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Research Article

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A coupled model of partial differential equations for uranium ores heap leaching and its parameters identification

Abstract: In this article, we consider a mathematical modelling problem in engineering of uranium ores heap leaching. Firstly, we deduce a mathematical model of uranium ores heap leaching by combining solute transportation equations with microbial chemical reactions. Secondly, an inverse problem, which is solved by the optimal perturbation method together with the Tikhonov regularization, is considered for identifying the parameters of the proposed mathematical model. Finally, numerical simulations are given for the forward problem and the inverse problem to show the pattern of uranium ores microbial heap leaching and verify the effectiveness of parameters identification, respectively.

Keywords: Uranium, heap leaching, inverse problem, parameters identification, mathematical modelling

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1 Introduction

High-grade uranium ore resources are in decline in the world and therefore more attentions are given to low-grade and complex uranium ores. The low-grade and complex uranium ores are difficult to be treated by the traditional methods, which have some disadvantages such as poor recovery, involvement of high process and energy cost, and increase in pollution load of water resources [2, 4]. Therefore, less energy cost uranium extraction techniques are becoming more attractive. One of these methods is heap leaching, which is implemented firstly for the recovery of gold from low-grade ores by cyanidation in the early 1970s, has developed into an important hydrometallurgical technology for the recovery of base metals [6, 16].

Uranium could also be recovered by micro-organisms that catalyze the oxidation and reduction of uranium and associated metals also, and hence influence their mobility in the environment [1]. Currently, microbial assisted heap leaching plays a greater role to recover valuable metals from various sulfide minerals or low grade ores. It also becomes the dominant model of treatment for low-grade uranium ores. Microbial leaching of ores depends primarily on bacterial processes which are the essential causes of natural weathering of sulfide minerals. To the authors' knowledge, few scholars [13, 15] discussed mathematical models on uranium ores heap leaching. The solute transportation models in the mobile and immobile regions were built respectively in their paper. However, the parameters of chemical reaction, like decomposition coefficient on heap leaching, are always hard to be known in advance. In this article, we try to combine the solute transportation models with microbial chemical reaction so as to identify parameters by means of the optimal perturbation algorithm and Tikhonov regularization.

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2 Forward problem and its numerical method

2.1 Mathematical model

Microbial assisted heap leaching is an industrial mining process to extract low grade precious and base metals from ore, typically involving the application of a leach solution to large heaps, width and depth of hundreds of meters, of run of mine ore. Usually, the placed microorganisms leach solution percolates through the heap, dissolving both the target and other metal species from various minerals, draining into storage ponds at the base of the heap. The chemical reactions which like an intricate network in the leaching process, induced a long-standing debate among scientists about whether the microbially assisted leaching of uranium ore is by direct or indirect mechanism, or both [8].

As we all known, uranium is most commonly found in the +4 oxidation state as UO_2. Hexavalent uranium is readily solubilized in acidic solution forming a uranyl cation with tetravalent uranium requiring oxidation, often by Ferric ions (Fe^{3+}) liberated from accessory pyrites or added during leaching. Pyrite (FeS_2) is the most abundant sulfide mineral in Earth's crust. Exposure of pyrite surfaces to oxygen and water results in the formation of sulfuric acid [11]. Ferric iron, an abundant alternative electron acceptor in many solutions which are an acid environment, interacts effectively with surface sulfur species and promotes pyrite dissolution.

There are two major mechanisms involved in microbial metal solubilization of sulfide minerals [7]. One is a direct mechanism that involves physical contact of the organism with the insoluble sulfide. Microorganisms oxidize the metal sulfides obtaining electrons directly from the reduced minerals. Another, indirect mechanism involves the Ferric–Ferrous cycle. The oxidation of reduced metals is mediated by the Ferric ions (Fe^{3+}) and this is formed by microbial oxidation of Ferrous ions (Fe^{2+}) present in the minerals. Ferric ions acts as an oxidant and oxidizes metal sulfides and is reduced to Ferrous ions that, in turn, can be microbially oxidized. Indeed, the model of direct and indirect metal leaching is still under discussion. In many cases, the 'direct' mechanism dominates over the 'indirect' one mostly because of the fact that the direct mechanism is conducted via direct physical contact of bacteria to the mineral surfaces. However, there is a clear fact that microorganisms accelerate reoxidation of ferrous iron in solution to generate ferric iron which chemically oxidizes the sulfur present in the ore. The bio-oxidation is about one hundred thousand times faster than the chemical oxidation [5]. The following figure (quoted from [3]) may illustrate the difference between direct and indirect mechanisms more clearly.

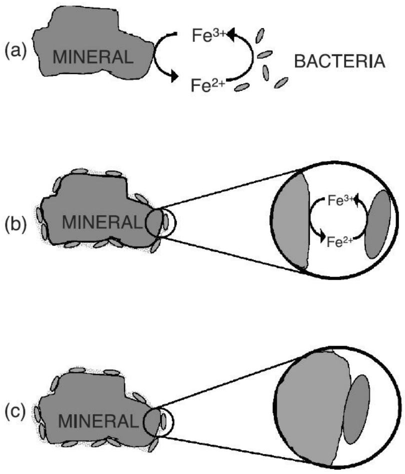

Figure 1. The three proposed mechanisms for the action of T. ferrooxidans on sulfide minerals. (a) The indirect mechanism, in which bacteria oxidize Ferrous ions in the bulk solution to Ferric ions and Ferric ions leach the mineral. (b) The indirect contact mechanism, in which attached bacteria oxidize Ferrous ions to Ferric ions within layer of bacteria and exopolymeric material, and the Ferric ions within this layer leach the mineral. (c) The direct contact mechanism, in which the bacteria directly oxidize the mineral by biological means, without any requirement for Ferric or Ferrous ions.

Owing to the complication of bioleaching, we consider some typical reactions as follows.

Direct mechanism. We have

$$\begin{cases} 4FeS_2 + 14O_2 + 4H_2O \xrightarrow{\text{Microbial}} 4FeSO_4 + 4H_2SO_4, \\ 4FeSO_4 + O_2 + 2H_2SO_4 \xrightarrow{\text{Microbial}} 2Fe_2(SO_4)_3 + 2H_2O. \end{cases} \tag{2.1}$$

Reactions (2.1) are bacterially catalyzed, and exemplify direct bacterial oxidation. However, as the oxidant, Ferric ions (Fe^{3+}) is bacterially produced by the second reaction of (2.1), it is classified as indirect bacterial oxidation. Thus, the second reaction of (2.1) can be described as direct mechanism and as indirect mechanism by oxidation of uranium from the last reaction of (2.5).

The reactions can be summarized as

$$4FeS_2 + 15O_2 + 2H_2O \xrightarrow{\text{Microbial}} 2Fe_2(SO_4)_3 + 2H_2SO_4. \tag{2.2}$$

Then, the direct mechanism can be described as

$$\begin{cases} 4FeS_2 + 15O_2 + 2H_2O \xrightarrow{\text{Microbial}} 2Fe_2(SO_4)_3 + 2H_2SO_4, \\ 2UO_2 + O_2 + 2H_2SO_4 \xrightarrow{\text{Microbial}} 2UO_2SO_4 + 2H_2O, \end{cases} \tag{2.3}$$

i.e.

$$\begin{cases} 4FeS_2 + 15O_2 + 2H_2O \xrightarrow{\text{Microbial}} 4Fe^{3+} + 8SO_4^{2-} + 4H^+, \\ 2UO_2 + O_2 + 4H^+ \xrightarrow{\text{Microbial}} 2UO_2^{2+} + 2H_2O. \end{cases} \tag{2.4}$$

The indirect mechanism refers to following reactions.

Indirect mechanism. We have

$$\begin{cases} FeS_2 + 8H_2O + 7Fe_2(SO_4)_3 \xrightarrow{\qquad} 8H_2SO_4 + 15FeSO_4, \\ 4FeSO_4 + 2H_2SO_4 + O_2 \xrightarrow{\text{Microbial}} 2Fe_2(SO_4)_3 + 2H_2O, \\ 2S + 3O_2 + 2H_2O \xrightarrow{\qquad} 2H_2SO_4, \\ UO_2 + Fe_2(SO_4)_3 \xrightarrow{\text{Microbial}} UO_2SO_4 + 2FeSO_4, \end{cases} \tag{2.5}$$

i.e.

$$\begin{cases} FeS_2 + 8H_2O + 14Fe^{3+} \xrightarrow{\qquad} 15Fe^{2+} + 2SO_4^{2-} + 16H^+, \\ 4Fe^{2+} + 4H^+ + O_2 \xrightarrow{\text{Microbial}} 4Fe^{3+} + 2H_2O, \\ 2S + 3O_2 + 2H_2O \xrightarrow{\qquad} 4H^+ + 2SO_4^{2-}, \\ UO_2 + 2Fe^{3+} \xrightarrow{\text{Microbial}} UO_2^{2+} + 2Fe^{2+}. \end{cases} \tag{2.6}$$

We consider a tube experiment of uranium heap leaching in a laboratory, and omit the third reaction from (2.6) because of the acid environment. Combining the direct and indirect mechanism, we get the following microbial chemical reactions:

$$4FeS_2 + 15O_2 + 2H_2O \xrightarrow{k_1} 4Fe^{3+} + 8SO_4^{2-} + 4H^+, \tag{2.7a}$$

$$2UO_2 + O_2 + 4H^+ \xrightarrow{k_2} 2UO_2^{2+} + 2H_2O, \tag{2.7b}$$

$$FeS_2 + 8H_2O + 14Fe^{3+} \xrightarrow{k_3} 15Fe^{2+} + 2SO_4^{2-} + 16H^+, \tag{2.7c}$$

$$4Fe^{2+} + 4H^+ + O_2 \xrightarrow{k_4} 4Fe^{3+} + 2H_2O, \tag{2.7d}$$

$$UO_2 + 2Fe^{3+} \xrightarrow{k_5} UO_2^{2+} + 2Fe^{2+}, \tag{2.7e}$$

where k_1 and k_3 represent the soil decomposition coefficient of FeS_2 into Fe^{3+} and into Fe^{2+} severally; k_4 is the liquid reaction coefficient of Fe^{2+} into Fe^{3+}; k_2 and k_5 are the soil decomposition coefficients of UO_2 into U^{6+} in two different chemical reactions.

As we known, the one-dimensional solute transportation can be stated as the hydrodynamic convection-diffusion equation (see [9, 10])

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2} - v\frac{\partial c(x,t)}{\partial x}, \tag{2.8}$$

where $x \in (0, L)$, $t \in (0, T_{\text{tol}})$, $c(x, t)$, D and v represent position, time, solute concentration, diffusion coefficient and solution flow rate respectively.

Actually, the microbial chemical reaction could be regarded as the source term of the convection-diffusion equations (2.8). Combining the chemical reactions (2.7) with the convection-diffusion equation (2.8), we obtain the following equations by using the **Schlogt molecular chemical kinetics model** (see [14]):

$$\begin{cases} \dfrac{\partial c_1}{\partial t} = D\dfrac{\partial^2 c_1}{\partial x^2} - v\dfrac{\partial c_1}{\partial x} + k_2 {s_2}^2 + k_5 s_2 {c_3}^2, \\ \dfrac{\partial c_2}{\partial t} = D\dfrac{\partial^2 c_2}{\partial x^2} - v\dfrac{\partial c_2}{\partial x} + k_3 s_1 {c_3}^{14} + k_5 s_2 {c_3}^2 - k_4 {c_2}^4, \\ \dfrac{\partial c_3}{\partial t} = D\dfrac{\partial^2 c_3}{\partial x^2} - v\dfrac{\partial c_3}{\partial x} + k_1 {s_1}^4 - k_3 s_1 {c_3}^{14} + k_4 {c_2}^4 - k_5 s_2 {c_3}^2, \end{cases} \tag{2.9}$$

where c_1, c_2, c_3 denote concentration hexavalent uranium ions (i.e. U^{6+}), Ferrous ions (i.e. Fe^{2+}) and Ferric ions (i.e. Fe^{3+}) in the liquid phase respectively; s_1, s_2 are concentration FeS_2 and UO_2 in the soil respectively.

Remark 1 (Combination details). To demonstrate how to combine the reactions (2.7) with equation (2.8), some details about the second equation of (2.9) will be given as follows.

The concentration c_2 refers to the reactions (2.7c), (2.7d) and (2.7e). As a source term of equation (2.8), we know it consists of three parts: $k_3 s_1 {c_3}^{14}$, $k_5 s_2 {c_3}^2$ and $-k_4 {c_2}^4$. The first part arises from (2.7c) and contains a plus sign, since (2.7e) produces Fe^{2+}. The left parts can be deduced from the same act of thinking.

Then, we have got a convection-diffusion system with strongly nonlinear sources term. At the beginning, the rate of reaction with respect to FeS_2 and UO_2 would be very fast. Then, the rate would be slow down as the contact area becoming more and more smaller between liquid and solid particles. Finally, the process will reach a steady state. To simulate the reactions, we assume that FeS_2 and UO_2 satisfy exponential decay during the reactions (2.7).

Let

$$\begin{aligned} & s_1 = s_1(0) \cdot e^{-(k_1+k_3)\cdot t}, && s_2 = s_2(0) \cdot e^{-(k_2+k_5)\cdot t}, \\ & r_1 = k_2, && r_2 = k_2 \cdot {s_2}^2(0), \\ & r_3 = k_5, && r_4 = k_5 \cdot s_2(0), \\ & r_5 = k_3, && r_6 = k_3 \cdot s_1(0), \\ & r_7 = k_4, && r_8 = k_1, \\ & r_9 = k_1 \cdot {s_1}^4(0). \end{aligned} \tag{2.10}$$

Then equations (2.9) can be rewritten as

$$\begin{cases} \dfrac{\partial c_1}{\partial t} = D\dfrac{\partial^2 c_1}{\partial x^2} - v\dfrac{\partial c_1}{\partial x} + r_2 \cdot e^{-2(r_1+r_3)\cdot t} + r_4 \cdot e^{-(r_1+r_3)\cdot t} \cdot c_3^2, \\ \dfrac{\partial c_2}{\partial t} = D\dfrac{\partial^2 c_2}{\partial x^2} - v\dfrac{\partial c_2}{\partial x} + r_6 \cdot e^{-(r_5+r_8)\cdot t} \cdot c_3^{14} + r_4 \cdot e^{-(r_1+r_3)\cdot t} \cdot c_3^2 - r_7 \cdot c_2^4, \\ \dfrac{\partial c_3}{\partial t} = D\dfrac{\partial^2 c_3}{\partial x^2} - v\dfrac{\partial c_3}{\partial x} + r_9 \cdot e^{-4(r_5+r_8)\cdot t} - r_4 \cdot e^{-(r_1+r_3)\cdot t} \cdot c_3^2 + r_7 \cdot c_2^4 - r_6 \cdot e^{-(r_5+r_8)\cdot t} \cdot c_3^{14}. \end{cases} \tag{2.11}$$

We have got the mathematical model of one-dimensional heap leaching with microbial chemical reaction by adding the initial and boundary conditions:

$$\begin{cases} c_i(x, 0) = 0, \\ c_i(0, t) = c_{i0}, \\ c_i(L, t) = \phi_i(t). \end{cases} \tag{2.12}$$

2.2 Numerical method for solving the forward problem

The forward problem of uranium ores heap leaching is to find concentrations $c_1(x,t)$, $c_2(x,t)$, $c_3(x,t)$ such that the couple partial differential equations (2.11)–(2.12) for given parameters and boundary conditions are valid. In this subsection, we utilize a numerical method for solving the forward problem based on the finite difference method. To this end, it is convenient to non-dimensionalize the equations (2.11) and (2.12) with the following substitutions.

Let

$$C_i = \frac{c_i}{c_{i0}}, \quad Z = \frac{x}{L}, \quad T = \frac{v \cdot t}{L}, \quad P = \frac{v \cdot L}{D}, \quad R_j = \frac{r_j \cdot L}{v}, \tag{2.13}$$

i.e.

$$c_i = c_{i0} \cdot C_i, \quad x = L \cdot Z, \quad t = \frac{T \cdot L}{v}, \quad r_j = \frac{R_j \cdot v}{L}, \tag{2.14}$$

where $i = 1, 2, 3$ and $j = 1, 2, \dots, 9$.

Substituting (2.14) into equations (2.11) and (2.12), we obtain

$$\begin{cases} \dfrac{\partial C_1}{\partial T} = \dfrac{1}{P} \cdot \dfrac{\partial^2 C_1}{\partial Z^2} - \dfrac{\partial C_1}{\partial Z} + \dfrac{R_2}{c_{10}} \cdot e^{-2(R_1+R_3)\cdot T} + \dfrac{R_4 \cdot c_{30}^2}{c_{10}} \cdot e^{-(R_1+R_3)\cdot T} \cdot C_3^2, \\ \dfrac{\partial C_2}{\partial T} = \dfrac{1}{P} \cdot \dfrac{\partial^2 C_2}{\partial Z^2} - \dfrac{\partial C_2}{\partial Z} + \dfrac{R_6 \cdot c_{30}^{14}}{c_{20}} \cdot e^{-(R_5+R_8)\cdot T} \cdot C_3^{14} + \dfrac{R_4 \cdot c_{30}^2}{c_{20}} \cdot e^{-(R_1+R_3)\cdot T} \cdot C_3^2 - R_7 \cdot c_{20}^3 \cdot C_2^4, \\ \dfrac{\partial C_3}{\partial T} = \dfrac{1}{P} \cdot \dfrac{\partial^2 C_3}{\partial Z^2} - \dfrac{\partial C_3}{\partial Z} - \dfrac{R_9}{c_{30}} \cdot e^{-4(R_5+R_8)\cdot T} - R_4 \cdot c_{30} \cdot e^{-(R_1+R_3)\cdot T} \cdot C_3^2 + \dfrac{R_7 \cdot c_{20}^4}{c_{30}} \cdot C_2^4 \\ \qquad - R_6 \cdot c_{30}^{13} \cdot e^{-(R_5+R_8)\cdot T} \cdot C_3^{14} \end{cases} \tag{2.15}$$

and

$$\begin{cases} C_i(Z,0) = 0, \quad i = 1,2,3, \\ C_i(0,T) = 1, \\ C_i(1,T) = \dfrac{\phi_i(T)}{c_{i0}}. \end{cases} \tag{2.16}$$

Then we are able to solve problem (2.15)–(2.16) by using the explicit finite difference scheme when the parameters D, v, c_{i0}, r_j, T_{tol}, L are given, that is, we use the approximations

$$\begin{cases} \dfrac{\partial C(z_j,t_k)}{\partial z} \simeq \dfrac{C(z_{j+1},t_k) - C(z_j,t_k)}{\Delta z}, \\ \dfrac{\partial^2 C(z_j,t_k)}{\partial z^2} \simeq \dfrac{C(z_{j+1},t_k) - 2C(z_j,t_k) + C(z_{j-1},t_k)}{\Delta z^2}, \\ \dfrac{\partial C(z_j,t_k)}{\partial t} \simeq \dfrac{C(z_j,t_{k+1}) - C(z_j,t_k)}{\Delta t} \end{cases} \tag{2.17}$$

instead of the derivatives in (2.15), respectively.

By Taylor series expansion, we know easily that the explicit finite difference scheme obtained from (2.17) has a first-order accurate approximation. But, it is efficient and stable for solving problem (2.15)–(2.16), which can be seen in the next numerical simulation.

3 Inverse problem and its numerical solutions

The inverse problem considered in this paper is to reconstructing unknown parameters R_j by some measurement data. To obtain approximate solutions of R_j, we formulate the inverse problem into a nonlinear optimization problem solved by a perturbation method.

First, we introduce some symbols. Let $R = (R_1, R_2, \dots, R_9)$, $C = (C_1, C_2, C_3)$, where $C_i(Z,T;R)$ denote solutions of the direct problem (2.15)–(2.16). By $\hat{C}_i(h,T) = \varphi(T)$ we denote some measurement data at the position h. Then the inverse problem of reconstructing R is turned into solving the minimum of the nonlinear functional

$$J(R) = \|C(h, T; R) - \varphi(T)\|^2 + \alpha \cdot \Omega(R), \tag{3.1}$$

where $0 < \alpha < 1$ represents a regularization parameter and $\Omega(R) = R^{T_r}R$ is a 2-norm stabilizing functional, where T_r means transposition of a matrix.

In order to solve the minimum of the nonlinear functional (3.1), we introduce the optimal perturbation algorithm which is a feasible means for this case (see [12]). Then problem (3.1) of solving the optimal parameters R is transformed into solving the optimal perturbation δR_n for a given R_n.

3.1 The optimal perturbation algorithm

Computing the optimal perturbation δR_n for a given R_n can be changed into solving another minimization of the functional

$$f(\delta R_n) = \|C(h, T; R_n + \delta R_n) - \varphi(T)\|^2 + \alpha \cdot \Omega(\delta R_n), \tag{3.2}$$

where δR_n is the minimizer of the functional (3.2). Then we can further identify R_{n+1} by means of the following iterate algorithm:

$$R_{n+1} = R_n + \delta R_n \quad \text{for } n = 0, 1, 2, \dots. \tag{3.3}$$

Taking advantage of the Taylor series expansion, we have

$$C(h, T; R_n + \delta R_n) = C(h, T; R_n) + \nabla^{T_r} C(h, T; R_n) \cdot \delta R_n + o(\delta R_n), \tag{3.4}$$

where

$$\nabla^{T_r} = \Big(\frac{\partial}{\partial R_1}, \frac{\partial}{\partial R_2}, \dots, \frac{\partial}{\partial R_9}\Big),$$

T_r means transposition of a matrix. Omitting the high-order infinitesimal term, we obtain

$$f(\delta R_n) = \|C(h, T; R_n) - \varphi(T) + \nabla^{T_r} C(h, T; R_n) \cdot \delta R_n\|^2 + \alpha \cdot \Omega(\delta R_n). \tag{3.5}$$

Discretizing T, i.e. $0 < T_1 < T_2 < \cdots < T_M$, we gain

$$f(\delta R_n) = \sum_{m=1}^{M} \big(C(h, T_m; R_n) - \varphi(T_m) + \nabla^{T_r} C(h, T_m; R_n) \cdot \delta R_n\big)^2 + \alpha \cdot (\delta R_n)^{T_r}(\delta R_n), \tag{3.6}$$

namely

$$f(\delta R_n) = (\delta R_n)^{T_r} B^{T_r} B(\delta R_n) + 2(\delta R_n)^{T_r} B^{T_r}(G - \hat{G}) + (G - \hat{G})^{T_r}(G - \hat{G}) + \alpha \cdot (\delta R_n)^{T_r}(\delta R_n), \tag{3.7}$$

where

$$G = \big(C(h, T_1; R_n), C(h, T_2; R_n), \dots, C(h, T_M; R_n)\big)^{T_r}, \tag{3.8}$$

$$\hat{G} = \big(\varphi(T_1), \varphi(T_2), \dots, \varphi(T_M)\big)^{T_r}, \tag{3.9}$$

$$B = (b_{m,i})_{M\times 9}, \quad b_{m,i} = \frac{C(h, T_m; R_n + \tau_i) - C(h, T_m; R_n)}{\tau_i}, \tag{3.10}$$

and $\tau = (\tau_1, \tau_2, \dots, \tau_9)$ is usually called the numerical differential step vector.

Solving the minimum of the functional (3.7) is equivalent to solving the canonical equation according to the least square method. So, we have got

$$(\alpha I + B^{T_r} B) \cdot (\delta R_n) = B^{T_r} \cdot (G - \hat{G}), \tag{3.11}$$

namely

$$(\delta R_n) = (\alpha I + B^{T_r} B)^{-1} \cdot B^{T_r} \cdot (G - \hat{G}). \tag{3.12}$$

Hence, the algorithm for identifying the unknown parameter R from some measurement data $\hat{C}(h, T) = \varphi(T)$ can be summed up in following three steps.

Algorithm 1. Identification for unknown parameter R_j.

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Given the initial guess $R_n$ and the numerical differential step vector $\tau$.
Step 1. $\varepsilon_k$ denotes the maximum of error function $\varepsilon_j = \|C_j(h, T; R_n) - \varphi_j(T)\|$, compute the matrices $G$, $\hat{G}$, and $B$ by using (3.8)–(3.10).
Step 2. Calculate $\delta R_n$ and $R_{n+1}$ by virtue of (3.12) and (3.3) respectively.
Step 3. Repeat Step 1 and Step 2 until $\|\delta R_n\| \le$ eps for a given precision eps in advance, and then $R_n$ is the optimum parameters.
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4 Numerical experiments

Before we successfully simulate the forward and inverse problems, we need to give the boundary conditions $\phi_i(t)$ that can be obtained by data fitting from the measurements at the right end point. Here, we study which model can be used to characterize the boundary conditions based on microbial chemical reaction equations.

Superposing the reaction equations (2.7), we have got the total effect equation

$$5FeS_2 + 17O_2 + 6H_2O + 3UO_2 + 8Fe^{3+} \xrightarrow{\text{Microbial}} 13Fe^{2+} + 3UO_2^{2+} + 10SO_4^{2-} + 12H^+. \tag{4.1}$$

With the passage of time, the concentration Fe^{3+} decreased at the same time, U^{6+} and Fe^{2+} on the rise from the above equation, so we make use of the logistic model to simulate this procedure. Let

$$\phi_i(t) = \frac{K_i}{1 + \left(\frac{K_i}{K_{i0}} - 1\right) \cdot e^{-q_i \cdot t}}, \tag{4.2}$$

where K_i, K_{i0} represent the maximum concentration and the initial concentration respectively. According to the reaction equations (2.7), we have got the following equations:

$$q_1 = k_2 + k_5, \quad q_2 = k_3 - k_4 + k_5, \quad q_3 = k_1 - k_3 + k_4 - k_5. \tag{4.3}$$

Then the boundary conditions $\phi_i(T)$ are built as follows after non-dimensional disposal:

$$\phi_1(T) = \frac{K_1}{1 + \left(\frac{K_1}{K_{10}} - 1\right) \cdot e^{-(R_1+R_3)\cdot T}}, \tag{4.4}$$

$$\phi_2(T) = \frac{K_2}{1 + \left(\frac{K_2}{K_{20}} - 1\right) \cdot e^{-(R_3+R_5-R_7)\cdot T}}, \tag{4.5}$$

$$\phi_3(T) = \frac{K_3}{1 + \left(\frac{K_3}{K_{30}} - 1\right) \cdot e^{-(R_8-R_3-R_5+R_7)\cdot T}}. \tag{4.6}$$

4.1 Numerical simulation for the forward problem

We consider the Dirichlet boundary condition $c_i(0, t) = c_{i0}$, $c_i(L, t) = \phi_i(t)$, $i = 1, 2, 3$, and assume that there is no chemical reaction at the beginning $c_i(x, 0) = 0$.

In the finite difference scheme (2.17), we take

$$\begin{gathered}
R = (1.243, 1.07, 2.125, 1.08, 5.205, 1.03, 8.125, 1.0909, 1.05),\\
\tau = (0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02, 0.02), \quad \text{eps} = 1\times 10^{-4},\\
c_{10} = 338.28\ \text{mg/L}, \quad c_{20} = 1062.9\ \text{mg/L}, \quad c_{30} = 104.42\ \text{mg/L}, \quad L = 0.45\ \text{m}, \quad h = 1,\\
v = 5.1\times 10^{-5}\ \text{m/s}\ \ (\text{i.e. } 0.1836\ \text{m/h}), \quad D = 1\times 10^{-9}\ \text{m}^2/\text{s}, \quad T_{\text{tol}} = 3456000\ \text{s}\ \ (\text{i.e. 40 days}),\\
K_1 = 338.28\ \text{mg/L}, \quad K_2 = 1062.9\ \text{mg/L}, \quad K_3 = 104.42\ \text{mg/L},\\
K_{10} = 0.5\ \text{mg/L}, \quad K_{20} = 0.1\ \text{mg/L}, \quad K_{30} = 3\ \text{mg/L}.
\end{gathered}$$

The time interval $[0, T]$ is divided into 85 segments,and the space interval $[0, 1]$ is also divided into 85 subintervals. Then we obtain approximate solutions of the forward problems by the finite difference scheme (2.17), which are listed in Figures 2–4 and show the variation of concentration rate with reaction time (days) in the C-t plane.

From Figure 2, we see that the percentage of Fe^{2+} rises after their reaction 4 days and 15 days reach to steady state. Figure 3 illustrates that the proportion of Fe^{3+} almost deplete after 24 days. The concentration of U^{6+} begin to climb after 3 days and about 17 days to stable state.

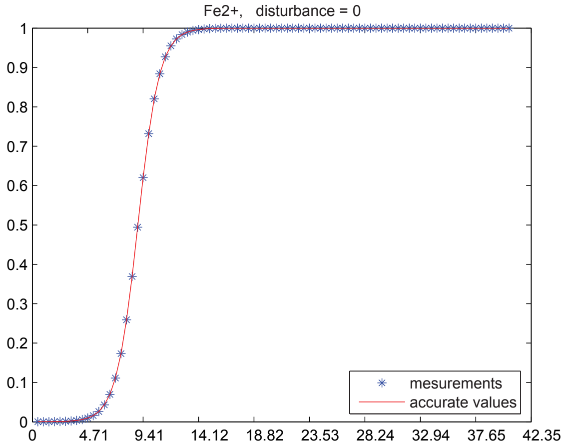

Figure 2. The percentage of Fe^{2+} with $\eta = 0$.

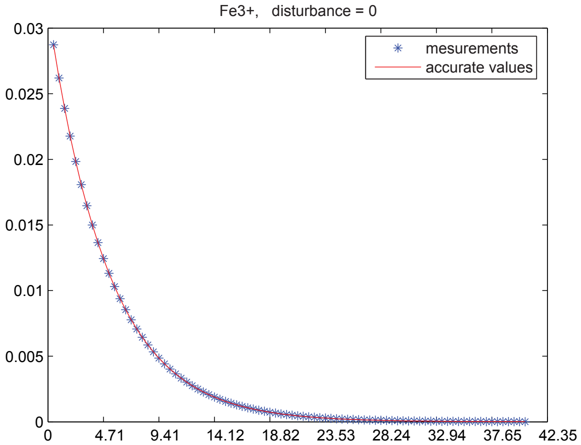

Figure 3. The percentage of Fe^{3+} with $\eta = 0$.

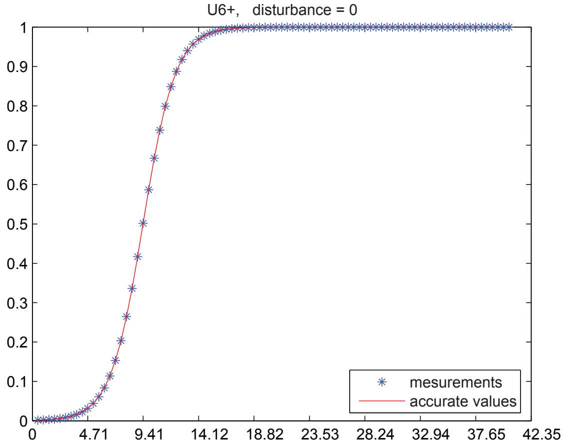

Figure 4. The percentage of U^{6+} with $\eta = 0$.

4.2 Simulation for the inverse problem

Assuming that parameters R_j, $j = 1, \ldots, 9$, are unknown, we now try to identify R_j, $j = 1, \ldots, 9$, from the final measurements $C(h, T) = (C_1(h, T), C_2(h, T), C_3(h, T))$. Considering the practically final measurements often contain some errors, we use the calculated value by adding some noises, i.e.

$$\hat{C} = C \cdot (1 + \eta \times \xi),$$

where C is the calculated value computed by the finite difference scheme as stated in Section 4.1, $\xi \in (-1, 1)$ are uniformly distributed random numbers, η represents the level of relative errors. In Algorithm 1, we take the iterative initial value

$$R_0 = (0.0775, 0.0775, 0.0775, 0.0775, 0.0775, 0.0775, 0.0775, 0.0775, 0.0775),$$

and use the following stoping criteria:

$$\theta = \text{average}\Big(\frac{|R - R_0|}{R}\Big). \tag{4.7}$$

Inverse results are listed in Table 1.

Error η	α	θ (%)	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	R_9
0	0.0050	5.8677	1.0775	1.0775	2.5811	1.0775	5.0403	1.0775	7.9523	1.041	1.0775
0.01	0.0098	7.7455	1.0775	1.0775	2.7226	1.0775	4.8489	1.0775	8.1532	1.2319	1.0775
0.05	0.0141	7.8993	1.0775	1.0775	2.7065	1.0775	4.8312	1.0775	8.1705	1.2492	1.0775

Table 1. The result of reconstructing R.

It can be seen that the optimal perturbation regularization method is feasible for the identification of parameter R in the uranium ores heap leaching from the above experimental results.

Remark 2. From the modeling process in Section 2, we know that R_j characterizes the rate of chemical reaction k_j. Usually, an experiment of uranium heap bioleaching needs several months or more to accomplish. The time cost is very expensive. Therefore, it is meaningful and beneficial for practical productions to improve the rate of chemical reaction k_j and decrease the time cost. The inverse problem considered in this paper maybe give an approach to achieve our goal.

5 Conclusion

In this paper, we mainly investigate a mathematical model and identify its parameters in engineering of uranium ores heap leaching. A mathematical model of uranium ores heap leaching is firstly formulated by combining solute transportation equations with microbial chemical reactions. Furthermore, based on the optimal perturbation method and the Tikhonov regularization, an inverse problem is taken into account for identifying the parameters of the proposed model. At last, the result of numerical simulations demonstrate feasibility of parameters identification for the uranium ores microbial heap leaching.

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