A Mathematical Model for a Disturbed Soil-column Experiment and Reconstruction of Breakthrough Data

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Abstract This paper deals with a mathematical model for a disturbed soil-column experiment, and inversion and reconstruction of the measured breakthrough data. Based on the analysis of the experimental process and the breakthrough data for eight kinds of ion solutes, a mathematical model describing transport behaviors of the solute ions in the column was established. Furthermore, the unknown parameters were determined by applying an optimal perturbation iteration algorithm, and the breakthrough data were reconstructed.

Key words Disturbed soil-column experiment; advection-dispersion equation; parameter inversion; optimal perturbation algorithm; data reconstruction

1 Introduction

It is important to characterize physical/chemical reactions quantitatively in the solute transport processes in the soil and groundwater. To understand the behaviors of the soil in the presence of infiltrating contaminants, soil-column experiments are often performed in the laboratory. There are disturbed and undisturbed soil-column experiments. The main purpose for a disturbed soil-column experiment is to investigate some definite solutes transport behaviors occurring in the column.

On soil-column experiments in the known literatures we have (c.f.[1, 2, 3], for instance), earlier researches were focused on the construction of mathematical models for solutes transportation. For example, Nielsen[1] gave a general equation of solute transport in unsaturated soils, and Van Genuchten[2] discussed solute transport models of two sites/two regions in the soils. With development of computational techniques, numerical methods are widely utilized on the researches of soil-column experiments. Kamra[3] obtained transport parameters of a Bromine ion by fitting the breakthrough data using CXTFIT software based on quite a few small soil-column experiments; Cui[4] studied transport mechanisms of Cd in unsaturated soils by equipping a set of apparatus controlled by a computer, and estimated the model parameters by using a gradient regularization algorithm. Recently, the authors[5, 6] have ever considered an undisturbed soil-column experiment with a linear solute transport model, and gave numerical inversions for the solutes ions transportation in the column by fitting the measured breakthrough data using an optimal perturbation algorithm.

In this paper, we will investigate a disturbed soil-column experiment carried out in Zibo, Shandong. Based on the analysis of the experimental process and the breakthrough data, a mathematical model describing transport behaviors of the solute ions in the column was established. By applying an optimal perturbation iteration algorithm, the unknown parameters were determined, and then the measured breakthrough data were reconstructed. The inversion results show that the computational reconstruction data are basically coincide with the measured breakthrough data, and the mathematical model and parameters can be utilized to describe and explain the experimental results and processes.

2 Experimental process and analysis

The experiment was carried out in a simple apparatus in a lab in Shandong University of Technology. The device is installed with a column of fine sands with diameter of 2mm, infiltrating bottle and sample

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collecting installation. The diameter of the lucite tube loading the soil-column is 18.6 cm, and the height of the column is 62 cm. After seeping the column with distilled water for 24 hours, the experiment was performed at normal temperature by infiltrating the column with artificial coal-mine water. By collecting water samples at the bottom, 23 samples were collected throughout 23 hours. All the samples were sent to tested and analyzed in Shandong General Inspecting Station of Geology and Environment, and then we have the so-called breakthrough data of positive ions of Ca$^{2+}$, Na$^{+}$, K$^{+}$ and Mg$^{2+}$, and negative ions of Cl$^-$, SO$_4^{2-}$, HCO$_3^-$, and NO$_3^-$, which are plotted in Figure 1, where the transverse axis denotes the experimental time [hr], and the vertical axis represents the measured breakthrough data [mg/L].

By Figure 1, we can find that Ca$^{2+}$, Na$^+$ and Mg$^{2+}$ in the liquid phase almost have same behaviors.
which go up quickly at the initial stage, and gradually tend to steady situations after 2-3 hours; however, there is a different performance for $K^+$. Although $K^+$ goes up rapidly during the initial stage of 3 hours, it is still in an increasing position at a slow speed after $t=3$ hr.

On the other hand, let us investigate behaviors of negative ions. $SO_4^{2-}$ and $Cl^-$ have the same tendency with $Ca^{2+}$, $Na^+$ and $Mg^{2+}$, but the situations are complicated for $HCO_3^-$ and $NO_3^-$. It is noticeable that initial concentration of $HCO_3^-$ in the inflow is almost zero, and the first sample (at $t=2/3$ hr) gives a higher concentration of $HCO_3^-$ which is 152.7mg/L. The reason maybe ascribes to the actions of free $CO_2$ in the inflow. From $t=2/3$ hr to $t=2$ hr, the concentration goes down rapidly, and it goes up quickly from $t=2$ hr to $t=6$ hr, after $t=6$ hr, it approaches to an equilibrium. For $NO_3^-$, even if it goes up rapidly at initial stage, and then goes down rapidly during the initial 2 and 3 hours, but it still goes down slowly and gradually after $t=3$ hr.

In the follows, based on the above analysis, a mathematical model describing the solutes transport behaviors will be given, and an optimal perturbation algorithm will be applied to determine the unknown parameters in the model.

3 Mathematical model

It is well-known that under suitable hypotheses, solute transportation in a homogeneous porous medium can be characterized via simple 1-D advection-dispersion equation. For the disturbed soil-column experiment discussed above, there are some physical/chemical reactions in the liquid and solid phases. In mathematics, we can utilize different source/sink terms adding at the right hand side of the equation to describe different solutes transportation in the column.

Firstly, based on the analysis in Section 2, $Ca^{2+}$, $Na^+$, $Mg^{2+}$, and $Cl^-$ with $SO_4^{2-}$ have similar behaviors resulting from convection and dispersion mechanisms. Without loss generality, let us take $SO_4^{2-}$ as example, and denote $c_1 = c_1(x,t)$ as its concentration in the liquid phase, then we have

$$\frac{\partial c_1}{\partial t} = a_L v \frac{\partial^2 c_1}{\partial x^2} - v \frac{\partial c_1}{\partial x}, \quad 0 < x < l, t_0 < t < T_{tol},$$

(1)

where $a_L$ is the longitudinal dispersivity, $v$ is the actual pore-water velocity, $l$ is the length of the column, and $t_0$ is the moment at which the first sample collected, $T_{tol}$ is the total infiltrating time.

Next, due to specialties of concentrations of $HCO_3^-$, $K^+$ and $NO_3^-$ varying with time, we can utilize source/sink terms depending upon time to describe their transport behaviors. Let us take $HCO_3^-$ as example, and denote $c_2 = c_2(x,t)$ as its concentration, then we have

$$\frac{\partial c_2}{\partial t} = a_L v \frac{\partial^2 c_2}{\partial x^2} - v \frac{\partial c_2}{\partial x} + \beta(t)c_2, \quad 0 < x < l, t_0 < t < T_{tol},$$

(2)

where $\beta(t)$ represents some physical/chemical reactions depending on the experimental time.

Finally, by the experiment, the initial conditions of Eq.(1) and Eq.(2) are

$$c_i(x,t_0) = (c_i(l,t_0) - c_{i0}) \cdot x^m / l^m + c_{i0}, \quad 0 \leq x \leq l, \quad i = 1,2$$

(3)

Here $m > 0$ is an unknown parameter determined later; and the boundary conditions are chosen as

$$c_i(0,t) = c_{i0}, \quad \frac{\partial c_i}{\partial x}(l,t) = 0, \quad t_0 \leq t \leq T_{tol}, \quad i = 1,2$$

(4)

Thus, a mathematical model describing solutes transport behaviors in the soil-column is established composed by Eq.(1) and Eq.(2) with initial boundary value conditions (3) and (4). Noting the parameter $m$ in initial condition (3) and the source/sink function $\beta = \beta(t)$ in Eq.(2) are all unknown, we need to determine them by inversion algorithms in order to reconstruct the measured breakthrough data. In the follows, we will take $HCO_3^-$ as example, and apply an optimal perturbation algorithm\cite{7} to determine the unknown parameters based on the measured breakthrough data. For the convenience of computing,
we will transform Eq.(2) and its initial boundary conditions to dimensionless forms.

Set \( C_2 = c_2 / c_{20} \), \( Z = x/l \), \( T = vt/l \), then we have

\[
\frac{\partial C_2}{\partial T} = \frac{a_l}{l} \frac{\partial^2 C_2}{\partial Z^2} - \frac{\partial C_2}{\partial Z} + \frac{l}{v} \beta(T)C_2.
\] (5)

The initial and boundary value conditions are transformed to:

\[
C_2(Z, T_0) = 1 + (c_2(l, t_0) / c_{20} - 1) \cdot Z^m,
\] (6)

\[
C_2(0, T) = 1, \frac{\partial C_2}{\partial Z}(1, T) = 0.
\] (7)

Now the problem left is to determine the unknown initial parameter \( m \) and the source function \( \beta(t) \) which can lead to an inverse problem of parameter identification. Therefore, we need additional information from the experiment. The additional condition we will utilize is the breakthrough data as plotted in Fig.1. Also by dimensionless to the real data, we have

\[
C_2(1, T_k) = C^*_2, \ k = 1, 2, \cdots, 23.
\] (8)

As a result, an inverse problem of determining the function \( \beta(t) \) and the parameter \( m \) is formulated by Eq.(5), the initial boundary condition (6)-(7), and the over-posed condition (8). In addition, we give the following a priori values of known parameters in the model: The initial concentration of \( \text{SO}_4^{2-} \) and \( \text{HCO}_3^- \) are \( c_{10} = 1023.2 \text{ mg/L} \) and \( c_{20} = 34.1 \text{ mg/L} \) respectively. The length of the column \( l = 0.62 \text{ m} \), the steady pore-water velocity \( v = 2.4 \times 10^{-5} \text{ m/s} \), and the longitudinal dispersivity \( a_L = 8.8 \times 10^{-3} \text{ m} \), the total infiltrating time \( T_{\text{tot}} = 23 \text{ hr} \).

4 Inversion and reconstruction

Suppose that \( \beta(T) = \sum_{i=1}^{N} a_i T_{i-1} \), and denote the unknown parameters as \( r = (a_1, a_2, \cdots, a_N, m) \). Following the methods used in paper [5], we will implement an optimal perturbation algorithm to determine the unknown vector \( r \).

(1) \( \text{HCO}_3^- \)

Set \( N = 5 \), and choose regularization parameter as \( \alpha = 0.08 \), initial iteration as \( r_0 = (0,0,\cdots,0,1) \), then by 50-time iterations which cost CPU time 133.5 s, we obtain the inversion parameters:

\[
\bar{r} = (-1.2587, 7.6652, -13.4345, 10.3152, -3.5836, 0.5832).
\]

Furthermore, substituting the computational parameters into the model to solve the forward problem Eq.(5) with (6)-(7), the breakthrough data can be reconstructed, which are plotted in Fig.2 (b) together with the real measured breakthrough data.

(2) \( \text{SO}_4^{2-} \)

Let us consider the inversion of \( \text{SO}_4^{2-} \). For Eq.(1) with corresponding initial boundary conditions, there is only one initial parameter \( m \) to be determined. Thus an optimal perturbation algorithm without regularization term can be utilized to carry out the inversion. By taking initial iteration value as 1, and regularization parameter as zero, the parameter can be determined by 7-time iterations costing CPU time 1.7 s which is \( m = 3.7588 \). Similarly as for \( \text{HCO}_3^- \), Fig.2 (a) plots the measured breakthrough data and the reconstructed data of \( \text{SO}_4^{2-} \).

With a similar method as used for inversion of \( \text{HCO}_3^- \), the unknown source/sink coefficient functions \( \beta(t) \) and the initial parameter \( m \) for \( \text{K}^- \) and \( \text{NO}_3^- \) can be determined respectively, and then
their breakthrough data can also be reconstructed. In Fig.2 (c) and (d), the measured breakthrough data and the reconstruction data of the two solutes ions are plotted, where $C_3$ and $C_4$ denote the dimensionless concentrations of $\text{K}^+$ and $\text{NO}_3^-$ respectively.

Fig.2. Real breakthrough data and reconstruction data, where (a), (b), (c) and (d) represent the inversion results of $\text{SO}_4^{2-}$, $\text{HCO}_3^-$, $\text{K}^+$ and $\text{NO}_3^-$, respectively.

References