theta_b^n\right] \\
&+\frac{1}{\Delta t}\sum_{n=0}^{N_t-1}(\delta d^{n+1}-\delta d^n)^T\mathcal{M}^T\left[\mathcal{M}(d^{n+1}-d^n) - \Delta t\theta_d^n\right] + o(\delta k_d).
\end{aligned} \tag{85}$$

In obtaining the last equality, we have used the property that $\delta b^n = O(\delta k_d)$ and $\delta d^n = O(\delta k_d)$ for $n = 0,1,\dots,N_t$. We note that $(\delta b^0,\dots,\delta b^{N_t})$ satisfies the following equations:

$$\begin{aligned}
&A^{n+1}\delta b^{n+1} + B(k_d)(\delta b^n + \delta b^{n+1}) - C^n\delta b^n = -B(\delta k_d)(\bar{b}^n + \bar{b}^{n+1}),\ n = \overline{0, N_t-1}, \\
&\delta b^0 = 0.
\end{aligned} \tag{86}$$

Similarly, $(\delta d^0,\dots,\delta d^{N_t})$ satisfies the following equations:

$$\begin{aligned}
&A^{n+1}\delta d^{n+1} + B(k_r)(\delta d^n + \delta d^{n+1}) - C^n\delta d^n - B(k_d)(\delta b^n + \delta b^{n+1}) \\
&\qquad = B(\delta k_d)(\bar{b}^n + \bar{b}^{n+1}) - B(\delta k_r)(\bar{d}^n + \bar{d}^{n+1}),\ n = \overline{0, N_t-1}, \\
&\delta d^0 = 0.
\end{aligned} \tag{87}$$

Let η^n and ξ^n, $n = 1,\dots,N_t$ be column vectors in $\mathbb{R}^{N_x+1}$. Taking the transpose of (86) and (87) and multiplying both sides by η^{n+1} and ξ^{n+1}, respectively, and taking the sum from $n=0$ to N_t-1, we obtain:

$$
\begin{aligned}
&\sum_{n=0}^{N_t-1}\left[(\delta b^{n+1})^T(A^{n+1})^T\eta^{n+1}+(\delta b^n+\delta b^{n+1})^T B^T(k_d)\eta^{n+1}-(\delta b^n)^T(C^n)^T\eta^{n+1}\right]\\
&+\sum_{n=0}^{N_t-1}\left[(\delta d^{n+1})^T(A^{n+1})^T\xi^{n+1}+(\delta d^n+\delta d^{n+1})^T B^T(k_r)\xi^{n+1}-(\delta d^n)^T(C^n)^T\xi^{n+1}\right]\\
&-\sum_{n=0}^{N_t-1}(\delta b^n+\delta b^{n+1})^T B^T(k_d)\xi^{n+1}\\
&=-\sum_{n=0}^{N_t-1}[B(\delta k_d)(\bar b^n+\bar b^{n+1})]^T(\eta^{n+1}-\xi^{n+1})-\sum_{n=0}^{N_t-1}[B(\delta k_r)(\bar d^n+\bar d^{n+1})]^T\xi^{n+1}.
\end{aligned}
\tag{88}
$$

We want to determine the vectors η^n and ξ^n, $n=1,\dots,N_t$ such that

$$
\begin{aligned}
&\sum_{n=0}^{N_t-1}(\delta b^{n+1}-\delta b^n)^T\mathcal{M}^T\left[\mathcal{M}(b^{n+1}-b^n)-\theta_b^n\right]\\
&+\sum_{n=0}^{N_t-1}(\delta d^{n+1}-\delta d^n)^T\mathcal{M}^T\left[\mathcal{M}(d^{n+1}-d^n)-\theta_d^n\right]\\
&=\sum_{n=0}^{N_t-1}[B(\delta k_d)(\bar b^n+\bar b^{n+1})]^T(\eta^{n+1}-\xi^{n+1})+\sum_{n=0}^{N_t-1}[B(\delta k_r)(\bar d^n+\bar d^{n+1})]^T\xi^{n+1}.
\end{aligned}
\tag{89}
$$

If (89) holds, then by substituting this equality into (88), we obtain

$$
\begin{aligned}
&\sum_{n=0}^{N_t-1}\left[(\delta b^{n+1})^T(A^{n+1})^T\eta^{n+1}+(\delta b^n+\delta b^{n+1})^T B^T(k_d)\eta^{n+1}-(\delta b^n)^T(C^n)^T\eta^{n+1}\right]\\
&+\sum_{n=0}^{N_t-1}\left[(\delta d^{n+1})^T(A^{n+1})^T\xi^{n+1}+(\delta d^n+\delta d^{n+1})^T B^T(k_r)\xi^{n+1}-(\delta d^n)^T(C^n)^T\xi^{n+1}\right]\\
&-\sum_{n=0}^{N_t-1}(\delta b^n+\delta b^{n+1})^T B^T(k_d)\xi^{n+1}\\
&=-\sum_{n=0}^{N_t-1}(\delta b^{n+1}-\delta b^n)^T\mathcal{M}^T\left[\mathcal{M}(b^{n+1}-b^n)-\theta_b^n\right]\\
&-\sum_{n=0}^{N_t-1}(\delta d^{n+1}-\delta d^n)^T\mathcal{M}^T\left[\mathcal{M}(d^{n+1}-d^n)-\theta_d^n\right].
\end{aligned}
$$

Rearranging the terms in the above equation, taking into account the fact that $\delta b^0=\delta d^0=0$, we have

$$
\begin{aligned}
&\sum_{n=1}^{N_t}(\delta b^n)^T(A^n)^T\eta^n+\sum_{n=1}^{N_t-1}(\delta b^n)^T B^T(k_d)\eta^{n+1}+\sum_{n=1}^{N_t}(\delta b^n)^T B^T(k_d)\eta^n-\sum_{n=1}^{N_t-1}(\delta b^n)^T(C^n)^T\eta^{n+1}\\
&+\sum_{n=1}^{N_t}(\delta d^n)^T(A^n)^T\xi^n+\sum_{n=1}^{N_t-1}(\delta d^n)^T B^T(k_r)\xi^{n+1}+\sum_{n=1}^{N_t}(\delta d^n)^T B^T(k_r)\xi^n-\sum_{n=1}^{N_t-1}(\delta d^n)^T(C^n)^T\xi^{n+1}\\
&-\sum_{n=1}^{N_t-1}(\delta b^n)^T B^T(k_d)\xi^{n+1}-\sum_{n=1}^{N_t}(\delta b^n)^T B^T(k_d)\xi^n\\
&=-\sum_{n=1}^{N_t}(\delta b^n)^T\mathcal{M}^T\left[\mathcal{M}(b^n-b^{n-1})-\theta_b^{n-1}\right]+\sum_{n=1}^{N_t-1}(\delta b^n)^T\mathcal{M}^T\left[\mathcal{M}(b^{n+1}-b^n)-\theta_b^n\right]\\
&-\sum_{n=1}^{N_t}(\delta d^n)^T\mathcal{M}^T\left[\mathcal{M}(d^n-d^{n-1})-\theta_d^{n-1}\right]+\sum_{n=1}^{N_t-1}(\delta d^n)^T\mathcal{M}^T\left[\mathcal{M}(d^{n+1}-d^n)-\theta_d^n\right].
\end{aligned}
$$

Hence,

$$
\begin{aligned}
&(\delta b^{N_t})^T\left\{(A^{N_t})^T\eta^{N_t}+B^T(k_d)\eta^{N_t}-B^T(k_d)\xi^{N_t}+\mathcal{M}^T[\mathcal{M}(b^{N_t}-b^{N_t-1})-\theta_b^{N_t-1}]\right\}\\
&+\sum_{n=1}^{N_t-1}(\delta b^n)^T\{(A^n)^T\eta^n+B^T(k_d)(\eta^n+\eta^{n+1})-(C^n)^T\eta^{n+1}-B^T(k_d)(\xi^n+\xi^{n+1})\\
&\qquad\qquad-\mathcal{M}^T[\mathcal{M}(b^{n+1}-2b^n+b^{n-1})-\theta_b^n+\theta_b^{n-1}]\}\\
&+(\delta d^{N_t})^T\left\{(A^{N_t})^T\xi^{N_t}+B^T(k_r)\xi^{N_t}+\mathcal{M}^T[\mathcal{M}(d^{N_t}-d^{N_t-1})-\theta_d^{N_t-1}]\right\}\\
&+\sum_{n=1}^{N_t-1}(\delta d^n)^T\{(A^n)^T\xi^n+B^T(k_r)(\xi^n+\xi^{n+1})-(C^n)^T\xi^{n+1}\\
&\qquad\qquad-\mathcal{M}^T[\mathcal{M}(d^{n+1}-2d^n+d^{n-1})-\theta_d^n+\theta_d^{n-1}]\}
\end{aligned}
$$

$= 0.$

From the last equation we can see that (89) holds if η^n and ξ^n, $n = 1, \dots, N_t$ satisfy the following problems:

$$A^{N_t}\xi^{N_t} + B^T(k_r)\xi^{N_t} = -\mathcal{M}^T[\mathcal{M}(d^{N_t} - d^{N_t-1}) - \theta_d^{N_t-1}], \tag{90}$$

$$(A^n)^T\xi^n + B^T(k_r)(\xi^n + \xi^{n+1}) - (C^n)^T\xi^{n+1} = \mathcal{M}^T[\mathcal{M}(d^{n+1} - 2d^n + d^{n-1}) - \theta_d^n + \theta_d^{n-1}],\ n = N_t - 1, \dots, 1. \tag{91}$$

$$A^{N_t}\eta^{N_t} + B^T(k_d)\eta^{N_t} - B^T(k_d)\xi^{N_t} = -\mathcal{M}^T[\mathcal{M}(b^{N_t} - b^{N_t-1}) - \theta_b^{N_t-1}], \tag{92}$$

$$(A^n)^T\eta^n + B^T(k_d)(\eta^n + \eta^{n+1}) - (C^n)^T\eta^{n+1} - B^T(k_d)(\xi^n + \xi^{n+1}) = \mathcal{M}^T[\mathcal{M}(b^{n+1} - 2b^n + b^{n-1}) - \theta_b^n + \theta_b^{n-1}],\ n = N_t - 1, \dots, 1. \tag{93}$$

Now it follows from (85) and (89) that

$$\begin{aligned}\mathcal{F}_1(\bar{k}_d, \bar{k}_r) - \mathcal{F}_1(k_d, k_r) &= \frac{1}{\Delta t}\sum_{n=0}^{N_t-1}[B(\delta k_d)(\bar{b}^n + \bar{b}^{n+1})]^T(\eta^{n+1} - \xi^{n+1}) \\ &+ \frac{1}{\Delta t}\sum_{n=0}^{N_t-1}[B(\delta k_r)(\bar{d}^n + \bar{d}^{n+1})]^T\xi^{n+1} + o(\delta k_b) + o(\delta k_r) \\ &= \frac{1}{\Delta t}\sum_{n=0}^{N_t-1}[B(\delta k_d)(b^n + b^{n+1})]^T(\eta^{n+1} - \xi^{n+1}) \\ &+ \frac{1}{\Delta t}\sum_{n=0}^{N_t-1}[B(\delta k_r)(d^n + d^{n+1})]^T\xi^{n+1} + o(\delta k_b) + o(\delta k_r).\end{aligned} \tag{94}$$

In obtaining the last equality, we have used the property that $\bar{b}^n - b^n = O(\delta k_d)$ and $\bar{d}^n - d^n = O(\delta k_d) + O(\delta k_r)$. It follows from (84) that

$$(B(k)u)^T v = \frac{\Delta t}{2}\left[\sum_{i=1}^{N_x-1} k_i u_i(v_i + v_{i+1}) + k_{N_x}u_{N_x}v_{N_x}\right]$$

for vectors $u = (u_0, \dots, u_{N_x})^T$ and $v = (v_0, \dots, v_{N_x})^T$. Hence,

$$\frac{\partial \mathcal{F}_1}{\partial k_{di}} = \frac{1}{2}\sum_{n=0}^{N_t-1}(b_i^n + b_i^{n+1})(\eta_i^{n+1} + \eta_{i+1}^{n+1} - \xi_i^{n+1} - \xi_{i+1}^{n+1}),\ i = \overline{0, N_x - 1}, \tag{95}$$

$$\frac{\partial \mathcal{F}_1}{\partial k_{dN_x}} = \frac{1}{2}\sum_{n=0}^{N_t-1}(b_{N_x}^n + b_{N_x}^{n+1})(\eta_{N_x}^{n+1} - \xi_{N_x}^{n+1}), \tag{96}$$

$$\frac{\partial \mathcal{F}_1}{\partial k_{ri}} = \frac{1}{2}\sum_{n=0}^{N_t-1}(d_i^n + d_i^{n+1})(\xi_i^{n+1} + \xi_{i+1}^{n+1}),\ i = \overline{0, N_x - 1}, \tag{97}$$

$$\frac{\partial \mathcal{F}_1}{\partial k_{rN_x}} = \frac{1}{2}\sum_{n=0}^{N_t-1}(d_{N_x}^n + d_{N_x}^{n+1})(\xi_{N_x}^{n+1}). \tag{98}$$

Thus, we have proved the following theorem concerning the gradient of the objective function $J_1(k_d, k_r)$.

Theorem 4.2. *The objective functional $\mathcal{F}_1(k_d, k_r)$ defined by (85) is differentiable and its partial derivatives are given by (95)–(98), where $\eta := (\eta^1, \dots, \eta^{N_t})$ and $\xi := (\xi^1, \dots, \xi^{N_t})$ are the solutions of the adjoint equations (90)–(93).*

Remark 4.2. The adjoint equations (90)–(93) can be written in a similar form as the discrete forward equations (76) and (77). Therefore, their solutions can be explicitly computed without solving linear systems. Indeed, by direct calculations, we obtain the following problem for ξ:

- For $n = N_t$:

$$\left(1 + a_{N_x}^{N_t} + \frac{\Delta t}{2}k_{rN_x}\right)\xi_{N_x}^{N_t} = -(d_{N_x}^{N_t} - d_{N_x}^{N_t-1} - \theta_d^{N_t-1}),$$

$$\left(1 + a_i^{N_t} + \frac{\Delta t}{2}k_{ri}\right)\xi_i^{N_t} + \left(1 - a_{i+1}^{N_t} + \frac{\Delta t}{2}k_{ri}\right)\xi_{i+1}^{N_t} = 0,\ i = \overline{N_x - 1, 0},$$

- For $n = N_t - 1, N_t - 2, \dots, 1$:

$$\left(1 + a_{N_x}^n + \frac{\Delta t}{2}k_{rN_x}\right)\xi_{N_x}^n + \left(1 - a_{N_x}^n + \frac{\Delta t}{2}k_{rN_x}\right)\xi_{N_x}^{n+1} = (d^{n+1} - 2d^n + d^{n-1}) - \theta_d^n + \theta_d^{n-1},$$

$$\left(1 + a_i^n + \frac{\Delta t}{2}k_{ri}\right)\xi_i^n + \left(1 - a_{i+1}^n + \frac{\Delta t}{2}k_{ri}\right)\xi_{i+1}^n - \left(1 + a_i^n - \frac{\Delta t}{2}k_{ri}\right)\xi_i^{n+1} - \left(1 - a_{i+1}^n - \frac{\Delta t}{2}k_{ri}\right)\xi_{i+1}^{n+1} = 0, \quad i = \overline{N_x - 1, 0}.$$

Similarly, the adjoint problem for η is written as follows.

- For $n = N_t$:

$$\left(1 + a_{N_x}^{N_t} + \frac{\Delta t}{2} k_{dN_x}\right) \eta_{N_x}^{N_t} = \frac{\Delta t}{2} k_{dN_x} \xi_{N_x}^{N_t} - (b_{N_x}^{N_t} - b_{N_x}^{N_t-1} - \theta_b^{N_t-1}),$$

$$\left(1 + a_i^{N_t} + \frac{\Delta t}{2} k_{di}\right) \eta_i^{N_t} + \left(1 - a_{i+1}^{N_t} + \frac{\Delta t}{2} k_{di}\right) \eta_{i+1}^{N_t} = \frac{\Delta t}{2} k_{di} (\xi_i^{N_t} + \xi_{i+1}^{N_t}),\ i = \overline{N_x - 1, 0},$$

- For $n = N_t - 1, N_t - 2, \ldots, 1$:

$$\left(1 + a_{N_x}^{n} + \frac{\Delta t}{2} k_{dN_x}\right) \eta_{N_x}^{n} + \left(1 - a_{N_x}^{n} + \frac{\Delta t}{2} k_{dN_x}\right) \eta_{N_x}^{n+1} - \frac{\Delta t}{2} k_{dN_x} \left(\xi_{N_x}^{n} + \xi_{N_x}^{n+1}\right)$$
$$= (b^{n+1} - 2b^n + b^{n-1}) - \theta_b^n + \theta_b^{n-1},$$

$$\left(1 + a_i^{n} + \frac{\Delta t}{2} k_{di}\right) \eta_i^{n} + \left(1 - a_{i+1}^{n} + \frac{\Delta t}{2} k_{di+1}\right) \eta_{i+1}^{n} - \left(1 + a_i^{n} - \frac{\Delta t}{2} k_{di}\right) \eta_i^{n+1}$$
$$- \left(1 - a_{i+1}^{n} - \frac{\Delta t}{2} k_{di}\right) \eta_{i+1}^{n+1} = \frac{\Delta t}{2} k_{di} \left(\xi_i^{n} + \xi_i^{n+1} + \xi_i^{n+1} + \xi_{i+1}^{n+1}\right), \quad i = \overline{N_x - 1, 0}.$$

Remark 4.3. We remark that the discrete adjoint problem was constructed for the discretized forward problem and objective functional. Therefore, we do not consider the convergence or approximation of this discrete adjoint problem.

4.3. Using the L^2 data

For comparison, we also consider the case of L^2 data. That means, assume that the following data are available:

$$b_L(t) := b(L, t), \quad d_L(t) := d(L, t).$$

In this case, we consider the following objective function:

$$\mathcal{F}_2(k_d, k_r) := \frac{\Delta t}{2} \sum_{n=1}^{N_t} \left[b_{N_x}^n - b_L^n\right]^2 + \frac{\Delta t}{2} \sum_{n=1}^{N_t} \left[d_{N_x}^n - d_L^n\right]^2 + \frac{\gamma}{2} \mathcal{R}(k_d, k_r)$$
$$:= \frac{\Delta t}{2} \sum_{n=1}^{N_t} \left[\mathcal{M} b^n - b_L^n\right]^2 + \frac{\Delta t}{2} \sum_{n=1}^{N_t} \left[\mathcal{M} d^n - d_L^n\right]^2 + \frac{\gamma}{2} \mathcal{R}(k_d, k_r), \tag{99}$$

where $b_L^n = b_L(t_n)$, and $d_L^n = d_L(t_n)$, and $\frac{\gamma}{2} \mathcal{R}(k_d, k_r)$ is a regularization term. Note that $\mathcal{M}$ is the same as in the previous case, i.e., $\mathcal{M} = [0, \ldots, 1]$.

We remark that due to the error estimates (69) and (70), the first minimization problem with data θ_b and θ_d is stable. However, the second minimization problem with the L^2 data b_L and d_L is not stable. Therefore, we add the regularization term to stabilize $J_2(k_d, k_r)$. We use Morozov's discrepancy principle to find the regularization parameter γ and stop minimization algorithms for $J_2(k_d, k_r)$.

Using a similar derivation as in obtaining Theorem 4.2, we also obtain the following result concerning the gradient of $\mathcal{F}_2(k_d, k_r)$.

Theorem 4.3. *Assume that $\mathcal{R}$ is a differential function of (k_d, k_r). Then, the objective functional $\mathcal{F}_2(k_d, k_r)$ defined by (99) is differentiable and its partial derivatives are given by*

$$\frac{\partial \mathcal{F}_2}{\partial k_{di}} = \frac{\Delta t}{2} \sum_{n=0}^{N_t-1} (b_i^n + b_i^{n+1})(\tilde{\eta}_i^{n+1} + \tilde{\eta}_{i+1}^{n+1} - \tilde{\xi}_i^{n+1} - \tilde{\xi}_{i+1}^{n+1}) + \gamma \frac{\partial \mathcal{R}}{\partial k_{di}}, \tag{100}$$

$$\frac{\partial \mathcal{F}_2}{\partial k_{dN_x}} = \frac{\Delta t}{2} \sum_{n=0}^{N_t-1} (b_{N_x}^n + b_{N_x}^{n+1})(\tilde{\eta}_{N_x}^{n+1} - \tilde{\xi}_{N_x}^{n+1}) + \gamma \frac{\partial \mathcal{R}}{\partial k_{dN_x}}, \tag{101}$$

$$\frac{\partial \mathcal{F}_2}{\partial k_{ri}} = \frac{\Delta t}{2} \sum_{n=0}^{N_t-1} (d_i^n + d_i^{n+1})(\tilde{\xi}_i^{n+1} + \tilde{\xi}_{i+1}^{n+1}) + \gamma \frac{\partial \mathcal{R}}{\partial k_{ri}}, \tag{102}$$

$$\frac{\partial \mathcal{F}_2}{\partial k_{rN_x}} = \frac{\Delta t}{2} \sum_{n=0}^{N_t-1} (d_{N_x}^n + d_{N_x}^{n+1})(\tilde{\xi}_{N_x}^{n+1}) + \gamma \frac{\partial \mathcal{R}}{\partial k_{rN_x}}, \tag{103}$$

for $i = 0, \ldots, N_x - 1$, where $\tilde{\eta} = (\tilde{\eta}^1, \ldots, \tilde{\eta}^{N_t})$ and $\tilde{\xi} = (\tilde{\xi}^1, \ldots, \tilde{\xi}^{N_t})$ are the solutions of the following adjoint equations

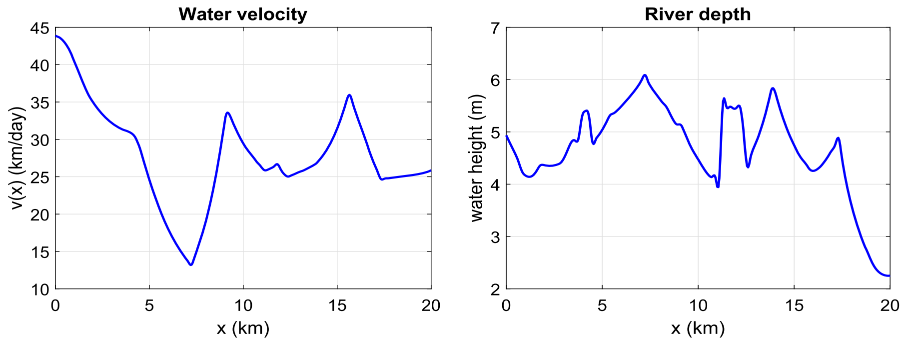
$$A^{N_t} \tilde{\xi}^{N_t} + B^T(k_r) \tilde{\xi}^{N_t} = -\Delta t \mathcal{M}^T [\mathcal{M} d^{N_t} - d_L^{N_t}], \tag{104}$$

$$(A^n)^T \xi^n + B^T(k_r)(\tilde{\xi}^n + \tilde{\xi}^{n+1}) - (C^n)^T \tilde{\xi}^{n+1} = -\Delta t \mathcal{M}^T [\mathcal{M} d^n - d_L^n], \tag{105}$$

$$A^{N_t} \tilde{\eta}^{N_t} + B^T(k_d) \tilde{\eta}^{N_t} - B^T(k_d) \tilde{\xi}^{N_t} = -\Delta t \mathcal{M}^T [\mathcal{M} b^{N_t} - b_L^{N_t}], \tag{106}$$

$$(A^n)^T \tilde{\eta}^n + B^T(k_d)(\tilde{\eta}^n + \tilde{\eta}^{n+1}) - (C^n)^T \tilde{\eta}^{n+1} - B^T(k_d)(\tilde{\xi}^n + \tilde{\xi}^{n+1})$$
$$= -\Delta t \mathcal{M}^T [\mathcal{M} b^n - b_L^n], \tag{107}$$

for $n = N_t - 1, \ldots, 1$.



(a) Water velocity (d) River depth

Fig. 1. Water velocity (a) and water depth (b) in the considered section of the Nhue-Day river.

4.4. Parametrization of the coefficients k_d and k_r

To reconstruct the coefficients $k_d(x)$ and $k_r(x)$, we parametrize them as follows.

$$k_d(x) \approx \sum_{n=1}^{N_b} q_{dn}\phi_n(x), \quad k_r(x) \approx \sum_{n=1}^{N_b} q_{rn}\phi_n(x),$$

where $N_b \in \mathbb{N}^+$ represents the number of basis functions chosen to approximate the coefficients and $\phi_1, \phi_2, \dots, \phi_{N_b}$ are known basis functions. In this paper, we choose ϕ_n as cosine functions:

$$\phi_n(x) = \cos((n-1)\pi x/L), \quad n = 1, 2, \dots, N_b.$$

For simplicity of notation, we denote by

$$q_d = (q_{d1}, q_{d2}, \dots, q_{dN_b})^T, \quad q_r = (q_{r1}, q_{r2}, \dots, q_{rN_b})^T$$

the vectors of parameters to be determined. We also denote the objective functions of (q_d, q_r) by $\mathcal{F}_1(q_d, q_r)$ and $\mathcal{F}_2(q_d, q_r)$. Then, the partial derivatives of the objective functions with respect to the new variables are given by

$$\frac{\partial \mathcal{F}_j}{\partial q_{dn}} = \sum_{i=0}^{N_x} \phi_n(x_i)\frac{\partial \mathcal{F}_j}{\partial k_{di}}, \quad \frac{\partial \mathcal{F}_j}{\partial q_{rn}} = \sum_{i=0}^{N_x} \phi_n(x_i)\frac{\partial \mathcal{F}_j}{\partial k_{ri}}, \quad j = 1, 2.$$

5. Numerical examples

In this section we present numerical examples to demonstrate the performance of the proposed algorithms for determining the coefficients k_d and k_r. In the following numerical examples, the domain and the parameters were chosen as realistic values in a river. More precisely, we considered a 10 km section of Nhue-Day river in Vietnam, i.e., $L = 10$. The time interval was chosen as $T = 2$ (day). The water velocity was obtained by solving a Saint-Venant's equation (see, e.g., [1], section 3.3) using real hydraulic and geological data from the selected river section. However, due to lack of experimental BOD and DO data, we use simulated BOD and DO data in this work. Numerical results with real BOD and DO data, which we are currently in the collection process, will be presented in our future work.

In our numerical tests, we assumed that the water velocity did not depend on time, that is $v(x,t) = v(x)$. Fig. 1 depicts the water velocity and river depth. The initial conditions were chosen as follows:

$$f_b(x) = f_d(x) = 1$$

and the boundary conditions were chosen to be

$$g_b(t) = 1 + 2\sin(2\pi t/T), \quad g_d(t) = 1.$$

The source function was chosen to be zero, i.e., there was no pollution source within the considered river section when the model coefficients were estimated.

The measured boundary data of both BOD and DO at $x = 10$ were obtained by solving the forward problem (1)–(4) and then perturbed with additive pseudo random noise of magnitude of 0.2. To avoid the so-called *inverse crime*, we used 401 grid points in the x-direction and 5761 points in the t-direction in solving the forward problem for generating the data, but doubled the grid sizes in both directions in solving the inverse problem. In all the tests, we chose the initial guesses of both k_d and k_r to be zero. The parameter τ in Morozov's discrepancy principle was chosen to be $\tau = 1.01$.

Example 1. In the first example, we reconstructed the coefficients $k_d(x)$ and $k_r(x)$ of the forms

$$k_d(x) = 1 + 0.4\sin(2\pi x/L), \quad k_r(x) = 1.5 + 0.5\sin(2\pi x/L). \tag{108}$$

To approximate these coefficients, we used 10 basis functions, i.e., $N_b = 10$. Figs. 2(a)–(b) depicts the reconstructed coefficients $k_d(x)$ and $k_r(x)$ together with the exact coefficients with data of BOD and DO corrupted with 5% additive random noise. The noise was generated by the Matlab

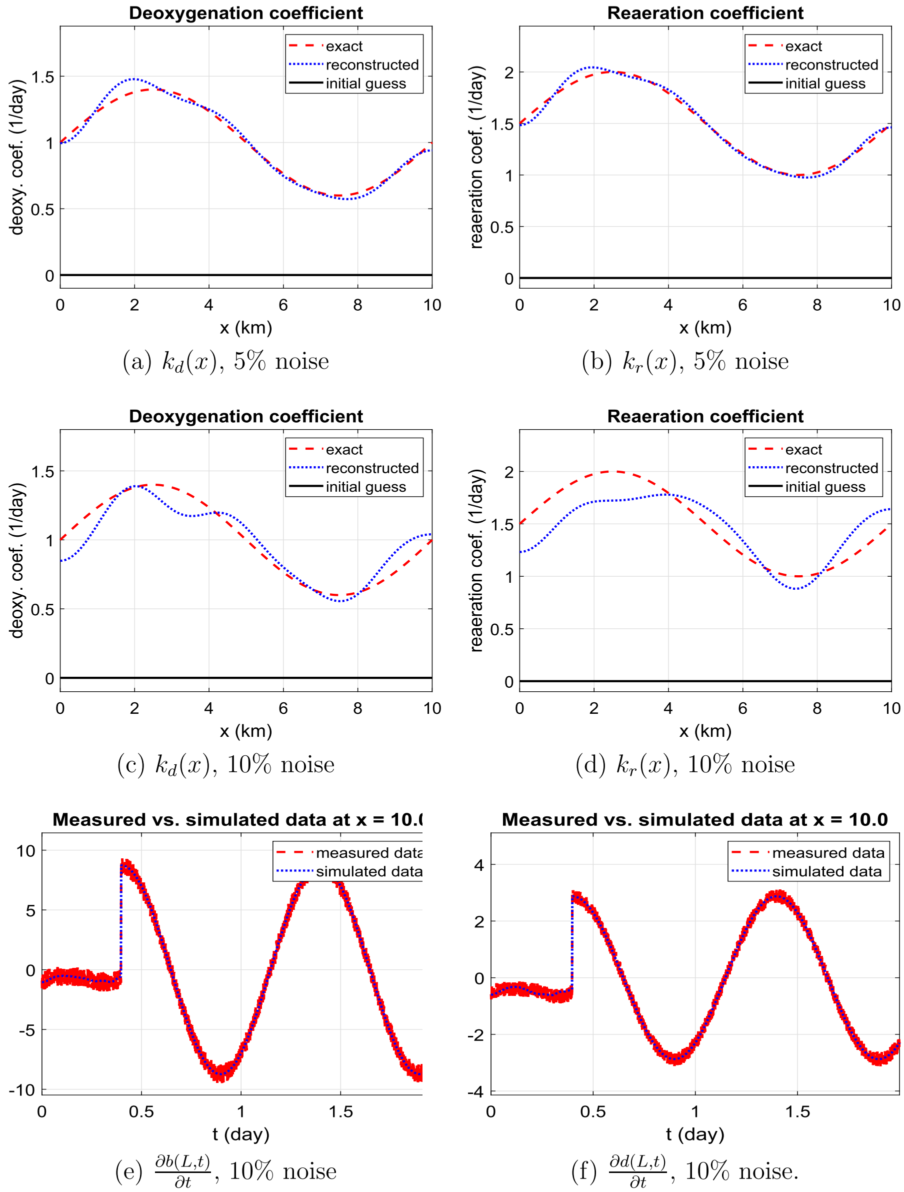


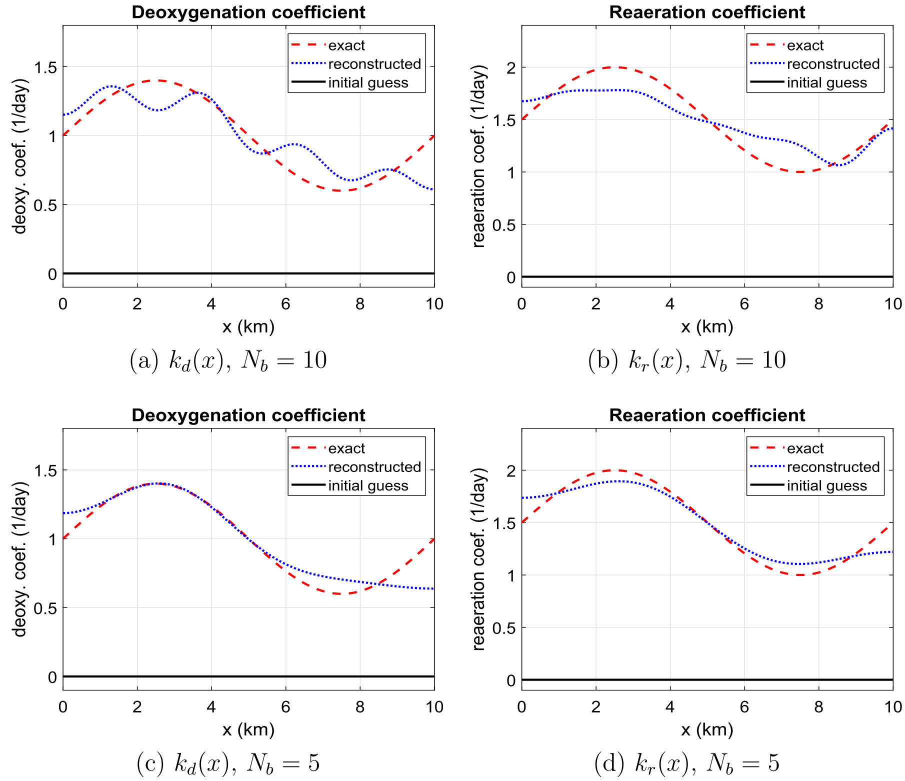
Fig. 2. Exact coefficients $k_d(x)$ and $k_r(x)$ in Example 1 and the reconstructed ones by minimizing the objective function $\mathcal{F}_1$. (a)-(b): reconstruction with 5% noise; (c)-(d): reconstruction with 10% noise; (e)-(f): data vs. simulation with the reconstructed coefficients at 10% noise. The algorithm was stopped using Morozov's discrepancy principle with $\tau = 1.01$.

function `rand`. These figures show that the reconstructions were very accurate for both k_d and k_r. To analyze the effect of the measurement noise on the reconstruction accuracy, we show in Figs. 2(c)–(d) the reconstructed coefficients with data corrupted by 10% measurement noise. We still can see from these figures that the coefficients were still reconstructed quite accurately. Figs. 2(e)–(f) depict the measured data and the solution of the forward problem associated with the reconstructed coefficients shown in Figs. 2(c)–(d). It is clear that the model fits well the measured data.

For comparison, in Fig. 3 we show the reconstruction results using the L^2 boundary data of BOD and DO, i.e., by minimizing the objective function $\mathcal{F}_2$ given by (99). In this test, we chose $\mathcal{R}$ as the standard Tikhonov regularization term, $\mathcal{R}(q) = |q|^2$ for a vector $q \in \mathbb{R}^{2N_b}$. To obtain the regularization parameter, we started the algorithm with $\gamma = 10^{-2}$ and then reduce it by half until Morozov's discrepancy principle is satisfied. Here we also chosen $\tau = 1.01$. At each value of γ, the iterative procedure was stopped when the first-order optimality condition was less than 10^{-6} or Morozov's discrepancy principle was satisfied.

For this algorithm, we tested two choices of the basis functions. Figs. 3(a)–(b) depict the results when 10 basis functions were used to approximate the coefficients, as in the previous test. Figs. 3(c)–(d) depict the results for 5 basis functions. The reason for reducing the number of basis functions was that the results with 10 basis functions looked more oscillating. Reducing the number of basis functions helps further stabilize the inverse problem. In this test, we used the same 5%-noise data set as in obtaining the results in Figs. 2(a)–(b). Comparing Fig. 2 with Fig. 3, we can see that the former was more accurate and stable even with a large number of basis functions. We note that unlike the objective function $\mathcal{F}_2$, no regularization method was needed in $\mathcal{F}_1$.

Example 2. In practice, some empirical formulas are widely used for the reaeration coefficient $k_r(x)$. One of them is the so-called O'Connor-Dobbins' formula given by (see, e.g., [14], chapter 10)



(a) $k_d(x)$, $N_b = 10$ (b) $k_r(x)$, $N_b = 10$

(c) $k_d(x)$, $N_b = 5$ (d) $k_r(x)$, $N_b = 5$

Fig. 3. Exact coefficients $k_d(x)$ and $k_r(x)$ in Example 1 and the reconstructed ones using the L^2 boundary data with 5% noise. (a)-(b): $N_b = 10$, $\tau = 1.03$; (c)-(d): $N_b = 5$, $\tau = 1.01$.

$$k_r(x) = 3.95(v(x))^{0.5}(h(x))^{-1.5},$$

where $v(x)$ is measured in meters per second and h is in meters. However, the unit of $k_r(x)$ is 1/day. In this example we reconstructed the same coefficient $k_d(x)$ as in Example 1 and coefficient $k_r(x)$ given by this O'Connor-Dobbins' formula. All parameters were chosen the same as in Example 1. For objective function $\mathcal{F}_1$, we chose 10 basis functions while for objective function $\mathcal{F}_2$ we chose 5 basis functions again for stability reason.

Figs. 4(a)–(b) show the reconstructed coefficients with $\mathcal{F}_1$. The algorithm was still able to reconstruct the coefficients quite accurately in this case. Note that the coefficient k_r has some sudden changes due to the sudden changes in the water velocity and the river depth as shown in Fig. 1. As a comparison, we show in Figs. 4(e)–(f) the results with $\mathcal{F}_2$. Again, the former looks more accurate than the latter.

6. Conclusions

We investigated a CIP of reconstructing the reaction coefficients in a system of advection-reaction equations from boundary data. The equations represent the evolution of the BOD and DO in a river. We proved stability estimates of the CIP and error estimates of the solution obtained by the least-squares method. Numerical results have demonstrated the efficiency of the proposed approach.

Data availability

No data was used for the research described in the article.

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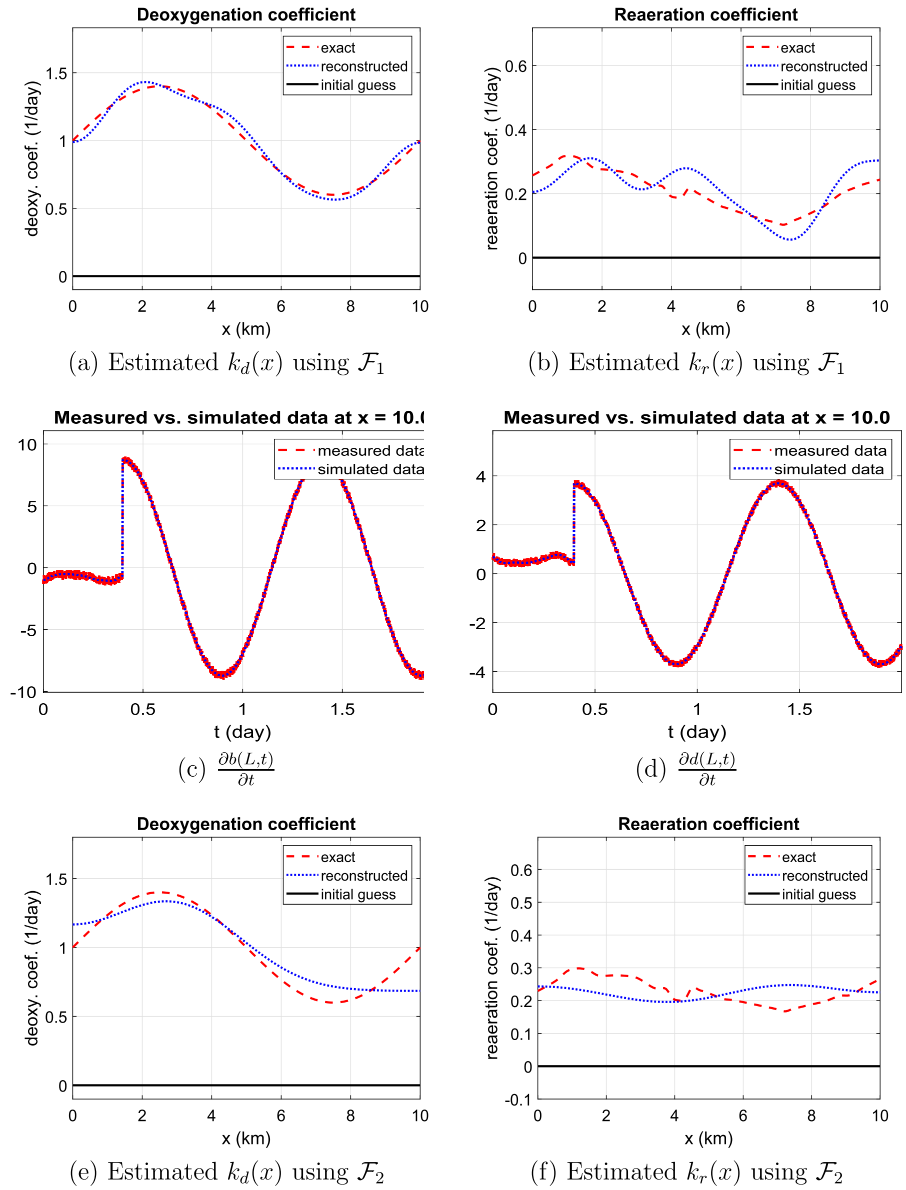

Fig. 4. Exact coefficients $k_d(x)$ and $k_r(x)$ in Example 2 and the reconstructed ones using data with 5% noise. (a)-(b): using objective function $\mathcal{F}_1$ with 10 basis functions; (c)-(d): measured vs. simulated data at $x = 10$; (e)-(f): using objective function $\mathcal{F}_2$ with 5 basis functions. Measurement noise is 5%.

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