Numerical modeling of biogeobattery system from microbial degradation of underground organic contaminant

Jing Xie^{1,2,3} · Yi-an Cui^{1,2,3} · Lijuan Zhang^{1,2,3} · Youjun Guo^{1,2,3} · Jiaxin Wang^{1,2,3} · Meryem Fanidi^{1,2,3} · Jianxin Liu^{1,2,3}

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Abstract

Redox fields observed near contaminated sites are related to electrochemical and electrobiological reactions. The term biogeobattery is used to describe the redox processes in underground organic contaminated sites which are biogeochemical systems, where bacteria, conductive minerals, oxygen, and organic contaminants create numerous anode–cathode pairs by transferring electrons from reducing areas under the water table or other anaerobic conditions to oxidizing areas above the water table. A numerical biogeobattery model established based on the geobattery and inert electrode model is the theoretical basis for numerical modeling. A coupled method of tetrahedral finite elements and hexahedral infinite elements is proposed for the algorithm basis of numerical modeling. Then a small-scale biogeochemical system and a field-scale landfill system are modeled using the numerical biogeobattery model and the finite–infinite element coupling method. The results suggest that the accuracy of the coupled method is superior to the finite element method. The amplitude change in the embedded redox field has a great effect on self-potential anomalies, while the gradient change in the embedded redox field has no significant impact on self-potential anomalies. The resolution of the surface self-potential decreases with the depth of biogeochemical systems. The biogeobattery model based on the inert electrode model is an effective numerical model in biogeochemical systems.

Keywords Numerical modeling · Biogeochemical system · Biogeobattery · Finite element · Infinite element

1 Introduction

The self-potential (SP) method uses electric potential anomalies measured by nonpolarizing electrodes at the Earth's surface or in wells to recognize geological, hydrological, biological, and chemical targets [1, 2]. As a passive source method, it is very efficient by getting rid of power supply. Mohd [3] measured the SP data in downhole to enhance the oil recovery monitoring. Safipour [4] studied an SP investigation to explore submarine massive sulfides. Zlotnicki [5] used the SP method to study volcano activities. Chen [6] used the SP skewness and kurtosis to forecast the earthquake. Roubinet [7] modeled SP signals in

fractured rock to identify hydraulically active fractures. Ikard [8] studied the surface–groundwater exchange by a floating SP dipole. Ahmed [9] implemented the joint inversion of hydraulic head and SP data associated with harmonic pumping tests. Because of its characteristics, the SP method is supposed to be applied to long-term monitoring of organic-rich contaminated sites or methods of remediation. Naudet [10, 11] and Revil [12] applied it to describe the redox front of contaminated sites. Arora [13] and Gallas [14] successfully monitored the leakage of landfills using this method. Martínez-Pagán [15] simulated the contamination diffusion process through laboratory experiments and verified the feasibility of this method to

✉ Yi-an Cui, cuiyian@csu.edu.cn | ¹School of Geosciences and Info Physics, Central South University, Changsha 410083, China. ²Hunan Key Laboratory of Non-ferrous Resources and Geological Hazard Detection, Changsha 410083, China. ³Key Laboratory of Metalorganic Prediction of Nonferrous Metals and Geological Environment Monitoring (Central South University), Ministry of Education, Changsha 410083, China.

monitor contamination. Placencia-Gomez [16] took it to investigate the leakage of tailing ponds. Also, Che-Alota [17] and Forte [18] used it to monitor the degradation of hydrocarbon contaminants in the environment. Rittgers [19] studied SP signals generated by the corrosion of buried metallic objects to explain the physical and chemical mechanisms of such electrical signals. Giampaolo [20] performed the monitoring of a crude oil-contaminated site using the SP method. Mao [21] studied the SP tomography by sandbox and field experiments and applied it to groundwater remediation and contaminant plumes. Abbas [22] analyzed the redox field distribution of an organic-rich contaminated site obtained by the inversion of SP data. Cui [23, 24] conducted the sandbox experiments to try to use the SP method to monitor the diffusion and migration of underground contamination. Graham [25] discussed the SP as a predictor of seawater intrusion in coastal groundwater boreholes. Fernandez [26] assessed whether combining electrical resistivity and SP measurements can map the zones affected by anaerobic degradation. These studies show that the laboratory or field observation of the SP method is fast and nondestructive, has no secondary pollution, has real-time monitoring, and is of low cost. And the SP method is sensitive to many kinds of signals associated with contaminant diffusion, such as seepage, redox processes, and microbial activities, which is applicable to the field of biogeophysical exploration, especially the detection and monitoring of underground organic contaminants.

There are two main contributions of measured SP data, namely the streaming potential associated with pore water flow or geothermal systems in saturated and unsaturated regions and the redox potential associated with redox processes of orebodies or organic contaminants. In environmental contamination investigations, abnormal redox potential gradients on the ground help determine the location of contaminants. Microorganisms (or bacteria) are believed to be responsible for these redox processes in contaminant plumes [10–13, 27–31], where every element of the redox interface (e.g., the water table) behaves like a dipole with cathodic half-cell reactions occurring at the upper, more oxidizing end, and anodic half-cell reactions at the lower, more reducing end [13]. Microorganisms support the migration of electrons which flow from the anode through the electrical circuit toward a terminal redox electron acceptor at the cathode [12]. Sato and Mooney [2] first attempted to construct a galvanic cell model to evaluate redox fields for the application of the SP method in mineral exploration. Krauskopf [32] studied the formula for the SP generated by redox reactions. The inert electrode model (IEM) proposed by Stoll [33] and Bigalke [34] is the formulation that takes into account the subsurface redox conditions and provides a mathematical

basis for calculating the theoretical redox field of minerals. Mendonça [35] conducted 2D forward and inversion studies of mineral redox potential based on the IEM. Castermant [36] calculated the distribution of the SP generated by redox reactions during underground metal corrosion. Mohamad Sadegh and Ali [37, 38] carried out the forward modeling and physical experiments of the SP based on geobattery models, and successfully inverted experimental observation data. Targeted numerical modeling of the redox processes is helpful to identify the characteristics of the SP anomalies caused by microbial degradation of organic contaminants. Accordingly, it can provide a forward algorithm and numerical foundation for applying the SP method in environmental contamination fields. In order to improve the calculation accuracy of numerical modeling, the Astley uni-directional mapping infinite element is introduced to realize an effective coupling of tetrahedral finite elements and hexahedral infinite elements in spacial and physical properties. Then based on theories of the geobattery and the IEM which provides a consistent electrochemical model and the SP fields from a set of current sources, a numerical biogeobattery model is established for the three-dimensional (3D) numerical modeling of redox potentials from the microbial degradation of organic contaminants.

2 Numerical biogeobattery model

2.1 Geobattery

In mineral exploration, the subsurface redox process is characterized by negative SP anomalies on the ground [39–41]. The main reason for the formation of orebody redox fields is the penetration of rainwater and the diffusion of oxygen, which forms an oxidizing environment in the shallow layer and a reducing environment in the deep. The orebody connects the shallow and deep regions, causing electrons to flow upward [35]. As a result, the upper part releases electrons to form the cathode of a battery and the lower part acquires electrons to form the anode. “Geobattery” is used to describe this system [2, 12, 32–38, 42].

2.2 Biogeobattery

The term “biogeobattery” coined by Revil and his coworkers [10–12, 29] is used to describe the electron-transfer mechanism of a biogeochemical system which is an interdisciplinary system of geophysics, geochemistry, and microbiology. Revil [12] proposed a biogeobattery linear model to explain the redox fields of thin, flat, and contaminated aquifers. Hubbard [43] and Fachin

[44] studied the SP data from an analog biogeobattery model through experiments. Also, Risgaard-Petersen [45] measured the electric fields generated in a biogeobattery model with microelectrodes.

In a biogeobattery system, the growth of bacterial colonies is associated with organic contaminants and oxygen levels. Therefore, those bacteria that can participate in the degradation of underground organic contaminants and produce redox processes are likely to be confined to the water table, where contaminated water mixes with oxygen-rich meteoric water [12, 13]. The electron-transfer mechanism can be summarized into three categories: (1) The first mechanism (named model I, see Fig. 1a) shows that conductive minerals and the bacteria are found near the water table [12, 13, 46–48]; (2) the second mechanism (named model II, see Fig. 1b) suggests that different bacterial populations form nanowire networks by conductive pili [49–51]; (3) the third mechanism (named model III, see Fig. 1c) shows that the filamentous bacteria can also transfer electrons alone [52].

2.3 Numerical biogeobattery model from IEM

All above-mentioned electron-transfer mechanisms shown in Fig. 1 are not isolated. As shown in Fig. 1d, a biogeochemical system in which the electron-transfer mechanism may contain one or two, even three mechanisms simultaneously can be simplified into an equivalent circuit, as shown in Fig. 1e. Based on the above discussion, a macroscopic numerical biogeobattery model is established where the model space is constrained by defining interfaces (e.g., the water table) and the thin, flat distribution of primary redox fields [12, 13, 22, 29]. Then the forward modeling of the numerical biogeobattery model can be realized through the IEM.

Numerical modeling of a biogeobattery model can be realized by solving the governing differential equation with numerical methods. The large sparse system of linear equations can be expressed as

$$\mathbf{K}\mathbf{u} = \mathbf{q} \quad (1)$$

where $\mathbf{K}$ is the $n \times n$ stiffness matrix which is obtained by the finite-infinite element coupling method in this paper,

Fig. 1 Sketches of three electron-transfer mechanisms in a biogeochemical system. **a** In model I, bacteria and (semi-) conductive minerals facilitate the transfer of electrons. **b** In model II, bacterial colonies form nanowire networks by conductive pili. **c** In model III, electrons transfer from donors to acceptors through insulated internal wires of filamentous bacteria. **d** Illustration of a biogeochemical system from microbial degradation of organic contaminants. **e** Illustration of an equivalent circuit of a biogeochemical system. Modified from [11, 12, 44, 52]

$\mathbf{u}$ is an n -dimensional vector with potential values that are unknown and need to be solved, $\mathbf{q}$ is an n -dimensional source vector, and n is the number of nodes.

Then, the k th value u_k of $\mathbf{u}$ can be expressed as

$$u_k = \mathbf{r}_k^T \mathbf{q} \quad (2)$$

where $\mathbf{r}_k^T$ is the k th row of the matrix $\mathbf{K}^{-1}$, $\mathbf{K}^{-1}$ represents the inverse matrix of $\mathbf{K}$.

The distribution of redox fields and current source densities is assumed to be situated at the thin, flat biogeobattery system which is near the water table and can be regarded as numerous micro-geobatteries (or dipoles) [12, 13, 22, 29]. Then current source intensities can be evaluated by the IEM approximately. The current term q_i can be expressed as [34, 35]

$$q_i = S_i[E_c - E_{h,i} - u_i] \quad (3)$$

where i represents the i th node of the biogeobattery, E_c represents the electrode potential (V), $E_{h,i}$ represents the redox potential (V), u_i is the electric potential (V), and S_i represents the electrical conductance (S).

Biogeobattery nodes with index $i \equiv i(a)$, $a = 1, \dots, N$ are assigned. Substitution of Eq. (2) into Eq. (3) gives

$$-E_{h,i} = \sum_{j=1}^N (r_{ij} q_j) + q_i R_i - E_c \quad (4)$$

where $R_i \equiv 1/S_i$ can be regarded as the electrical resistance (Ω).

The charge conservation condition is taken as the $N+1$ th equation, and then the matrix form of Eq. (4) can be written as

$$\begin{pmatrix} E_{h,1} \\ E_{h,2} \\ \vdots \\ E_{h,N} \\ 0 \end{pmatrix} = - \begin{pmatrix} r_{1,1} + R_1 & r_{1,2} & \cdots & r_{1,N} & 1 \\ r_{2,1} & r_{2,2} + R_2 & \cdots & r_{2,N} & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ r_{N,1} & r_{N,2} & \cdots & r_{N,N} + R_N & 1 \\ 1 & 1 & \cdots & 1 & 0 \end{pmatrix} \times \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_N \\ -E_c \end{pmatrix} \quad (5)$$

where r_{ij} is the j th entry of vector $\mathbf{r}_i$, i and j represent the nodeID of biogeobattery nodes. Solve Eq. (5) and then get the unknown currents q_i in the biogeochemical system.

3 Finite-infinite element coupling method

3.1 Boundary value problem

The Poisson equation in a biogeobattery model can be expressed as

$$\nabla \cdot (\sigma \nabla u) = -2 \sum_{i=1}^N q_i \delta(A_i) \in \Omega \quad (6)$$

where σ is the electric conductivity, $\delta(A_i)$ represents the Dirac delta function of point A_i .

On the air-Earth interface, electric potentials satisfy

$$\mathbf{n} \cdot \sigma \nabla u = 0 \in \Gamma_s \quad (7)$$

On the infinite boundary, the coupling of finite elements and infinite elements is achieved.

3.2 Infinite element

Ungless first proposed the concept of the infinite element [53]. The infinite elements are generally grouped into three types: Astley-mapping infinite elements [54, 55], Bettess mapping infinite elements [56, 57], and Burnett multipole expansion infinite elements [58, 59]. Compared with finite elements, infinite elements are more suitable for solving infinite region problems. The essence of infinite elements is an extension of finite elements in infinite domain or semi-infinite domain problems. Infinite elements can be introduced to couple with finite elements at model boundaries to deal with truncated boundary problems. The finite-infinite element coupling method has also been successfully applied to the direct current resistivity method [60, 61], the electromagnetic method [62, 63], and other geophysical fields.

The coupled relationship between finite elements and the Astley-mapping infinite elements [54, 55] is shown in Fig. 2. The infinite elements have directionalities which take the point M at the center of the ground as the only starting point of the mapping and radially map to infinity through the boundary nodes of the finite elements.

As shown in Fig. 3, the uni-directional infinite element starts from nodes 1, 2, 3, and 4 then passes through the middle nodes 5, 6, 7, and 8, respectively, to infinity. The attenuation degree of the SP in the infinite element can be controlled by the distance from M to the surface S_{5678} . Meanwhile, the electric potential values of the four nodes at infinity are zero, which are not considered.

The positive direction of ξ points to infinity, and spatial coordinates of any point in infinite elements can be expressed as

$$\begin{cases} x = \sum_{i=1}^8 M_i(\xi, \eta, \zeta) x_i = M_1 x_1 + M_2 x_2 + \cdots + M_8 x_8 \\ y = \sum_{i=1}^8 M_i(\xi, \eta, \zeta) y_i = M_1 y_1 + M_2 y_2 + \cdots + M_8 y_8 \\ z = \sum_{i=1}^8 M_i(\xi, \eta, \zeta) z_i = M_1 z_1 + M_2 z_2 + \cdots + M_8 z_8 \end{cases} \quad (8)$$

Fig. 2 Coupled relationship of finite elements and infinite elements where the regular hexahedral meshes at the middle of the model are finite elements and the radial hexahedral meshes at around and bottom are infinite elements

where ξ, η , and ζ are local coordinates in parent elements, $x_1, x_2, \dots, x_8, y_1, y_2, \dots, y_8$, and $z_1, z_2, \dots, z_8$ are spatial coordinates of infinite element nodes, $M_i(\xi, \eta, \zeta)$ represents the mapping function which can be expressed as

$$\begin{cases} M_1 = -\frac{\xi(1-\eta)(1+\zeta)}{2(1-\xi)} \\ M_2 = -\frac{\xi(1+\eta)(1+\zeta)}{2(1-\xi)} \\ M_3 = -\frac{\xi(1+\eta)(1-\zeta)}{2(1-\xi)} \\ M_4 = -\frac{\xi(1-\eta)(1-\zeta)}{2(1-\xi)} \end{cases}, \begin{cases} M_5 = \frac{(1+\xi)(1-\eta)(1+\zeta)}{4(1-\xi)} \\ M_6 = \frac{(1+\xi)(1+\eta)(1+\zeta)}{4(1-\xi)} \\ M_7 = \frac{(1+\xi)(1+\eta)(1-\zeta)}{4(1-\xi)} \\ M_8 = \frac{(1+\xi)(1-\eta)(1-\zeta)}{4(1-\xi)} \end{cases} \quad (9)$$

The SP value of any point in infinite elements can be expressed as

$$u = \sum_{i=1}^8 N_i(\xi, \eta, \zeta) u_i \quad (10)$$

where N_i is the shape function which satisfies

$$\begin{cases} N_1 = -\frac{\xi(1-\xi)^2(1-\eta)(1+\zeta)}{16} \\ N_2 = -\frac{\xi(1-\xi)^2(1+\eta)(1+\zeta)}{16} \\ N_3 = -\frac{\xi(1-\xi)^2(1+\eta)(1-\zeta)}{16} \\ N_4 = -\frac{\xi(1-\xi)^2(1-\eta)(1-\zeta)}{16} \end{cases}, \begin{cases} N_5 = \frac{(1-\xi^2)(1-\xi)(1-\eta)(1+\zeta)}{8} \\ N_6 = \frac{(1-\xi^2)(1-\xi)(1+\eta)(1+\zeta)}{8} \\ N_7 = \frac{(1-\xi^2)(1-\xi)(1+\eta)(1-\zeta)}{8} \\ N_8 = \frac{(1-\xi^2)(1-\xi)(1-\eta)(1-\zeta)}{8} \end{cases} \quad (11)$$

3.3 Infinite element analysis

In finite elements, the Jacobi matrix is calculated by the shape function, while the Jacobi matrix in infinite elements is calculated by the mapping function, which can be expressed as

$$[J] = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} = \sum_{i=1}^8 \begin{bmatrix} \frac{\partial M_i}{\partial \xi} x_i & \frac{\partial M_i}{\partial \xi} y_i & \frac{\partial M_i}{\partial \xi} z_i \\ \frac{\partial M_i}{\partial \eta} x_i & \frac{\partial M_i}{\partial \eta} y_i & \frac{\partial M_i}{\partial \eta} z_i \\ \frac{\partial M_i}{\partial \zeta} x_i & \frac{\partial M_i}{\partial \zeta} y_i & \frac{\partial M_i}{\partial \zeta} z_i \end{bmatrix} \quad (12)$$

$$= \begin{bmatrix} \frac{\partial M_1}{\partial \xi} & \frac{\partial M_2}{\partial \xi} & \dots & \frac{\partial M_8}{\partial \xi} \\ \frac{\partial M_1}{\partial \eta} & \frac{\partial M_2}{\partial \eta} & \dots & \frac{\partial M_8}{\partial \eta} \\ \frac{\partial M_1}{\partial \zeta} & \frac{\partial M_2}{\partial \zeta} & \dots & \frac{\partial M_8}{\partial \zeta} \end{bmatrix} \begin{bmatrix} x_1 y_1 z_1 \\ x_2 y_2 z_2 \\ \vdots \\ x_8 y_8 z_8 \end{bmatrix}$$

Fig. 3 Mapping process of infinite element. **a** Sub-element; **b** parent element

Let $\partial N_i/\partial x = F_{ix}$, $\partial N_i/\partial y = F_{iy}$, and $\partial N_i/\partial z = F_{iz}$, then the stiffness matrix of any infinite element can be expressed as

$$K_{ij} = \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 [F_{ix} F_{jx} + F_{iy} F_{jy} + F_{iz} F_{jz}] [J] d\xi d\eta d\zeta \quad (13)$$

where $i, j = 1, \dots, 8$, and K_{ij} represent the stiffness value of infinite elements.

3.4 Finite-infinite element coupling

As shown in Fig. 4, in order to fit complex terrains better, all hexahedral finite elements are further subdivided into tetrahedral finite elements. The stiffness matrix of every finite element and infinite element is $n \times n$ dimensional, where n is the number of element nodes and it is 4 and 8 in tetrahedral finite elements and hexahedral infinite elements, respectively. In the coupled process, just the stiffness matrix values calculated by finite elements and infinite elements are added to the corresponding position of the total stiffness matrix according to the nodeID, respectively.

$$\begin{bmatrix} \dots & \dots & \dots \\ \dots & K_{ij} & \dots \\ \dots & \dots & \dots \end{bmatrix} = \begin{bmatrix} \dots & \dots & \dots \\ \dots & K_{ij}^1 & \dots \\ \dots & \dots & \dots \end{bmatrix} + \begin{bmatrix} \dots & \dots & \dots \\ \dots & K_{ij}^2 & \dots \\ \dots & \dots & \dots \end{bmatrix} \quad (14)$$

where K_{ij} represents the stiffness value of the coupled method, K_{ij}^1 is the stiffness value of finite elements, K_{ij}^2 is the stiffness value of infinite elements, and i and j are nodeID.

4 Numerical modeling

4.1 Algorithm validation

The correctness and effectiveness of the coupled method are verified by a point source model (see

Fig. 5) in homogeneous half-space. In this validation model, the finite element region with dimensions (length $\times$ width $\times$ height) of 15 m $\times$ 15 m $\times$ 10 m is subdivided into $30 \times 30 \times 20$ hexahedral elements, the background resistivity is 100 Ω -m, and the point source with 1 amp is at the surface center. The accuracy of the coupled method with different infinite element dimensions in the mapping direction is also discussed. As shown in Fig. 6, when the term "Multiple," which means the multiple of the infinite element dimension in the mapping direction to the distance from the mapping origin M to the boundary of the finite element region, is 2.5, the minimum mean-square error (MSE) is 0.0292 (see Fig. 6a). The result of the ground SP curves (see Figs. 6b–c) shows that the accuracy of the coupled method is better than the traditional finite element method with the mixed boundary condition (MSE = 0.3158) or the Dirichlet boundary condition (MSE = 3.2570) under the same subdivision conditions, and the results of the coupled method coincide exactly with the analytical solution. The "Multiple" is set as 2.5 in the following models.

Fig. 5 Point source model, where A is the point source, Γ_s is the air-Earth interface, Γ_∞ is the infinite boundary

Fig. 4 A hexahedral finite element is subdivided into five tetrahedral finite elements while the number of nodes does not change

Fig. 6 Algorithm validation of the coupled method. **a** Accuracy of the coupled method with different infinite element dimensions, where the term “Multiple” means the multiple of the infinite element dimension in the mapping direction to the distance

from the mapping origin M to the boundary of the finite element region; **b** Electrical potential curves of different conditions, where the “Multiple” is 2.5; **c** The relative error of the three conditions to the analytical solution, where the “Multiple” is 2.5

Fig. 7 Resistivity model profile with a biogeobattery (10 Ω -m), which are embedded in four decay rates of redox potentials with depth, embedded in a 100 Ω -m half-space. All the biogeobattery nodes are considered as source points. A, B, C, and D represent four decay rates, respectively

4.2 Test—variable redox decay of biogeobattery

The 2D cross-sectional structure of the 3D geoelectric model is shown in Fig. 7. The resistivity (100 Ω -m) model has dimensions of 5 m $\times$ 5 m $\times$ 5 m. A thin, flat biogeobattery system (10 Ω -m) with dimensions of 3 m $\times$ 3 m $\times$ 0.2 m is embedded into this model. The water table is at a depth of 0.5 m, and presupposed four redox fields shown in Fig. 7 are embedded into the biogeobattery to evaluate the dependence of SP anomalies on redox fields. The redox potentials A–D shown in Fig. 7 start from 50 mV at a depth of 0.4 m and decrease to preset values at a depth of 0.6 m, which are –50, –50, 0, and 20 mV, respectively [35]. Assume that R_i equals to zero.

The numerical results (see Fig. 8) show that in cases A and B, larger SP anomalies obtained from higher redox amplitudes are observed. Correspondingly, smaller SP anomalies are obtained in cases C and D. There is an important conclusion that the gradient change in the embedded redox field has no obvious effect on SP anomalies, which is of great significance on field measurements of primary redox fields in contaminated sites.

4.3 Small-scale biogeobattery system

In a small-scale biogeobattery system, the microcolonies are distributed regionally. So, they can be considered as individual biogeobatteries. As shown in Fig. 9, a small-scale (0.1 m $\times$ 0.1 m) model with three microcolonies is modeled to explore the SP anomalies of micro-biogeobatteries. As discussed in the Test part, for SP anomalies, the gradient change in redox potentials is negligible. So, the numerical model can be simplified by only considering the redox potential values at the cathode interface and anode interface. Here, they are set as 10 mV and –10 mV, respectively. When the microcolonies are at a shallow depth (see Fig. 10a), the ground SP anomalies can distinguish the distributions and even the geometries of these individual biogeochemical systems easily. As the depth increases, the ground SP anomalies gradually become blurred and finally present a regional negative anomaly (see Figs. 10b–c), while in a field-scale biogeochemical system, the water table is usually located at a depth of decimeters or even meters. Thus, the ground SP anomaly in field is a macroscopic response of the whole system.

4.4 Field-scale landfill model

In a field-scale biogeochemical system, the water table with rich organic matters and dissolved oxygen can be

Fig. 8 Surface SP anomalies from biogeobatteries with variable redox decay. **a** Result from redox A shown in Fig. 7; **b** result from redox B shown in Fig. 7; **c** result from redox C shown in Fig. 7; **d** result from redox D shown in Fig. 7

Fig. 9 Resistivity model of three small-scale biogeobatteries where the resistance and the resistivity of biogeobatteries, and the background resistivity are 1 Ω , 1 Ω -m, and 100 Ω -m, respectively

considered as a thin, flat macro-biogeobattery model. The system usually exists in landfills, where microbial activities drive electrochemical reactions and establish electron-transfer structures through nanowire networks, microorganisms and (semi-) conductive minerals, or filamentous

bacteria. These mechanisms can connect the cathode and anode of a field-scale biogeobattery quickly and facilitate the transfer of electrons in separated space, which also means that the resistance parameter is very small in a biogeochemical system.

A landfill model (see Fig. 11) with complex terrains has dimensions of 100 m $\times$ 100 m $\times$ 50 m, where the biogeobattery space with dimensions of 32 m $\times$ 32 m $\times$ 1 m is constrained by defining the water table and a thin, flat distribution of redox fields. For the thickness of each layer and its resistivity value (see Fig. 11), refer to Naudet [11]. Here, the redox potential values at the cathode interface and the anode interface are set as 300 mV and -300 mV, respectively. R_i equals to 1 Ω . The result (see Fig. 12) suggests that the landfill model with a biogeochemical system has obvious negative SP anomalies on the ground surface.

Fig. 10 Surface SP anomalies from the small-scale biogeobattery system. **a** Microcolonies are at a depth of 2–3 cm; **b** microcolonies are at a depth of 4–5 cm; **c** microcolonies are at a depth of 8–9 cm

Fig. 11 Resistivity model of a landfill in a field-scale biogeochemical system

5 Discussion

In this paper, a numerical biogeobattery model and a new numerical modeling method based on the IEM and the finite–infinite element coupling, respectively, are presented to simplify the evaluation of SP anomalies from biogeochemical systems which may easily occur in environments with rich organic matters and an

oxidation–reduction interface such as marine sedimentary environments and underground contaminated sites. The numerical examples provide the foundation of data inversion and interpretation in environmental contamination problems like microbial degradation of underground organic contaminants and help to promote the application effect of the SP method in underground contamination detection and monitoring. The numerical result of the effect of preset redox fields and its gradient changes on the ground SP anomaly in the Test part is the same with the work of Mendonça [35], and it provides numerical support and help to simplify the measurement work. The small-scale biogeobattery model and the field-scale landfill model show the negative SP anomaly on the ground, which is consistent with the field work of Naudet [10, 11, 30], Revil [12], Arora [13], Abbas [22], and Linde [29]. The SP surveying is a promising method for environmental problems and can be applied to laboratory experiments or field work relating to 3D time-lapse (4D) monitoring of underground contaminants.

Fig. 12 Surface SP anomalies from the landfill model in a field-scale biogeochemical system

6 Conclusion

The numerical modeling results of the Algorithm Validation and the Test part suggest that (1) the coupled method has high precision, easy implementation, and good processing effects on truncation boundary problems; (2) at least for these models considered here, the preset redox field amplitude is an important factor affecting ground SP anomalies; (3) however, the gradient change in the embedded redox field has no significant effect on ground SP anomalies, which is the foundation of considering a thin, flat IEM as a biogeobattery model. The numerical results in the small-scale biogeochemical system and the field-scale landfill model further show that the biogeobattery model from the IEM is an effective numerical model in biogeochemical systems.

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Compliance with ethical standard

Conflict of interest The authors declare that they have no conflict of interest.

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