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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]).