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Reconstructing the Absorption Function in a Quasi-Linear Sorption Dynamic Model via an Iterative Regularizing Algorithm

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Abstract. This study addresses the parameter identification problem in a system of time-dependent quasi-linear partial differential equations (PDEs). Using the integral equation method, we prove the uniqueness of the inverse problem in nonlinear PDEs. Moreover, using the method of successive approximations, we develop a novel iterative algorithm to estimate sorption isotherms. The stability results of the algorithm are proven under both *a priori* and *a posteriori* stopping rules. A numerical example is given to show the efficiency and robustness of the proposed new approach.

AMS subject classifications: 65N15, 65N30

Key words: Inverse problem, quasi-linear dynamic model, uniqueness, method of successive approximations, stability.

1 Introduction

In this study, we consider the inverse problem of estimating function $\varphi(\cdot)$ in the following quasi-linear dynamic sorption model:

$$u_x + a_t = 0, \quad 0 < x < l, \quad 0 < t < T, \tag{1.1a}$$

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$$a_t = \varphi(u) - a, \qquad 0 < x < l, \quad 0 < t < T, \tag{1.1b}$$
$$u(0,t) = \mu(t), \qquad 0 \le t \le T, \tag{1.1c}$$
$$a(x,0) = 0, \qquad 0 \le x \le l, \tag{1.1d}$$

where $u(x,t)$ is the gas concentration in the pores of the tube between the sorbent grains, which depends on the metric argument x, and changes from the left input end of the sorption tube where $x=0$ to the right outlet section of the tube where $x=l$; the function $a(x,t)$ takes the values of the concentration of gas inside the sorbent grains depending on the same arguments. Function $\mu(t)$ represents the concentration of the input gas flow. Function $\varphi(\cdot)$ is a scaling factor that indicates the ratio of the gas concentration outside the sorbent grains to that inside the sorbent grains, depending on the external gas concentration. This quantity $\varphi(\cdot)$ is called the sorption isotherm, which describes the course of the chemical absorption of a particular gas by a certain sorbent. For the physical background of the dynamic sorption model, we refer to [21,24] and the references therein.

Although determining the values of sorption isotherms is extremely important in physical chemistry, it presents significant experimental difficulties, particularly in dynamic processes. A modern technique for obtaining sorption isotherms involves solving an inverse problem so that the simulated dynamic quantity coincides with the actual experimental results. During the last decades, certain inverse problems in estimating sorption isotherms and other parameters in some dynamic PDE models have been intensively studied, for example, [3,5,10,14,20,22,23,25–27,29–31]. We also refer to [1,2,7,8,12,15–19,28] for more related inverse problem studies. The main contribution of this work is twofold. First, we provide the uniqueness results for the nonlinear inverse problem of recovering the sorption isotherm function $\varphi(\cdot)$ in the PDE model (1.1a)-(1.1d). Second, we develop an iterative regularization algorithm for the efficient reconstruction of sorption isotherms.

This paper is structured as follows. In the next section, we perform a theoretical analysis for both the forward and inverse problems of (1.1a)-(1.1d). Section 3 describes the development of an iterative approach for solving the inverse problem of estimating sorption isotherms. A convergence analysis of the approach is also presented. In Section 4, numerical simulations for a model problem are presented. Finally, concluding remarks are given in Section 5.

2 Analysis of the forward and inverse problems

We begin with the well-posedness of the forward model (1.1a)-(1.1d), which was investigated decades ago by Denisov [6, Theorem 2.1] and [4, Theorem 5.4.1] with the study of properties of the solution for the problem (1.1a)-(1.1d) (see [4, Theorem 5.4.2]).

Theorem 2.1. *Let the functions $\mu(\cdot)$ and $\varphi(\cdot)$ satisfy the following conditions.*

$$\mu(t)\in C^1[0,T], \quad \mu'(t)>0 \qquad \text{for all } t\in[0,T], \quad \mu(0)=0, \tag{2.1a}$$

$$\varphi(s)\in C^1(\mathbb{R}), \quad \varphi'(s)\in(0,\varphi_0] \qquad \text{for all } s\in\mathbb{R}, \quad \varphi(0)=0. \tag{2.1b}$$

Then, there exists a unique pair of functions $(u,a)\in C^1(\bar{Q})\times C^1(\bar{Q})$ satisfying problem (1.1a)-(1.1d), *where $Q:=\{(x,t):0<x<l,\ 0<t<T\}$ and $\bar{Q}$ is the closure of Q.*

Theorem 2.2. *Let the functions $\mu(\cdot)$ and $\varphi(\cdot)$ satisfy the following conditions* (2.1a)-(2.1b), *and the pair of functions (u,a) is the solution of the problem* (1.1a)-(1.1d), *then*

$$\begin{aligned} &u_t(x,t)>0, \quad a_t(x,t)>0 && \text{for all } x\in[0,l], \quad t\in[0,T], \\ &0\le u(x,t)\le\mu(\tau) \quad 0\le a(x,t)\le\varphi(\mu(\tau)) && \text{for all } x\in[0,l], \quad t\in[0,\tau], \quad \tau\in(0,T]. \end{aligned}$$

From Eq. (1.1b), in the form of a linear inhomogeneous ordinary differential equation $a_t+a=\varphi(u)$ with the initial condition (1.1d), we derive the integral equation

$$a(x,t)=\int_0^t e^{-(t-\tau)}\varphi(u(x,\tau))d\tau, \quad (x,t)\in\bar{Q}. \tag{2.2}$$

Furthermore, from Eq. (1.1a), in the form of a nonlinear inhomogeneous ordinary differential equation,

$$u_x(x,t)=-\varphi(u(x,t))+\int_0^t e^{-(t-\tau)}\varphi(u(x,\tau))d\tau, \quad (x,t)\in\bar{Q},$$

with the initial condition (1.1c), we obtain the integral equation of Type II for the solution function $u(x,t)$ in $\bar{Q}$:

$$u(x,t)=\mu(t)-\int_0^x\varphi(u(s,t))ds+\int_0^x\int_0^t e^{-(t-\tau)}\varphi(u(s,\tau))d\tau ds, \tag{2.3}$$

which can be further used to obtain the function $a(x,t)$ using formula (2.2).

Remark 2.1. The solution of Eq. (2.3) is obtained numerically using the method of successive approximations based on equality (2.3) in the form of a recurrent formula.

In this study, we focused on the following inverse problem:

Problem 2.1 (IP). Recover the sorption isotherm φ in some regions as well as the solutions (u,a) of the system (1.1a)-(1.1d) with a known boundary function $\mu(t)$ satisfying (2.1a) from the noisy measurement of dynamical boundary velocity $h_\delta(t)\in\dot{C}[0,T]:=\{h(t)\in C[0,T]:h(0)=0\}$ of $h(t)\equiv u_x(0,t)$.

Remark 2.2. For data with lower regularity (e.g., $h_\delta(t)\in L^2[0,T]$), a smoothing technique can be employed to obtain smoothed data $h_\delta(t)\in\dot{C}[0,T]$ (see [9, Section 4.2] or [13, Section 4]).

Since the spectrum of differential operator has a accumulation point at infinity, the inverse problem (**IP**) is ill-posed in the sense that a tiny perturbation of the measurement data $h_\delta(t)$ may give a large change in the conventional resolution of φ. Therefore, for the problem of noisy data $h_\delta(t)$, some regularization methods should be employed to obtain meaningful function φ. With Tikhonov regularization, the inverse problem (**IP**) can be converted to the following minimization problem:

$$\min_{\tilde{\varphi} \text{ satisfies (2.1b)}} \|h_\delta(t)-u_x(0,t;\tilde{\varphi})\|^2_{L^2[0,T]}+\varepsilon\mathcal{R}(\tilde{\varphi}), \tag{2.4}$$

where u solves (1.1a)-(1.1d) with a given $\tilde{\varphi}$ [†], $\varepsilon>0$ is the regularization parameter, and $\mathcal{R}(\tilde{\varphi})$ denotes the regularization term, which reflects the *a priori* information of sorption isotherm φ.

There are two essential difficulties when employing the solution model (2.4). First, it is difficult to select appropriate regularization term $\mathcal{R}$ as well as regularization parameter ε in practice. By the standard argument of regularization theory of inverse problems, the optimal choices of these two quantities depend on the ground truth φ, which is unknown in real-world problems. Second, even both $\mathcal{R}$ and ε are given, the numerical realization of the PDE-constrained optimization problem (2.4) is a hard task since it is a non-convex optimization with a nonlinear PDEs constraint. Therefore, the main purpose of this work is to find a new replacement model instead of (2.4), which would be much simpler but sufficiently accurate.

To obtain an equation with respect to the function $\varphi(\cdot)$, Eq. (2.3) can be differentiated using argument x to obtain the result in the form of an equation

$$\varphi(u(x,t))=\int_0^t e^{-(t-\tau)}\varphi(u(x,\tau))d\tau-u_x(x,t), \quad (x,t)\in\bar{Q}.$$

With variable substitutions $s=u(0,t)$ and $\theta=u(0,\tau)$, we derive the equation for $x=0$:

$$\varphi(s)=\int_0^{\mu^{-1}(s)}\frac{e^{-\left(\mu^{-1}(s)-\mu^{-1}(\theta)\right)}}{\mu'(\mu^{-1}(\theta))}\varphi(\theta)d\theta-u_x(0,\mu^{-1}(s)), \quad s\in[0,\mu(T)]. \tag{2.5}$$

Eq. (2.5) is an affine Volterra integral equation of Type II. It can be used with a given perturbation $h_\delta(t)$ instead of the exact measurement $h(t)\equiv u_x(0,t)$ to solve the inverse problem with approximate determination of the function $\varphi(s)$ using the method of successive approximations from the equation

$$\varphi(s)=\int_0^{\mu^{-1}(s)}\frac{e^{-\left(\mu^{-1}(s)-\mu^{-1}(\theta)\right)}}{\mu'(\mu^{-1}(\theta))}\varphi(\theta)d\theta-h_\delta(\mu^{-1}(s)), \quad s\in[0,\mu(T)],$$

or for the composite function $\varphi(\mu(t))\equiv\psi(t)$ from the equation

$$\psi(t)=\int_0^t e^{-(t-\tau)}\psi(\tau)d\tau-h_\delta(t), \quad t\in[0,T], \tag{2.6}$$

[†]It is not difficult to show that $u_x(0,t;\tilde{\varphi}(\cdot))=-\tilde{\varphi}(\mu(t))+\int_0^t e^{-(t-\tau)}\tilde{\varphi}(\mu(\tau))d\tau$.

with the subsequent transition to the function $\varphi(s)$ in the form

$$\varphi(s)=\psi(\mu^{-1}(s)), \quad s\in[0,\mu(T)]. \tag{2.7}$$

Before proving the uniqueness of (**IP**), we provide a definition of mild solutions of (**IP**).

Definition 2.1. *A triad of functions* $(\varphi(s),u(x,t),a(x,t))$ *is called a mild solution of* (**IP**) *if* $\varphi(s)$, $u(x,t)$, $a(x,t)$ *satisfy* (1.1a)-(1.1d) *with conditions* (2.1a), $h_\delta(t)=u_x(0,t)\in\dot{C}[0,T]$, $u,a\in C^1(\bar{Q})$, *and* φ *satisfies*

$$\varphi(s)\in C^1[(0,\mu(T)], \quad \varphi'(s)\in(0,\varphi_0], \quad s\in[0,\mu(T)], \quad \varphi(0)=0. \tag{2.8}$$

Theorem 2.3. *The inverse problem* (**IP**) *has no more than one mild solution.*

Proof. Define

$$A:C[0,T]\to C[0,T], \quad A\psi(t):=\int_0^t e^{-(t-\tau)}\psi(\tau)d\tau. \tag{2.9}$$

Evidently, A is a bounded linear operator on the Banach space $C[0,T]$ with

$$\begin{aligned}\|A\|\equiv\|A\|_{\mathcal{L}(C[0,T],C[0,T])}&:=\frac{\|A\psi(\tau)\|_{C[0,T]}}{\|\psi(\tau)\|_{C[0,T]}}=\frac{\left\|\int_0^t e^{-(t-\tau)}\psi(\tau)d\tau\right\|_{C[0,T]}}{\|\psi(\tau)\|_{C[0,T]}}\\&\le\left\|\int_0^t e^{-(t-\tau)}d\tau\right\|_{C[0,T]}=\|1-e^{-t}\|_{C[0,T]}=1-e^{-T}<1.\end{aligned}$$

According to [11, Theorem 2.14], $I-A$ has a bounded inverse on $C[0,T]$ given by the Neumann series

$$(I-A)^{-1}=\sum_{k=0}^{\infty}A^k. \tag{2.10}$$

Hence, Eq. (2.6) has a unique solution

$$\psi=-(I-A)^{-1}h_\delta, \tag{2.11}$$

that gives $\varphi(s)$ by the formula (2.7).

Now, let there exist two solutions $(\varphi_1(\cdot),u_1(x,t),a_1(x,t))$ and $(\varphi_2(\cdot),u_2(x,t),a_2(x,t))$ of (**IP**) with initial functions $\mu(t)$ and $h_\delta(t)$. If the functions $\varphi_1(\mu(t))=\psi_1(t)$ and $\varphi_2(\mu(t))=\psi_2(t)$ satisfy the Eq. (2.6), then, consequently, the uniqueness of (**IP**) solution follows from the equalities $\psi(t)=\psi_1(t)=\psi_2(t)$ as the unique solution of Eq. (2.6) and from relations (2.7). □

Remark 2.3. The existence of solutions (u,a) can not be guaranteed by Theorem 2.2 due to the possibility of violation of sufficient condition (2.1b).

Remark 2.4. The conditions (2.1): $\mu(t)\in C^1[0,T]$, do not allow the conclusivity of the function $\mu(t)$ on the segment $[0,T]$ as $\lim_{t\to T}\mu(t)=\infty$, since according to Weierstrass's first theorem about the limitation of a continuous function defined on the segment. All mathematical results in this paper are obtained under conditions (2.1). Of the physico-chemical correspondences, the function $\mu(t)$ determines the concentration of a substance (absorbed gas) at a point, and is also a limited value. A mathematical problem can be considered with an integrable function $\mu(t)$, for example, from space $L_2[0,T]$. Such an expansion would require a separate study.

3 An iterative algorithm

According to the proof of Theorem 2.3, the partial sums

$$\psi_n := -\sum_{k=0}^{n} A^k h_\delta$$

of the Neumann series (2.10) satisfy $\psi_{n+1}=A\psi_n-h_\delta$ for all $n\geq 0$. Hence, the Neumann series (2.10) is related to successive approximations using the following theorem.

Proposition 3.1. *for any measurement $h_\delta(t)\in\dot{C}[0,T]$, the successive approximations*

$$\psi_{n+1}=A\psi_n-h_\delta,\quad n=0,1,\dots, \tag{3.1}$$

with an arbitrary $\psi_0\in\dot{C}[0,T]$ converge in $\dot{C}[0,T]$ to the unique solution of $\psi=A\psi-h_\delta$.

Proof. This follows from [11, Theorem 2.15]. □

Remark 3.1. Condition (2.1b) is not used in Section 3. In particular, ψ_n may not satisfy (2.1b) in general.

Now we are in a position to give the main result of this work–two stability results for the iterative algorithm (3.1). To that end, let $\psi^\dagger$ be the unique solution of the equation $\psi=A\psi-u_x(0,t)$ such that $\varphi^\dagger(s)=\psi^\dagger(\mu^{-1}(s))$, $(u(x,t;\varphi^\dagger(s)),a(x,t;\varphi^\dagger(s)))$ is the unique mild solution of (**IP**). Moreover, suppose that the measurement dynamical data $h_\delta(t)$ obeys the deterministic noise model

$$\|h_\delta(t)-h(t)\|_{C[0,T]}\leq\delta \tag{3.2}$$

with a known noise level $\delta>0$.

The following theorem provides the stability for the iterative algorithm (3.1), which indicates that the numerical $\psi_{n(\delta)}$ converges to the true solution $\psi^\dagger$ after appropriate steps.

Theorem 3.1 (A priori stopping rule)**.** *If the stopping index $n=n(\delta)$is selected such that $n\geq C\cdot\ln(\delta^{-1})$ with $C>1/\ln(1/\|A\|)$, then the iterative algorithm* (3.1) *exhibits the linear convergence rate, i.e.,*

$$\|\psi_{n(\delta)}-\psi^{\dagger}\|_{C[0,T]}=\mathcal{O}(\delta) \quad \text{as} \quad \delta\to 0. \tag{3.3}$$

Proof. Let ψ_δ be the unique solutions of equations $\psi=A\psi-h_\delta$. Then, from (3.2) and (2.10), using the inequalities

$$\|(I-A)^{-1}\|\leq\sum_{k=0}^{\infty}\|A^k\|\leq\sum_{k=0}^{\infty}\|A\|^k=(1-\|A\|)^{-1},$$

we derive

$$\|\psi_\delta-\psi^{\dagger}\|_{C[0,T]}\leq\|(I-A)^{-1}(h_\delta-u_x(0,t))\|_{C[0,T]}\leq\|(I-A)^{-1}\|\delta\leq(1-\|A\|)^{-1}\delta. \tag{3.4}$$

Furthermore, by selecting $n(\delta)$ (i.e., $n\geq C\cdot\ln(\delta^{-1})$ with $C>1/\ln(1/\|A\|)$), we deduce that for all $\delta\in(0,1]$,

$$\|A\|^{n(\delta)}\leq\delta. \tag{3.5}$$

Finally, according to successive formula (3.1), we obtain

$$\psi_n-\psi_\delta=A(\psi_{n-1}-\psi_\delta)=\cdots=A^n(\psi_0-\psi_\delta), \tag{3.6}$$

which, using inequalities (3.4), (3.5), and $\|A\|<1$, implies that

$$\begin{aligned}\|\psi_{n(\delta)}-\psi^{\dagger}\|_{C^1[0,T]}&\leq\|\psi_{n(\delta)}-\psi_\delta\|_{C[0,T]}+\|\psi_\delta-\psi^{\dagger}\|_{C[0,T]}\\&\leq\|A^n\|\|\psi_0-\psi_\delta\|_{C[0,T]}+\|\psi_\delta-\psi^{\dagger}\|_{C[0,T]}\\&\leq\|A\|^n(\|\psi_0-\psi^{\dagger}\|_{C[0,T]}+\|\psi^{\dagger}-\psi_\delta\|_{C[0,T]})+\|\psi_\delta-\psi^{\dagger}\|_{C[0,T]}\\&\leq\|A\|^n\|\psi_0-\psi^{\dagger}\|_{C[0,T]}+2\|\psi_\delta-\psi^{\dagger}\|_{C[0,T]}\\&\leq(\|\psi_0-\psi^{\dagger}\|_{C[0,T]}+2(1-\|A\|)^{-1})\delta.\end{aligned} \tag{3.7}$$

This yields the required estimation in (3.3). □

Theorem 3.2 (A posteriori stopping rule)**.** *If the iteration of* (3.1) *is terminated according to the following stopping rule,*

$$\|\psi_{n(\delta)+1}-\psi_{n(\delta)}\|_{C[0,T]}\leq c\cdot\delta<\|\psi_{n+1}-\psi_n\|_{C[0,T]}, \quad 0\leq n<n(\delta), \tag{3.8}$$

for some $c>0$. Then,

$$n(\delta)=\mathcal{O}(\ln(\delta^{-1})) \quad \text{and} \quad \psi_{n(\delta)}\to\psi^{\dagger} \quad \text{in} \quad C[0,T] \quad \text{as} \quad \delta\to 0. \tag{3.9}$$

Proof. The well-posedness of the stopping rule (3.8) follows from the following relation:

$$\|\psi_{n+1}-\psi_n\|_{C[0,T]}=\|A(\psi_n-\psi_{n-1})\|_{C[0,T]}=\cdots=\|A^n(\psi_1-\psi_0)\|_{C[0,T]}\to 0 \tag{3.10}$$

as $n\to\infty$.

Let $\{\delta_k\}$ be a sequence converging to 0 as $k\to\infty$, and let h_{δ_k} be a corresponding sequence of noisy data with

$$\|h_{\delta_k}(t)-h(t)\|_{C[0,T]}\le\delta_k.$$

For each tuple (δ_k,h_{δ_k}), denote by $n_k=n(\delta_k)$ the corresponding terminating time point determined from (3.8).

To prove this assertion, we distinguish between two cases: (i) n_k has a finite accumulation point n_* or (ii) $n_k\to\infty$ as $k\to\infty$.

For case (i), there exists an index k_0 such that for all $k>k_0: n_k\equiv n_*$. Consequently, estimates (3.9) hold because ψ_{n_*} is the unique solution of $\psi=A\psi+h$.

Now, consider case (ii). Using (3.7), we deduce that

$$\|\psi_{n_k}-\psi^\dagger\|_{C[0,T]}\le\|A\|^{n_k}\|\psi_0-\psi^\dagger\|_{C[0,T]}+2\|\psi_{\delta_k}-\psi^\dagger\|_{C[0,T]}\to 0$$

as $k\to\infty$, where $\|A\|^{n_k}\to 0$ when $n_k\to\infty$.

Finally, by combining (3.8) and (3.10), we deduce the following:

$$c\delta_k<\|\psi_{n_k}-\psi_{n_k-1}\|_{C[0,T]}\le\|A^{n_k}(\psi_1-\psi_0)\|_{C[0,T]}\le\|A\|^{n_k-1}\|\psi_1-\psi_0\|_{C[0,T]},$$

which implies that

$$n(\delta)\le 1+\ln\Big(\|\psi_1-\psi_0\|_{C[0,T]}c^{-1}\delta^{-1}\Big)\Big/\ln(\|A\|^{-1}).$$

Thus, we complete the proof. □

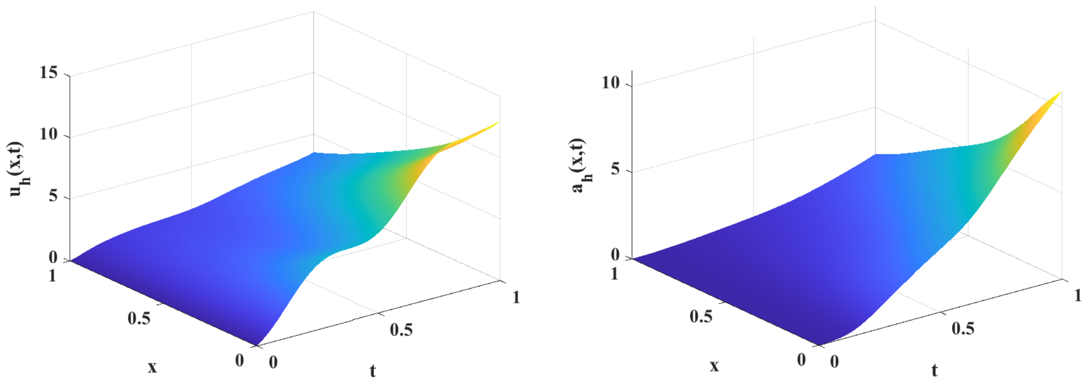
4 Numerical examples

In this section, we present numerical experiments to illustrate the theoretical predication of the convergence analysis developed in the previous sections. In the simulations ‡, we consider nonlinear functions $\varphi^\dagger(u)=2u-\sin(u)$ and $\mu(t)=13t-\cos(4\pi t)+1$ in (1.1b) and (1.1c), respectively. Such choices of φ and μ satisfy both of conditions (2.1a)-(2.1b) in Theorem 2.1. Moreover, we set $l=1$ and $T=1$.

First, the experiment is concerned with the finite difference method for solving (1.1a)-(1.1d). We employ the backward finite difference scheme to discrete (1.1a) and (1.1b) for both space and time domain and obtain the following discrete scheme:

$$\begin{cases} A_n^{k+1}=A_n^k+\Delta t[\varphi(U_n^k)-A_n^k], \\ U_{n+1}^k=U_n^k-\dfrac{h}{\Delta t}(A_n^{k+1}-A_n^k), \end{cases} \tag{4.1}$$

‡All the computations were performed on a dual core PC with 16.00 GB RAM with MatLab version R2021b.



(a) Numerical solution of u_h (b) Numerical solution of a_h

Figure 1: Numerical results of solutions u_h and a_h. Parameters: $l=1$, $T=1$, $\varphi^{\dagger}(u)=2u-\sin(u)$, $\mu(t)=13t-\cos(4\pi t)+1$.

where the time step Δt is set to be equal to the mesh size h. In this numerical scheme we compute A_n^{k+1} in the $(k+1)$-th time step by using the results A_n^k and U_n^k in the k-th time step, and then use the obtained A_n^{k+1} to calculate U_{n+1}^k in the $(n+1)$-th mesh step. The convergent results in space at a fixed time point $t=1$ are reported in Table 1, where $||\cdot||_2$ represents the standard L^2-norm and the subscript $_N$ denotes the numerical solutions on the highest mesh level (i.e., $h=1/640$ in our experiments). In this work, u_N and a_N are used to be the surrogates for exact quantities u and a, respectively.

We notice that the relative errors for $\frac{||u_n-u_{n+1}||_2}{||u_N||_2}$ and $\frac{||a_n-a_{n+1}||_2}{||a_N||_2}$ both converge in 2 order as h goes to zero. The numerical results for $u(x,t)$ and $a(x,t)$ in terms of x and t are depicted in Fig. 1.

We also present the computed results in Fig. 2 to verify Theorem 2.2 in Section 2. Figs. 2(a) and (b) show that both $u_t(x,t)>0$ and $a_t(x,t)>0$ for all $x\in[0,1]$, $t\in[0,1]$. Moreover, Figs. 2(c) and (d) indicate that $0\le u(x,t)\le\mu(\tau)$ and $0\le a(x,t)\le\varphi(\mu(\tau))$ for all $x\in[0,1]$, $t\in[0,\tau]$ and $\tau\in(0,1]$. These numerical results demonstrate that our numeri-

Table 1: Convergence of the errors at t=1. Parameters: l=1, T=1, $\varphi^{\dagger}(u)$=$2u-\sin(u)$, $\mu(t)$=$13t-\cos(4\pi t)+1$.

t	h	$\frac{\|\|u_n-u_{n+1}\|\|_2}{\|\|u_N\|\|_2}$	order	$\frac{\|\|a_n-a_{n+1}\|\|_2}{\|\|a_N\|\|_2}$	order
1	1/10	1.0000E−03	–	1.8000E−03	–
	1/20	6.0251E−04	2.4533	1.3000E−03	1.9186
	1/40	3.8040E−04	2.2851	9.4890E−04	2.0165
	1/80	2.5346E−04	2.1652	6.7200E−04	2.0372
	1/320	1.7393E−04	2.1023	4.7508E−04	2.0407
	1/640	1.2116E−04	2.0711	3.3582E−04	2.0401

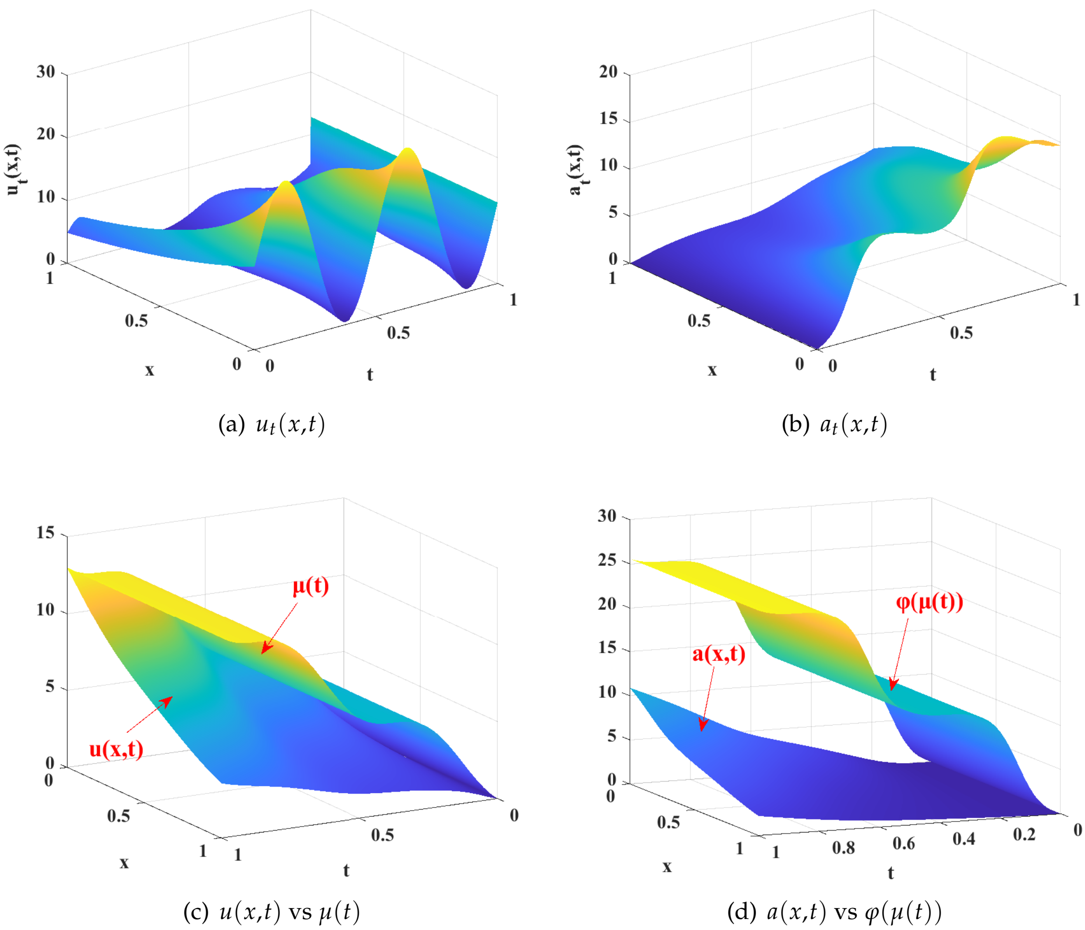


Figure 2: Properties of solutions $u(x,t)$ and $a(x,t)$. Parameters: $l=1$, $T=1$, $\varphi^{\dagger}(u)=2u-\sin(u)$, $\mu(t)=13t-\cos(4\pi t)+1$.

cal scheme (4.1) is structure-preserving (namely positivity-preserving and boundedness-preserving).

Now, we investigate the inverse problems (**IP**) with both noise-free and noisy data. First, by the introduced finite difference method (4.1) we obtain the numerical solution $h(t)=u_x(0,t)$, which is identified as the exact measurement data. Then, uniformly distributed noises with the magnitude δ' are added to $h(t)$ to obtain the noise data $h_\delta(t)$:

$$h_\delta(t)=[1+\delta'\cdot(2\text{Rand}-1)]\cdot h(t), \tag{4.2}$$

where Rand returns a pseudo-random value drawn from a uniform distribution on $[0,1]$. Since (4.2) generates non-smoothing data in $L^2(0,T)$, we have to smooth it as shown in Remark 2.2. Denote by $h_\delta^s(t)$ the smoothed noisy data by using the cubic spline method

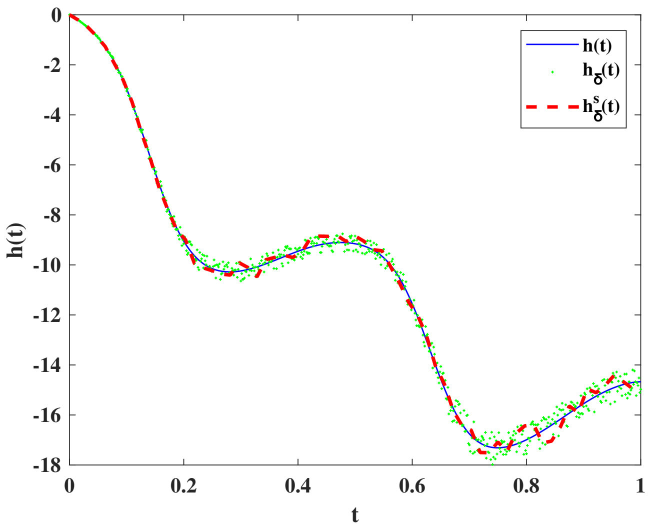


Figure 3: Exact measurement $h(t)$, noisy measurement $h_\delta(t)$ with $\delta'=0.04$, and smoothed noisy measurement $h^s_\delta(t)$, whose noise level is $\delta_2=60\%$ $(\delta_\infty=0.04)$. Other parameters: $l=1$, $T=1$, $\varphi^\dagger(u)=2u-\sin(u)$, $\mu(t)=13t-\cos(4\pi t)+1$.

(i.e., "spline" in MatLab). In our experiment we use both L^2-norm and C-norm to measure the noise level, which is defined as follows,

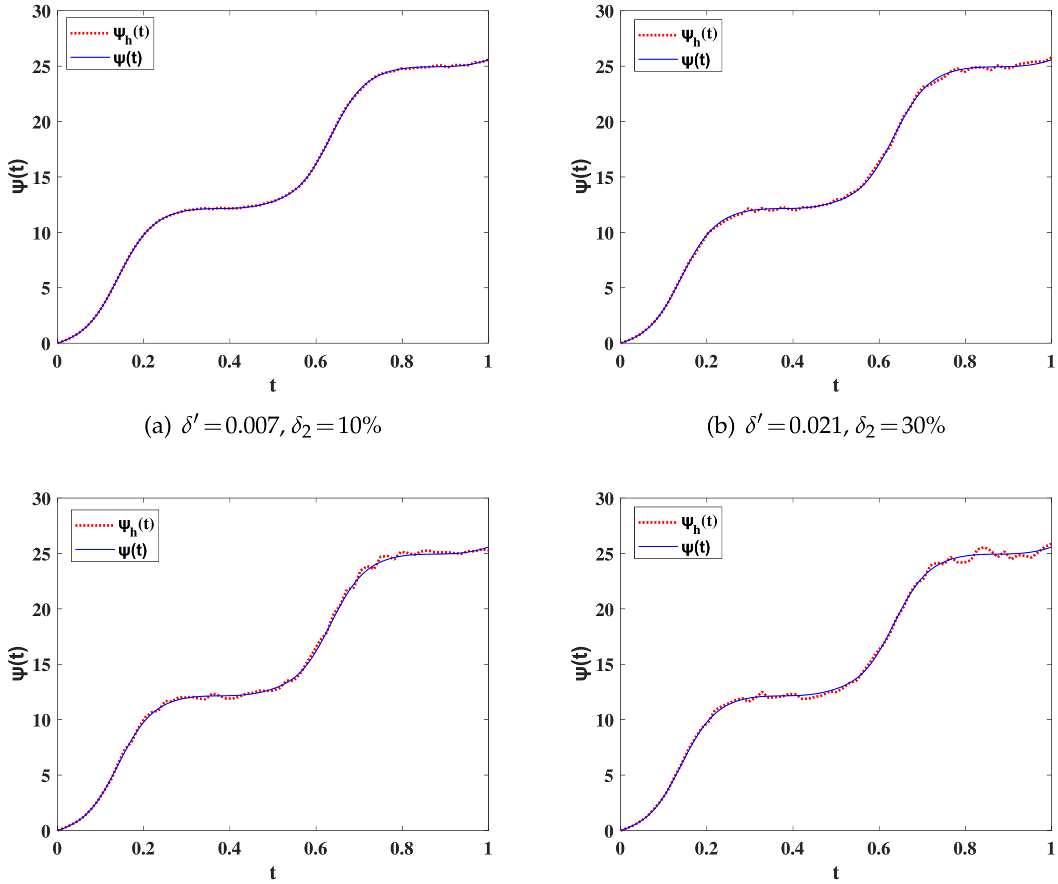
$$\delta_2=||h^s_\delta(t)-h(t)||_2, \qquad \delta_\infty=||h^s_\delta(t)-h(t)||_\infty.$$

Numerical experiments indicate that $\delta'\approx\delta_\infty$ if the mentioned parameters is applied for our model problem. To visualize the data processing, we plot the noise free dynamical boundary velocity $h(t)$, the noisy data $h_\delta(t)$ with $\delta'=0.04$ (consequently, $\delta_2=60\%$ and $\delta_\infty=0.04$), and the smoothed noisy data $h^s_\delta(t)$ in Fig. 3.

Now we carry on the iterative algorithm (3.1) introduced in Section 3 for problem (1.1a)-(1.1d) based on the above results. By the *a posteriori* stopping rule (3.8) in Theorem 3.2, we set the tolerance to be $c\delta'$ with $c=0.01$ and δ' defined in (4.2). This means that the iteration stops when the error between two successive iterations is less than $c\delta'$. From the relation (2.7), we see that $\psi^\dagger(t)=2s-\sin(s)$ with $s=13t-\cos(4\pi t)+1$, where $0\le t\le 1$ in this numerical example. Let $F(t)=A\psi(t)$, the discrete form for the iterative algorithm (3.1) is as following:

$$\begin{cases} F_n(t_{k+1})=\dfrac{F_n(t_k)+\Delta t\cdot\psi_n(t_{k+1})}{1+\Delta t}, \\ \psi_{n+1}=F_n-h_\delta, \end{cases} \tag{4.3}$$

with the initial guess $\psi_0=t$. According to the iterative algorithm, we first calculate F_n, that is $A\psi_n$, on the n-th iteration, then submit it into the second equation to update ψ_{n+1}.



(a) $\delta'=0.007$, $\delta_2=10\%$

(b) $\delta'=0.021$, $\delta_2=30\%$

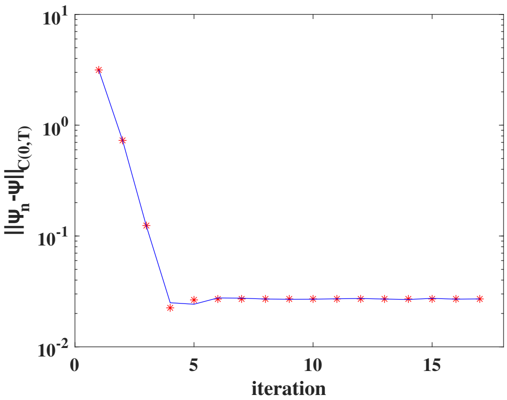
(c) $\delta'=0.035$, $\delta_2=50\%$

(d) $\delta'=0.04$, $\delta_2=60\%$

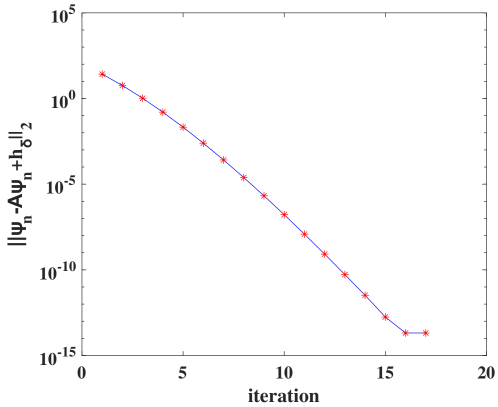
Figure 4: Numerical results $\psi_h(x,t)$ vs true result for different noise levels.

In this case we test the iterative algorithm both for $h(t)$ without noise and $h_\delta(t)$ with different noise levels. The numerical results for the iterative algorithm are shown in Fig. 4 and Table 2. We see that the iteration number decreases with the noise level increasing, which numerically proves the *a posteriori* stopping rule. For all cases with different noise levels, the numerical solution converges to the true solution as the error $||\psi_{n(\delta)}-\psi^\dagger||_{C(0,T)}$ goes to 0. Fig. 4 presents the numerical results $\psi_h(x,t)$ for different noise levels. It can be seen that oscillations become severer when the noise level gets higher, but still end with a convergent result, which proves that our iterative algorithm is robust with respect to the noise even for high leveled ones.

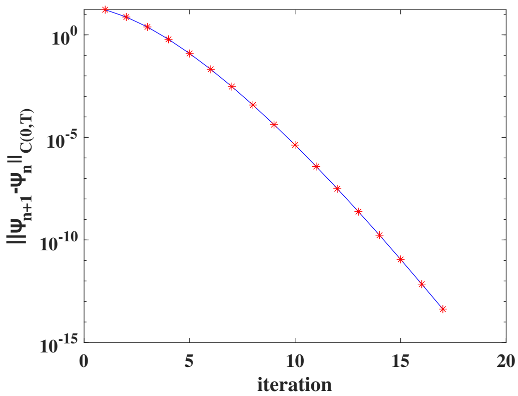
We end this section by dynamic behaviors of iteration scheme (3.1) with noise-free data in Fig. 5. From Fig. 5(a), we see that the error $||\psi_h-\psi||_{C(0,T)}$ converges nearly to 0 in just several iterations. We also give the residual error $||\psi_n-A\psi_n+h_\delta||_2$ and the increment



(a) Evolution of solution error



(b) Evolution of residual error



(c) Evolution of the increment $||\psi_{n+1}-\psi_n||_{C(0,T)}$ in the *a posteriori* stopping rule

Figure 5: Dynamics of quantities $||\psi_h-\psi||_{C(0,T)}$, $||\psi_n-A\psi_n+h_\delta||_2$ and $||\psi_{n+1}-\psi_n||_{C(0,T)}$ in the noise-free case.

$||\psi_{n+1}-\psi_n||_{C(0,T)}$ on each iteration in Figs. 5(b) and (c). For both cases the errors present a fast convergent results as iteration getting higher.

5 Conclusions

In this paper, we derived a Volterra integral equation for a nonlinear inverse problem in PDEs, which can be used not only for proving the the uniqueness of considered inverse problem but also for developing an efficient inversion solver. Both theoretical analysis and numerical simulations showed that our new inversion solver is stable and efficient. Finally, we mention that our methodology can be extended to the following more com-

Table 2: Convergent results for different noise levels.

δ_∞	δ_2	Iteration numbers	$\|\|\psi_{n(\delta)}-\psi^\dagger\|\|_{C(0,T)}$
0.02%	0.3%	13	3.0400E−02
0.075%	1%	11	3.9900E−02
0.15%	2%	10	5.1900E−02
0.2%	3%	8	6.0200E−02
0.7%	5%	7	1.4580E−01
1%	15%	6	1.9880E−01
4%	60%	5	6.9360E−01

plicated cases, which will be reported in the future: (i) System (1.1a)-(1.1c) with non-vanishing initial data $a(x,0)=a_0(x)$ such that $a_0\in C^1(0,l)$ and $a_0'(x)\leq 0$ for all $x\in(0,l)$; (ii) the transport equation $u_x+u_t+a_t=0$ and (1.1b) with appropriate boundary condition; (iii) the transport equation with diffusion $u_x+u_t+a_t=Du_{xx}$ and (1.1b), where D represents the diffusion parameter.

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