

Article

Three-Dimensional Spectral Induced Polarization (SIP) Forward Modelling Based on Piecewise Linear Continuous Geoelectric Model Using Finite Elements and Recursive Inversion

Haifei Liu ^{1,2}, Daowei Zhu ^{1,*}, Yingjie Zhao ¹, Rujun Chen ^{1,2}, Talal M. S. Alqadhi ¹ and Chunming Liu ^{1,*}

¹ School of Geosciences and Info-Physics, Central South University, Changsha 410083, China; 207187@csu.edu.cn (H.L.); chrujun@csu.edu.cn (R.C.)

² Hunan Key Laboratory of Nonferrous Resources and Geological Disaster Exploration, Central South University, Changsha 410083, China

* Correspondence: 245011098@csu.edu.cn (D.Z.); liuchunming@csu.edu.cn (C.L.)

Abstract

Petrophysical parameters of rocks and ores, influenced by composition, porosity, temperature, and pressure, are generally distributed uniformly or continuously in space—relatively homogeneous within individual geological units and varying smoothly across stratigraphic transition zones and contact boundaries. Based on this geological characteristic, this paper establishes a three-dimensional (3-D) piecewise linear continuous spectral parameter model to compute forward responses of apparent spectral parameters under low-frequency current excitation. The calculation follows a two-step workflow: finite-element forward simulation of multi-frequency apparent complex resistivity, followed by recursive inversion to obtain apparent spectral parameters. The subsurface medium is discretized with hexahedral meshes, with four Cole–Cole parameters (zero-frequency resistivity, chargeability, time constant, and frequency exponent) assigned to each mesh node. Linear interpolation is adopted for complex resistivity and potential within each element, ensuring piecewise linear continuity of both physical properties and simulated fields. To improve accuracy, the total complex potential is decomposed into a primary field from the source current and a secondary field from complex conductivity variations, and the corresponding boundary value problem and variational form are derived. On this basis, we implement the finite-element algorithm for 3-D piecewise linear continuous media and the recursive inversion algorithm for spectral parameters, and develop an interactive 3-D SIP forward modeling program. Comparison with analytical solutions for a continuous layered model shows good agreement, with relative errors below 1.5% for the real part and 3.8% for the imaginary part of apparent complex resistivity. Two numerical cases—a cubic anomaly in homogeneous half-space and a sandbox model—further verify the performance of the proposed method.

Keywords: 3-D SIP forward modeling; piecewise linear continuous geoelectric model; Cole-Cole model; finite element method; recursive inversion

MSC: 65N30; 86A22

Received: 29 April 2026

Revised: 27 May 2026

Accepted: 29 June 2026

Published: 2 July 2026

Copyright: © 2026 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license.

1. Introduction

The spectral induced polarization (SIP) method is a classical frequency-domain geoelectrical exploration technique. Physically, it arises from the polarization effect of rock and ore particles under alternating excitation electric fields: charged species in pore water and the rock matrix accumulate and migrate at medium interfaces, producing pronounced frequency-dependent polarization responses. Owing to its multi-parameter measurement capability and rich spectral information, SIP has been widely applied in various geological and engineering fields. In mineral exploration, SIP effectively delineates disseminated sulfide mineralization zones and distinguishes ore-bearing rocks from barren host rocks by extracting chargeability and time constant parameters [1]. For hydrogeological investigations, SIP provides quantitative constraints on pore structure, water saturation, and hydraulic conductivity of aquifers [2]. In environmental geophysics, time-lapse SIP monitoring tracks the migration of hydrocarbon contaminants and heavy metal plumes, and characterizes biodegradation processes in porous media [3,4]. Furthermore, emerging biogeophysical studies have confirmed the sensitivity of imaginary conductivity to subsurface microbial activity, extending the application scope of SIP to biogeochemical process monitoring [4–6].

To characterize the SIP responses of rocks and ores, several mathematical models have been proposed, including the Cole–Cole model [7], the Debye decomposition model [8], and the Warburg model [9]. Among these, the Cole–Cole model has gained the most widespread adoption, and numerous modified forms have been developed to describe the physical properties of rocks and ores [10]. Given its versatility and maturity, the Cole–Cole model is adopted in this study as the theoretical basis for constructing the three-dimensional geoelectric model.

With the growing application of the SIP method, the development of efficient and accurate forward modeling algorithms has become a key research focus in SIP data processing. The objective of SIP forward modeling is to predict the SIP responses of subsurface geological structures based on electrode array measurements. Existing numerical simulation methods for SIP mainly include the integral equation method, the finite-difference method (FDM), and the finite element method (FEM). When applied to complex geological structures, the integral equation method and FDM generally suffer from simulation errors due to grid approximation [11–16]. In contrast, FEM has been extensively employed in geoelectromagnetic numerical simulations owing to its flexible mesh generation capability [17–22], which enables accurate representation of complex geological structures. Despite these advances, most existing SIP numerical simulation methods assume piecewise-uniform physical property parameters in geoelectric models. However, the physical properties of subsurface media are typically influenced by factors such as composition, porosity, and temperature, resulting in continuous spatial variations. Consequently, piecewise-uniform modeling approaches produce stepwise approximations of subsurface media, which may compromise the fidelity of SIP response simulation for continuously varying anomalies.

In addition to forward modeling, estimating apparent spectral parameters from multi-frequency apparent complex resistivity data is essential for investigating the spectral characteristics of subsurface targets. Early spectral parameter estimation methods mainly relied on nonlinear least-squares iterative inversion [11,23,24]. However, these methods are highly dependent on initial parameter estimates and tend to converge to local minima. Xiang et al. [25] proposed a direct inversion method based on multiple least-squares estimation combined with optimal search techniques for calculating Cole–Cole spectral parameters, which ensures global convergence. Furthermore, to reduce the dependence on initial parameter values, several stochastic inversion approaches have been proposed for estimating Cole–Cole spectral parameters, including simulated annealing [17,26,27], genetic algorithms [28], and Bayesian inversion [29,30]. Nevertheless, practical

challenges remain in balancing computational efficiency, stability, and ease of implementation for spectral parameter estimation.

To address the above limitations in both forward simulation and spectral parameter estimation, this study proposes a two-step approach for SIP forward modeling based on a three-dimensional (3-D) continuous geoelectric model. The approach first computes multi-frequency apparent complex resistivity using the finite element method, and then estimates apparent spectral parameters using a recursive inversion algorithm. During the simulation, the physical property parameters of the geoelectric model are assumed to vary in a piecewise linearly continuous manner. To mitigate the influence of point-source singularities, a primary–secondary field decomposition strategy is employed. A finite-element numerical simulation algorithm is developed for the complex-domain potential field of the 3-D continuous medium model, and the Symmetric Successive Over-Relaxation Preconditioned Conjugate Gradient (SSOR-PCG) method is adopted to efficiently solve large-scale complex-coefficient linear systems. Building on the Cole–Cole model, a recursive inversion algorithm for spectral parameter estimation is further proposed, which eliminates the need for manual initialization and is both straightforward and computationally efficient.

Based on the proposed algorithm, a full-process interactive three-dimensional SIP finite element forward modeling program is developed for continuous geoelectric media. Several numerical test cases are designed to verify the reliability of the algorithm, including a three-layer model with analytical solution comparison, a cuboid ore body model with continuously graded spectral parameters, and a sandbox physical model with boundary correction. Finally, the advantages, limitations, and potential research directions of the presented algorithm are discussed.

2. 3-D Piecewise Linear Continuous SIP Model Parameterization

The petrophysical parameters of subsurface rocks and ores are governed by lithology, porosity, temperature and pressure. These parameters are relatively homogeneous within an individual geological unit and vary smoothly and continuously in stratigraphic transition zones and formation contact interfaces. For macro-scale geophysical prospecting, this paper adopts a three-dimensional piecewise linear continuous geoelectric model with spectral parameters to perform low-frequency SIP forward modeling. The proposed model conforms to the actual spatial distribution characteristics of petrophysical properties, which can describe uniform physical properties inside geological units and gradual property variations at formation boundaries.

The subsurface Cole–Cole spectral parameters, zero-frequency resistivity ρ_0 , chargeability m , time constant τ , and frequency exponent c , vary continuously with subsurface conditions and can be treated as continuous functions of spatial coordinates.

Numerical 3-D simulation requires discretizing the continuous spectral parameters into a geoelectric model defined by discrete mesh nodes; this discretization procedure is termed model parameterization. As illustrated in Figure 1, the entire computational domain Ω is partitioned into a set of hexahedral elements to realize the parameterization of the continuous geoelectric model. Each hexahedral element is defined by spectral parameters assigned to its eight vertices.

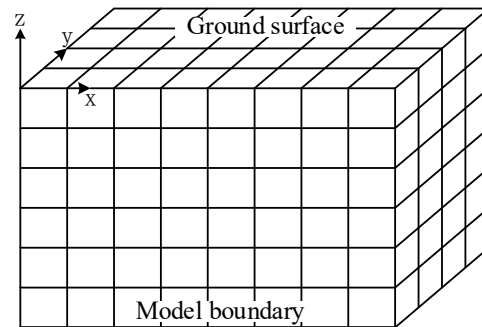


Figure 1. Parameterization of the SIP model using a hexahedral discretization scheme.

Substituting the vertex-specific spectral parameters $(\rho_{0j}, m_j, \tau_j, c_j)$ into the Cole-Cole model [7], the complex resistivity at vertex j is written as:

$$\rho_j(i\omega) = \rho_{0j} \left\{ 1 - m_j \left[1 - \frac{1}{1 + (i\omega\tau_j)^{c_j}} \right] \right\}, j = 1, 2, \dots, 8 \quad (1)$$

For finite-element computation, linear interpolation is applied within each hexahedral element. Complex resistivity is assumed to change linearly between the eight vertices of one element, which guarantees piecewise linear continuity of both medium physical properties and simulated electric fields over the full modeling domain.

Laboratory multi-frequency measurements on rock blocks, ore outcrops and drill core samples indicate that the complex resistivity spectra of most rock and ore types can be fully characterized by the four Cole-Cole parameters. Accordingly, a complete 3-D geoelectric model can be constructed by discretizing the research domain Ω into hexahedral meshes and assigning a set of Cole-Cole parameters to every mesh node.

3. Boundary Value Problem and Variational Formulation of the Complex Potential Field

3.1. Boundary Value Problem of the Complex Potential Field

The transmitting frequencies of the alternating-current source used in the spectral induced polarization (SIP) method are sufficiently low (typically < 100 Hz); therefore, displacement currents and electromagnetic induction effects can be neglected. Under this quasi-static approximation, the governing differential equation for the complex electrical potential in the three-dimensional (3-D) complex resistivity forward problem is given by:

$$\nabla \cdot [\sigma(i\omega) \nabla v(i\omega)] = -I(i\omega) \delta(A), \quad \in \Omega \quad (2)$$

where ω is the angular frequency, $i = \sqrt{-1}$, $v(i\omega)$ is the complex potential field induced by the alternating-current $I(i\omega)$, $\delta(A)$ is the Dirac delta function centered at the location of the point current source A on the surface or underground, and $\sigma(i\omega)$ is the complex conductivity of the study domain Ω , which is the reciprocal of complex resistivity $\rho(i\omega)$.

To solve Equation (2), appropriate boundary conditions must be specified. On the ground surface Γ_s , since no current flows through the air-ground interface Γ_s , the normal derivative of the complex potential $v(i\omega)$ is

$$\partial v(i\omega) / \partial n = 0, \quad \in \Gamma_s \quad (3)$$

On the outer boundaries of the computational domain Γ_∞ , it is assumed that the electrical inhomogeneities within the study area Ω do not significantly affect the potential distribution of the background medium Γ_∞ . Under this assumption, the potential field

generated by a point source A located underground and its image source A' relative to the ground surface can be expressed as

$$v(i\omega) = \frac{c}{r_A} + \frac{c}{r_{A'}}, \quad \in \Gamma_\infty \quad (4)$$

where c is a constant, and r_A and $r_{A'}$ denote the distances from the source A and A' , its image source, to the boundary Γ_∞ , respectively. When the boundary Γ_∞ is sufficiently far away, Equation (4) provides the first boundary approximation. The outward normal derivative of the complex potential $v(i\omega)$ in Equation (4) is then given by

$$\frac{\partial v(i\omega)}{\partial n} = -\frac{c}{r_A^2} \cos(\mathbf{r}_A, \mathbf{n}) - \frac{c}{r_{A'}^2} \cos(\mathbf{r}_{A'}, \mathbf{n}), \quad \in \Gamma_\infty \quad (5)$$

where $\cos(\mathbf{r}_A, \mathbf{n})$ and $\cos(\mathbf{r}_{A'}, \mathbf{n})$ denote the direction cosines between the radius vectors $\mathbf{r}_A$ and $\mathbf{r}_{A'}$ and the outward normal vector $\mathbf{n}$ at the boundary surface, respectively. Substituting Equation (4) into Equation (5) yields the mixed boundary condition

$$\partial v(i\omega) / \partial n + Dv(i\omega) = 0, \quad \in \Gamma_\infty \quad (6)$$

where $D = [r_A^2 \cos(\mathbf{r}_A, \mathbf{n}) + r_{A'}^2 \cos(\mathbf{r}_{A'}, \mathbf{n})] / [(r_A + r_{A'})r_A r_{A'}]$. Equation (1) and boundary conditions Equations (3) and (6) together define the boundary value problem for the total complex potential field:

$$\begin{cases} \nabla \cdot [\sigma(i\omega) \nabla v(i\omega)] = -I(i\omega) \delta(A), \quad \in \Omega \\ \partial v(i\omega) / \partial n = 0, \quad \in \Gamma_s \\ \partial v(i\omega) / \partial n + Dv(i\omega) = 0, \quad \in \Gamma_\infty \end{cases} \quad (7)$$

Numerical solutions of this boundary value problem often exhibit reduced accuracy near the source location. To address this issue, the singularity removal technique proposed by Lowry et al. [31] is adopted. The total complex conductivity $\sigma(i\omega)$ is decomposed into a background conductivity $\sigma_0(i\omega)$ and an anomalous conductivity $\sigma_a(i\omega) = \sigma(i\omega) - \sigma_0(i\omega)$. Accordingly, the total complex potential $v(i\omega)$ is decomposed into a background (primary) potential $u_0(i\omega)$ and an anomalous (secondary) potential $u(i\omega)$, i.e., $v(i\omega) = u_0(i\omega) + u(i\omega)$. Substituting this decomposition into Equation (7) yields the boundary value problem for the anomalous complex potential field generated by an alternating point current source:

$$\begin{cases} \nabla \cdot [\sigma(i\omega) \nabla u(i\omega)] = -\nabla \cdot [\sigma_a(i\omega) \nabla u_0(i\omega)], \quad \in \Omega \\ \partial u(i\omega) / \partial n = 0, \quad \in \Gamma_s \\ \partial u(i\omega) / \partial n + Du(i\omega) = 0, \quad \in \Gamma_\infty \end{cases} \quad (8)$$

The background (primary) potential is defined as

$$u_0(i\omega) = \frac{I}{4\pi\sigma_0(i\omega)} \left(\frac{1}{r_{AP}} + \frac{1}{r_{A'P}} \right) \quad (9)$$

where r_{AP} and $r_{A'P}$ are the distances from the transmitting point source A and its image source A' to the observation point P , respectively.

3.2. Variational Formulation of the Anomalous Potential Field

We derive the finite-element discretization via complex variational calculus. Since both the electric potential and conductivity are complex-valued, the real-valued energy minimization principle for real elliptic PDEs cannot be directly applied. Instead, we solve for stationary points of a real-valued functional constructed over complex fields.

We first define the complex conjugate inner product on the computational domain Ω :

$$\langle f, g \rangle_{\Omega} = \int_{\Omega} f \bar{g} d\Omega$$

where the overline $\overline{(\cdot)}$ denotes the complex conjugate operator. In the complex variational calculus, the complex function $u(i\omega)$ and its conjugate $\bar{u}(i\omega)$ are treated as two independent variables. The variation of the gradient term satisfies:

$$\delta[\nabla u(i\omega)] = \nabla[\delta u(i\omega)], \quad \delta[\nabla \bar{u}(i\omega)] = \nabla[\delta \bar{u}(i\omega)]$$

From the complex variational principle, the exact solution to the governing differential equation renders the corresponding real-valued functional stationary. For the boundary value problem described in Equation (8), we construct the real-valued functional as follows [32]:

$$F[u(i\omega), \bar{u}(i\omega)] = \int_{\Omega} \left\{ \frac{1}{2} \sigma \nabla u(i\omega) \cdot \nabla \bar{u}(i\omega) + \sigma_a \nabla u_0(i\omega) \cdot \nabla \bar{u}(i\omega) \right\} d\Omega \quad (10)$$

Taking the first-order variation of Equation (10) with respect to the conjugate field $\bar{u}(i\omega)$, we obtain:

$$\delta F[u(i\omega), \bar{u}(i\omega)] = \int_{\Omega} [\sigma(i\omega) \nabla u(i\omega) + \sigma_a(i\omega) \nabla u_0(i\omega)] \cdot \nabla \delta \bar{u}(i\omega) d\Omega \quad (11)$$

We employ the standard vector identity

$$\nabla \cdot (\mathbf{A} \varphi) = \nabla \cdot \mathbf{A} \varphi + \mathbf{A} \cdot \nabla \varphi$$

and the divergence theorem

$$\int_{\Omega} \nabla \cdot (\mathbf{A} \varphi) d\Omega = \int_{\Gamma} (\mathbf{A} \cdot \mathbf{n}) \varphi d\Gamma$$

to derive the integration-by-parts formula:

$$\int_{\Omega} \mathbf{A} \cdot \nabla \varphi d\Omega = \int_{\Gamma} (\mathbf{A} \cdot \mathbf{n}) \varphi d\Gamma - \int_{\Omega} \nabla \cdot (\mathbf{A} \varphi) d\Omega$$

In the above expression, $\mathbf{A}$ stands for an arbitrary vector test function and φ for an arbitrary scalar test function. The boundary $\Gamma = \Gamma_s + \Gamma_{\infty}$ encloses the full computational domain Ω .

Let $\mathbf{A} = \sigma(i\omega) \nabla u(i\omega) + \sigma_a(i\omega) \nabla u_0(i\omega)$ and $\varphi = \delta \bar{u}(i\omega)$. Substituting this relation into Equation (11) to reorganize the variational term gives

$$\begin{aligned} \delta F[u(i\omega), \bar{u}(i\omega)] &= \int_{\Gamma_s + \Gamma_{\infty}} \left(\sigma(i\omega) \frac{\partial u(i\omega)}{\partial n} + \sigma_a(i\omega) \frac{\partial u_0(i\omega)}{\partial n} \right) \delta \bar{u}(i\omega) d\Gamma \\ &\quad - \int_{\Omega} [\nabla \cdot (\sigma(i\omega) \nabla u(i\omega) + \sigma_a(i\omega) \nabla u_0(i\omega))] \delta \bar{u}(i\omega) d\Omega \end{aligned} \quad (12)$$

Substituting the governing Equation (8) into Equation (12) simplifies the variational equality to

$$\begin{aligned} \delta F[u(i\omega), \bar{u}(i\omega)] &= - \int_{\Gamma_{\infty}} [\sigma(i\omega) Du(i\omega) + \sigma_a(i\omega) Du_0(i\omega)] \delta \bar{u}(i\omega) d\Gamma \\ &= - \delta \int_{\Gamma_{\infty}} D \left[\frac{1}{2} \sigma(i\omega) u(i\omega) \bar{u}(i\omega) + \sigma_a(i\omega) u_0(i\omega) \bar{u}(i\omega) \right] d\Gamma \end{aligned} \quad (13)$$

Equivalently, moving the boundary variational term to the left-hand side gives

$$\begin{aligned} &\delta \left\{ F[u(i\omega), \bar{u}(i\omega)] + \int_{\Gamma_{\infty}} D \left[\frac{1}{2} \sigma(i\omega) u(i\omega) \bar{u}(i\omega) + \sigma_a(i\omega) u_0(i\omega) \bar{u}(i\omega) \right] d\Gamma \right\} \\ &= \delta \left\{ \int_{\Omega} \left[\frac{1}{2} \sigma(i\omega) \nabla u(i\omega) \cdot \nabla \bar{u}(i\omega) + \sigma_a(i\omega) \nabla u_0(i\omega) \cdot \nabla \bar{u}(i\omega) \right] d\Omega \right. \\ &\quad \left. + \int_{\Gamma_{\infty}} D \left[\frac{1}{2} \sigma(i\omega) u(i\omega) \bar{u}(i\omega) + \sigma_a(i\omega) u_0(i\omega) \bar{u}(i\omega) \right] d\Gamma \right\} = 0 \end{aligned}$$

In summary, the boundary value problem given by Equation (8) is equivalent to the following variational formulation [30]:

$$F[u(i\omega), \bar{u}(i\omega)] = \int_{\Omega} \left[\frac{1}{2} \sigma(i\omega) \nabla u(i\omega) \nabla \bar{u}(i\omega) + \sigma_a(i\omega) \nabla u_0(i\omega) \cdot \nabla \bar{u}(i\omega) \right] d\Omega \\ + \int_{\Gamma_{\infty}} D \left(\frac{1}{2} \sigma(i\omega) u(i\omega) \bar{u}(i\omega) + \sigma_a(i\omega) u_0(i\omega) \bar{u}(i\omega) \right) d\Gamma \\ \delta F[u(i\omega), \bar{u}(i\omega)] = 0 \quad (14)$$

4. Formulation of the Finite Element Equation

4.1. Element Subdivision

The model domain Ω is discretized into hexahedral elements, as shown in Figure 1. The integral form of Equation (14) is then decomposed into elemental integrals, yielding

$$F[u(i\omega), \bar{u}(i\omega)] = \sum_{\Omega} \int_{\Omega} \left[\frac{1}{2} \sigma(i\omega) \nabla u(i\omega) \nabla \bar{u}(i\omega) + \sigma_a(i\omega) \nabla u_0(i\omega) \cdot \nabla \bar{u}(i\omega) \right] d\Omega \\ + \sum_{\Gamma_{\infty}} \int_{\Gamma_{\infty}} \left[\frac{1}{2} D \sigma(i\omega) u(i\omega) \bar{u}(i\omega) + D \sigma_a(i\omega) u_0(i\omega) \bar{u}(i\omega) \right] d\Gamma \quad (15)$$

4.2. Linear Interpolation

To enable the finite element method to simulate continuous geoelectric earth models, it is assumed that, within each hexahedral element, the primary and secondary complex potentials, complex conductivity, and anomalous complex conductivity vary as linear functions of the Cartesian coordinates x , y , and z .

$$u_0(i\omega) = \sum_{j=1}^8 n_j u_{0j}(i\omega), \quad u(i\omega) = \sum_{j=1}^8 n_j u_j(i\omega), \quad \sigma(i\omega) = \sum_{j=1}^8 n_j \sigma_j(i\omega), \quad \sigma_a(i\omega) = \sum_{j=1}^8 n_j \sigma_{aj}(i\omega) \quad (16)$$

where $u_{0j}(i\omega)$, $u_j(i\omega)$, $\sigma_j(i\omega)$ and $\sigma_{aj}(i\omega)$ are the primary complex potential, secondary complex potential, conductivity, and anomalous conductivity at the corner node J of a hexahedral element ($J=1, 2, \dots, 8$), defined in the global coordinate system, are denoted (see Figure 2a). The functions n_j are linear shape functions defined as [32]:

$$n_j = \frac{1}{8} (1 + \xi_j \xi) (1 + \eta_j \eta) (1 + \zeta_j \zeta), \quad (j=1, 2, \dots, 8) \quad (17)$$

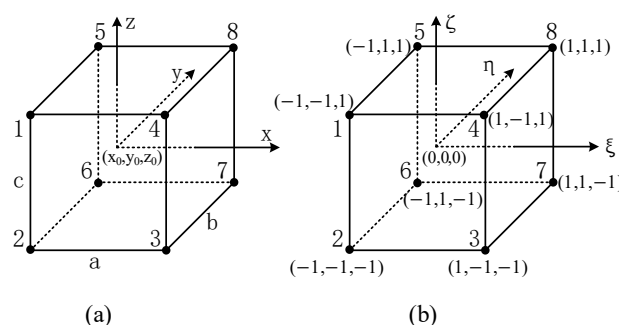


Figure 2. Hexahedral element in the global coordinate system (a) and in the local coordinate system (b) for FE modeling.

In Equation (17), (ξ_j, η_j, ζ_j) denote the local coordinates of the corner point j in the natural coordinate system (ξ, η, ζ) (see Figure 2b). A key step in the finite element method is the transformation between the global coordinates (x, y, z) and the corresponding local coordinates (ξ, η, ζ) , given by

$$x = x_0 + \frac{a}{2}\xi, \quad y = y_0 + \frac{b}{2}\eta, \quad z = z_0 + \frac{c}{2}\zeta \quad (18)$$

where x_0, y_0 and z_0 are the coordinates of the center of the hexahedral element, and a, b and c are the length, width, and height of the element, respectively. This transformation simplifies the evaluation of the integrals in Equation (15). Using Equations (16)–(18), the volume integrals in Equation (15) can be evaluated analytically in the local coordinate system.

4.3. Element Integration

(1) The volume element integration of Equation (15).

The volume integral in Equation (15) can be expressed as

$$\int_e \frac{1}{2} \sigma(i\omega) \nabla u(i\omega) \nabla \bar{u}(i\omega) d\Omega = \int_e \frac{1}{2} \sigma(i\omega) \left[\frac{\partial u(i\omega)}{\partial x} \frac{\partial \bar{u}(i\omega)}{\partial x} + \frac{\partial u(i\omega)}{\partial y} \frac{\partial \bar{u}(i\omega)}{\partial y} + \frac{\partial u(i\omega)}{\partial z} \frac{\partial \bar{u}(i\omega)}{\partial z} \right] dx dy dz = \frac{1}{2} \bar{\mathbf{u}}_e(i\omega)^T \mathbf{S}_{1e} \mathbf{u}_e(i\omega) \quad (19)$$

where $\mathbf{S}_{1e} = (S_{1jk})$, $S_{1jk} = S_{1kj}$, $\mathbf{u}_e(i\omega) = [u_j(i\omega)]^T$, $j, k = 1, 2, \dots, 8$.

$$k_{1jk} = \int_e \sum_{l=1}^8 n_l \sigma_l(i\omega) \left(\frac{\partial n_j}{\partial x} \frac{\partial n_k}{\partial x} + \frac{\partial n_j}{\partial y} \frac{\partial n_k}{\partial y} + \frac{\partial n_j}{\partial z} \frac{\partial n_k}{\partial z} \right) dx dy dz = \frac{1}{288} \sum_{l=1}^8 \left[\left(\frac{bc}{a} \alpha_{jkl} + \frac{ac}{b} \beta_{jkl} + \frac{ab}{c} \gamma_{jkl} \right) \cdot \sigma_l(i\omega) \right]$$

and

$$\left. \begin{aligned} \alpha_{jkl} &= [\xi_j \xi_k] [3 + (\eta_j \eta_k + \eta_j \eta_l + \eta_k \eta_l)] [3 + (\zeta_j \zeta_k + \zeta_j \zeta_l + \zeta_k \zeta_l)] / 4 \\ \beta_{jkl} &= [\eta_j \eta_k] [3 + (\xi_j \xi_k + \xi_j \xi_l + \xi_k \xi_l)] [3 + (\zeta_j \zeta_k + \zeta_j \zeta_l + \zeta_k \zeta_l)] / 4 \\ \gamma_{jkl} &= [\zeta_j \zeta_k] [3 + (\xi_j \xi_k + \xi_j \xi_l + \xi_k \xi_l)] [3 + (\eta_j \eta_k + \eta_j \eta_l + \eta_k \eta_l)] / 4 \end{aligned} \right\}, (j, k, l = 1, 2, \dots, 8) \quad (20)$$

The specific values of these integration coefficients are given in Appendix A.

Similarly, for the following integral:

$$\int_e \sigma_a(i\omega) \nabla u_0(i\omega) \cdot \nabla \bar{u}(i\omega) d\Omega = \int_e \sigma_a(i\omega) \left[\frac{\partial \bar{u}(i\omega)}{\partial x} \frac{\partial u_0(i\omega)}{\partial x} + \frac{\partial \bar{u}(i\omega)}{\partial y} \frac{\partial u_0(i\omega)}{\partial y} + \frac{\partial \bar{u}(i\omega)}{\partial z} \frac{\partial u_0(i\omega)}{\partial z} \right] dx dy dz = \bar{\mathbf{u}}_e(i\omega)^T \mathbf{S}'_{1e} \mathbf{u}_{0e}(i\omega) \quad (21)$$

where $\mathbf{S}'_{1e} = (S'_{1jk})$, $S'_{1jk} = S'_{1kj}$, $\mathbf{u}_{0e}(i\omega) = [u_{0j}(i\omega)]^T$, $j, k = 1, 2, \dots, 8$.

$$S'_{1jk} = \int_e \sum_{l=1}^8 n_l \sigma_{al}(i\omega) \left(\frac{\partial n_j}{\partial x} \frac{\partial n_k}{\partial x} + \frac{\partial n_j}{\partial y} \frac{\partial n_k}{\partial y} + \frac{\partial n_j}{\partial z} \frac{\partial n_k}{\partial z} \right) dx dy dz = \frac{1}{288} \sum_{l=1}^8 \left[\left(\frac{bc}{a} \alpha_{jkl} + \frac{ac}{b} \beta_{jkl} + \frac{ab}{c} \gamma_{jkl} \right) \cdot \sigma_{al}(i\omega) \right]$$

where the definitions of α_{jkl} , β_{jkl} and γ_{jkl} are consistent with those in Equation (20).

(2) The boundary element integration of Equation (15)

The boundary element integration in Equation (15) is more complex and requires simplification. First, it is assumed that one surface $\overline{1234}$ of the hexahedral element lies on an infinite boundary. Under this assumption, the distance from the source point A to any point on the plane $\overline{1234}$ can be considered approximately constant, i.e., the integrand D is treated as uniform over the surface. Therefore, the boundary integral Γ_e in Equation (15) can be approximated as

$$\int_{\Gamma_e} \left[\frac{1}{2} D \sigma(i\omega) u(i\omega) \bar{u}(i\omega) + D \sigma_a(i\omega) u_0(i\omega) \bar{u}(i\omega) \right] d\Gamma = \frac{1}{2} D \cdot \int_{\Gamma_e} \sigma(i\omega) u(i\omega) \bar{u}(i\omega) d\Gamma + D \cdot \int_{\Gamma_e} \sigma_a(i\omega) u_0(i\omega) \bar{u}(i\omega) d\Gamma \quad (22)$$

$$= \frac{1}{2} \bar{\mathbf{u}}_e(i\omega)^T \mathbf{S}_{2e} \mathbf{u}_e(i\omega) + \bar{\mathbf{u}}_e(i\omega)^T \mathbf{S}'_{2e} \mathbf{u}_{0e}(i\omega)$$

where $\mathbf{S}_{2e} = (S_{2jk})$, $S_{2jk} = S_{2kj}$, $\mathbf{S}'_{2e} = (S'_{2jk})$, $S'_{2jk} = S'_{2kj}$, $\mathbf{u}_{0e}(i\omega) = [u_{0j}(i\omega)]^T$, $\mathbf{u}_e(i\omega) = [u_j(i\omega)]^T$, $j, k = 1, 2, \dots, 4$.

$$S_{2jk} = D \cdot \int_{\overline{1234}} \sum_{l=1}^4 n_l \sigma_l(i\omega) (n_j n_k) \Big|_{\eta=-1} dx dz = D \frac{ac}{144} \sum_{l=1}^4 [\delta_{jkl} \cdot \sigma_l(i\omega)]$$

$$S'_{2jk} = D \cdot \int_{\overline{1234}} \sum_{l=1}^4 n_l \sigma_{al}(i\omega) (n_j n_k) \Big|_{\eta=-1} dx dz = D \frac{ac}{144} \sum_{l=1}^4 [\delta_{jkl} \cdot \sigma_{al}(i\omega)]$$

in which

$$\delta_{jkl} = \left[3 + (\xi_j \xi_k + \xi_j \xi_l + \xi_k \xi_l) \right] \left[3 + (\zeta_j \zeta_k + \zeta_j \zeta_l + \zeta_k \zeta_l) \right] / 4, \quad (j, k, l = 1, 2, \dots, 4) \quad (23)$$

Subsequently, the nodal coordinates of surface $\overline{1234}$ in the local coordinate system are substituted into Equation (23), yielding the corresponding coefficients of the lower triangular matrix.

$$\begin{bmatrix} \delta_{11} \\ \delta_{21} \\ \delta_{31} \\ \delta_{41} \end{bmatrix} = \begin{bmatrix} 9 & 3 & 1 & 3 \\ 3 & 3 & 1 & 1 \\ 3 & 9 & 3 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}, \quad \begin{bmatrix} \delta_{33} \\ \delta_{41} \\ \delta_{42} \\ \delta_{43} \\ \delta_{44} \end{bmatrix} = \begin{bmatrix} 1 & 3 & 9 & 3 \\ 3 & 1 & 1 & 3 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 3 & 3 \\ 3 & 1 & 3 & 1 \end{bmatrix}$$

The same procedure applies to other element surfaces $\overline{1234}$ that lie on the infinite boundary.

4.4. Complex Stiffness Matrix Assembly

The element stiffness matrices $\mathbf{S}_{1e}, \mathbf{S}_{2e}, \mathbf{S}'_{1e}, \mathbf{S}'_{2e}$ are obtained by summing the integrals in Equations (19), (21), and (22) over each finite element e , and subsequently assembling them into the global stiffness matrix associated with the global nodal system, yielding

$$F_e[u(i\omega), \bar{u}(i\omega)] = \frac{1}{2} \bar{\mathbf{u}}_e(i\omega)^T (\mathbf{S}_{1e} + \mathbf{S}_{2e}) \mathbf{u}_e(i\omega) + \bar{\mathbf{u}}_e(i\omega)^T (\mathbf{S}'_{1e} + \mathbf{S}'_{2e}) \mathbf{u}_{0e}(i\omega) = \frac{1}{2} \bar{\mathbf{u}}_e(i\omega)^T \mathbf{S}_e \mathbf{u}(i\omega) + \bar{\mathbf{u}}_e(i\omega)^T \mathbf{S}'_e \mathbf{u}_0(i\omega)$$

where $\mathbf{u}(i\omega)$ and $\mathbf{u}_0(i\omega)$ denote the column vectors of all nodal variables $u(i\omega)$ and $u_0(i\omega)$ respectively; $\mathbf{S}_e$ and $\mathbf{S}'_e$ are the corresponding expansion (assembly) matrices of $\mathbf{S}_{1e} + \mathbf{S}_{2e}$ and $\mathbf{S}'_{1e} + \mathbf{S}'_{2e}$ respectively. By summing over all elements $F_e[u(i\omega), \bar{u}(i\omega)]$, $F[u(i\omega), \bar{u}(i\omega)]$, Equation (24) can be expressed as

$$F[u(i\omega), \bar{u}(i\omega)] = \sum_e F_e[u(i\omega), \bar{u}(i\omega)] = \frac{1}{2} \bar{\mathbf{u}}(i\omega)^T \sum_e \mathbf{S}_e \mathbf{u}(i\omega) + \bar{\mathbf{u}}(i\omega)^T \sum_e \mathbf{S}'_e \mathbf{u}_0(i\omega) = \frac{1}{2} \bar{\mathbf{u}}(i\omega)^T \mathbf{S} \mathbf{u}(i\omega) + \bar{\mathbf{u}}(i\omega)^T \mathbf{S}' \mathbf{u}_0(i\omega) \quad (24)$$

Using Equation (24), the first variation of the functional $F[u(i\omega), \bar{u}(i\omega)]$ with respect to $\bar{\mathbf{u}}(i\omega)$ is given by

$$\delta F[u(i\omega), \bar{u}(i\omega)] = \delta \bar{\mathbf{u}}(i\omega)^T [\mathbf{S} \mathbf{u}(i\omega) + \mathbf{S}' \mathbf{u}_0(i\omega)] \quad (25)$$

The functional is minimized by setting its first variation to zero, which yields the final finite element governing equation:

$$\mathbf{S} \mathbf{u}(i\omega) = -\mathbf{S}' \mathbf{u}_0(i\omega) \quad (26)$$

where the resulting system matrices $\mathbf{S}$ and $\mathbf{S}'$ are symmetric and sparse, with non-zero elements distributed sparsely. By solving Equation (26), the anomalous potentials at all grid nodes under different angular frequencies and transmitting points can be obtained.

5. Symmetric Successive Over-Relaxation Preconditioned Conjugate Gradient Method (SSOR-PCG)

The efficiency of three-dimensional spectral induced polarization finite-element simulations largely depends on the efficiency of solving the resulting linear system. Considering that the coefficient matrix $\mathbf{S}$ is large, sparse, and symmetric, the SSOR-PCG method is employed to solve Equation (26). In addition, the non-zero elements of the matrix are stored using the Compressed Sparse Row (CSR) format to reduce memory consumption.

First, the coefficient matrix $\mathbf{S}$ is decomposed as

$$\mathbf{S} = \mathbf{C} + \mathbf{D} + \mathbf{C}^T \quad (27)$$

The corresponding SSOR preconditioning matrix is defined as [33]

$$\mathbf{M} = \frac{1}{(2-\omega)} \left(\frac{\mathbf{D}}{\omega} + \mathbf{C} \right) \left(\frac{\mathbf{D}}{\omega} \right)^{-1} \left(\frac{\mathbf{D}}{\omega} + \mathbf{C} \right)^T \quad (28)$$

where $\mathbf{C}$ is a strictly lower triangular matrix, $\mathbf{D}$ is a diagonal matrix, ω denotes the relaxation factor, with a typical range of (1,2)

The iterative procedure of the SSOR-PCG method is summarized as follows:

(1) Initialization

$$\mathbf{x}_0 = 0, \mathbf{g}_0 = \mathbf{b} - \mathbf{K}\mathbf{x}_0, \mathbf{p}_0 = \mathbf{h}_0 = \mathbf{M}^{-1}\mathbf{g}_0 \quad (29)$$

(2) Iterative process

$$\begin{cases} \alpha_j = (\mathbf{g}_j, \mathbf{h}_j) / (\mathbf{p}_j, \mathbf{S}\mathbf{p}_j) \\ \mathbf{x}_{j+1} = \mathbf{x}_j + \alpha_j \mathbf{p}_j \\ \mathbf{g}_{j+1} = \mathbf{g}_j - \alpha_j \mathbf{S}\mathbf{p}_j \\ \mathbf{h}_{j+1} = \mathbf{M}^{-1}\mathbf{g}_{j+1} \\ \beta_{j+1} = (\mathbf{g}_{j+1}, \mathbf{h}_{j+1}) / (\mathbf{g}_j, \mathbf{h}_j) \\ \mathbf{p}_{j+1} = \mathbf{h}_{j+1} + \beta_{j+1} \mathbf{p}_j \end{cases} \quad (30)$$

(3) Convergence criterion

$$(\mathbf{g}_{j+1}, \mathbf{h}_{j+1}) / (\mathbf{g}_0, \mathbf{h}_0) < \varepsilon_c$$

The iteration continues until the convergence condition is satisfied, where ε is set as 10^{-10} , a prescribed tolerance.

In iterative Equation (30), $\langle \cdot, \cdot \rangle$ denotes the inner product; $j=0,1,2,\dots$ represents the iteration index; $\mathbf{g}$ and $\mathbf{p}$ are the gradient and conjugate direction vectors, respectively; $\mathbf{h}$ is an intermediate auxiliary vector; and α_j and β_{j+1} are scalar coefficients representing the update parameters associated with $\mathbf{x}$ and $\mathbf{p}$, respectively.

In the above computation, it is not necessary to explicitly store the preconditioner matrix $\mathbf{M}$. The solution of the linear system $\mathbf{h}_{j+1} = \mathbf{M}^{-1}\mathbf{g}_{j+1}$ does not require direct matrix inversion. Instead, it can be rewritten as a triangular system, and solved efficiently in the form $\mathbf{M}\mathbf{h}_{j+1} = \mathbf{g}_{j+1}$ using Gaussian elimination with forward and backward substitution to obtain $\mathbf{h}_{j+1}$. Since this process involves only sparse lower- and upper-triangular operations with a small number of non-zero elements, the computational cost remains low.

The relaxation factor in Equation (28) is a key parameter affecting the convergence speed of the algorithm. We have conducted detailed tests to determine its optimal value. When using the SSOR-PCG method to solve the complex-coefficient linear equations in Equation (26), multiple relaxation factors are selected within the range [1,1.9] with a step of 0.05 to test the algorithm's convergence performance. As shown in Figure 3, the SSOR-PCG method achieves the optimal convergence speed when the relaxation factor is 1.45. Therefore, we adopt 1.45 as the optimal relaxation factor.

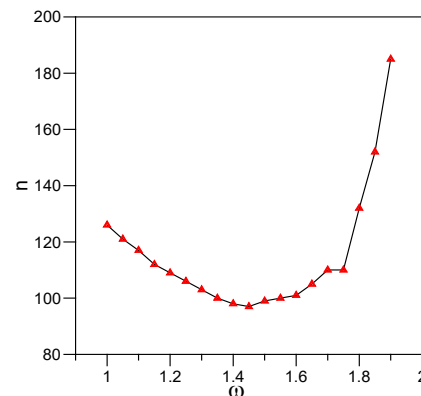


Figure 3. Iteration counts of SSOR-PCG under different relaxation factors.

6. Recursive Inversion of Apparent Spectral Parameters

The total complex potential $v(i\omega)$ is obtained by superposing the anomalous potential $u(i\omega)$ and the background potential $u_0(i\omega)$, i.e., $v(i\omega) = u_0(i\omega) + u(i\omega)$. The apparent complex resistivity $\rho_a(i\omega)$ of the subsurface medium can then be calculated using Equation (31):

$$\rho_a(i\omega) = C_a \frac{\Delta v(i\omega)}{I(i\omega)} \quad (31)$$

where the geometric array coefficient C_a is defined as:

$$C_a = \frac{4\pi}{\frac{1}{AM} + \frac{1}{A'M} - \frac{1}{AN} - \frac{1}{A'N} + \frac{1}{BN} + \frac{1}{B'N} - \frac{1}{BM} - \frac{1}{B'M}}$$

where AM , $A'M$, ..., $B'M$ denote the distances between the transmitting electrodes (or their image electrodes) and the receiving electrodes.

According to the Cole-Cole model in Equation (1), four spectral parameters are involved: zero-frequency resistivity, chargeability, time constant, and frequency exponent. Therefore, at least four complex resistivity measurements at different transmitting frequencies are required to estimate these parameters.

After completing the three-dimensional finite-element simulation of the apparent complex resistivity, the spectral parameters corresponding to each observation array are further estimated by transforming the multi-frequency apparent complex resistivity into apparent spectral parameters. It is assumed that the apparent complex resistivity of the polarized body also satisfies the Cole-Cole model, yielding:

$$\rho_a(i\omega) = \rho_{0a} \left\{ 1 - m_a \left[1 - \frac{1}{1 + (i\omega\tau_a)^{c_a}} \right] \right\} \quad (32)$$

where ρ_{0a} is the apparent zero-frequency resistivity, m_a is the apparent chargeability, τ_a is the apparent time constant, and c_a is the apparent frequency exponent.

The recursive inversion procedure for estimating the apparent spectral parameters is summarized as follows.

- (1) Given the apparent complex resistivity values $\rho_{af}(\omega_1), \rho_{af}(\omega_2), \dots, \rho_{af}(\omega_n)$, calculated using the FEM at frequencies satisfying $\omega_1 < \omega_2 < \dots < \omega_n$. The optimal apparent spectral parameters determined at the end of the inversion process are denoted by ρ_o, m_o, τ_o and c_o . The convergence tolerance is set to $\varepsilon_r = 10^{-6}$, and the maximum iteration number is denoted by $n_{\max}$. The root-mean-square error of the optimal solution E1 is initialized to FLT_MAX.

- (2) Let $\rho_{0a} = \rho_{af}(\omega_1)$, then compute

$$m_a(\omega_j) = \frac{\rho_{0a} - \rho_{af}(\omega_j)}{\rho_{0a}}, \quad j = 2, 3, \dots, n. \quad (33)$$

and define $m_a = m_a(\omega_n)$.

- (3) Using m_a and $m_a(\omega_j)$ from Step (2), compute

$$n_a(\omega_j) = \frac{m_a - m_a(\omega_j)}{m_a}, \quad j = 2, 3, \dots, n-1 \quad (34)$$

- (4) Select all pairs $n_a(\omega_j), n_a(\omega_k)$ where $j = 2, 3, \dots, n-2$ and $k = j+1, \dots, n-1$. the apparent frequency exponent c_a is then computed using

$$c_a = \frac{2 \sum_{j=2}^{n-2} \sum_{k=j+1}^{n-1} \left\{ \ln \left[\frac{1 - n_a(\omega_j)}{1 - n_a(\omega_k)} \right] \cdot n_a(\omega_k) \right\} / \ln \frac{\omega_j}{\omega_k}}{(n-2)(n-3)} \quad (35)$$

- (5) Using $n_a(\omega_j), j = 2, 3, \dots, n-1$, the apparent time constant τ_a is calculated as

$$\tau_a = \sum_{j=2}^{n-1} \left\{ \frac{1}{i\omega_j} \left(\frac{1 - n_a(\omega_j)}{n_a(\omega_j)} \right)^{\frac{1}{c_a}} \right\} / (n-2) \quad (36)$$

- (6) Calculation the root-mean-square error

$$E_2 = \sqrt{\Phi / n} \quad (37)$$

where $\Phi = \sum_{j=1}^n [\lg(A_j) - \lg(B_j)]^2 + [\lg(C_j) - \lg(D_j)]^2$

$$A_j = |\rho_{af}(\omega_j)|, \quad B_j = |\rho_a(\omega_j)|, \quad C_j = -\tan^{-1} \frac{\text{Im}[\rho_{af}(\omega_j)]}{\text{Re}[\rho_{af}(\omega_j)]}, \quad D_j = -\tan^{-1} \frac{\text{Im}[\rho_a(\omega_j)]}{\text{Re}[\rho_a(\omega_j)]}$$

where $\rho_{af}(\omega_j)$ and $\rho_a(\omega_j)$ denote the apparent complex resistivities obtained from the finite element method and the Cole-Cole model (Equation [32]), respectively.

If $|E_1 - E_2| < \varepsilon_r$ or $\text{Iter} > n_{\max}$, the iterative process terminates, and the optimal spectral parameters ρ_o , m_o , τ_o and c_o are output. Otherwise, if $E_2 < E_1$, the apparent spectral parameters are updated according to $\rho_{0a} \Rightarrow \rho_o$, $m_a \Rightarrow m_o$, $\tau_a \Rightarrow \tau_o$, $c_a \Rightarrow c_o$, and the procedure returns to Step (7).

(7) Recalculate $n_a(\omega_j)$ using the current estimates of τ_a and c_a

$$n_a(\omega_j) = \frac{1}{1 + (i\omega_j\tau_a)^{c_a}}, \quad j = 1, 2, \dots, n \quad (38)$$

(8) Calculate the updated $m_a(\omega_1)$ and ρ_{0a} using the recalculated $n_a(\omega_1)$

$$m_a(\omega_1) = m_a[1 - n_a(\omega_1)] \quad (39)$$

$$\rho_{0a} = \frac{\rho_{af}(\omega_1)}{(1 - m_a(\omega_1))} \quad (40)$$

(9) Calculate $m_a(\omega_j)$

$$m_a(\omega_j) = \frac{\rho_{0a} - \rho_{af}(\omega_j)}{\rho_{0a}}, \quad j = 2, 3, \dots, n \quad (41)$$

(10) Calculate m_a

$$m_a = \frac{m_a(\omega_n)}{1 - n_a(\omega_n)} \quad (42)$$

Increment the iteration counter: $\text{Iter} = \text{Iter} + 1$, then return to step (4) to repeat the process.

7. Modeling Experiment

7.1. Accuracy Validation on a Transition-Layer Model

To validate the accuracy of the three-dimensional (3-D) complex resistivity simulation based on the finite element method, we calculate vertical electrical sounding curves for a three-layer geoelectric model with a linear transitional layer via both the FEM and the analytical solution [34] (see Appendix B).

The stratigraphic configuration of this model is illustrated in Figure 4. The assigned Cole-Cole spectral parameters for each formation are listed as follows: the overlying homogeneous layer has a zero-frequency resistivity $\rho_{01} = 10 \Omega \cdot \text{m}$, chargeability $m_1 = 15\%$, time constant $\tau_1 = 3\text{s}$ and relaxation exponent $c_1 = 0.5$; the underlying basement half-

space is defined with $\rho_{02} = 100\Omega \cdot \text{m}$, $m_3 = 2\%$, $\tau_3 = 0.2\text{s}$ and $c_3 = 0.2$. A 2 m thick transitional layer is sandwiched between the upper layer and the basement half-space. Within this transitional layer, all Cole-Cole spectral parameters vary linearly and continuously with depth from the bottom boundary of the overlying layer to the top boundary of the basement half-space, which achieves a smooth transition of petrophysical properties between the two main formations.

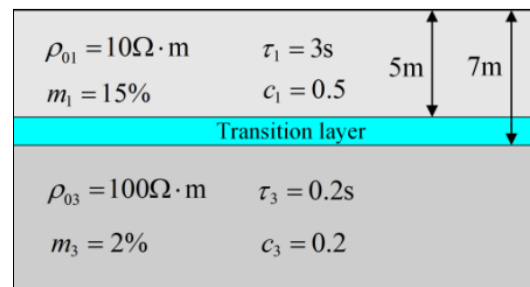


Figure 4. Three-layer earth model with a transitional layer.

For the vertical electrical sounding numerical test, a symmetrical Schlumberger array is adopted for forward simulation. The half-spacings of the current electrode pair AB/2 are set as 0.5 m, 1 m, 2 m, 4 m, 8 m, 12 m, 16 m, 20 m, 25 m, 30 m, 40 m, 50 m, 70 m, 90 m, 120 m, 150 m, 220 m, 320 m in sequence. The half-spacing of the potential electrode pair MN/2 is fixed to one-fifth of the corresponding AB/2 half-spacing at each measurement station. The excitation frequencies are defined as 2^j Hz, where the exponent j ranges from -4 to 3 with integer intervals.

Corresponding to the three-layer transitional geoelectric model, the computational domain is divided into an inner research subdomain and outer extended absorbing subdomains. The inner research area covering the electrode layout is designed to be a square region of 640 m $\times$ 640 m. An extended zone with a width of 1880 m is appended outward along all five boundaries of the inner research area to eliminate artificial boundary effects in finite-element calculations. The entire computational domain (including the inner research zone and outer extended zones) is discretized with a total of 562,280 nodes; the number of discretized nodes along the x-, y-, and z- directions are 134, 100, and 42, respectively. During mesh discretization, two grid elements are arranged between every pair of adjacent electrodes to guarantee the simulation accuracy of measuring points near the field sources.

A total of 288 forward modelling runs are required for the finite-element simulation of this geoelectric model, calculated as 8 frequencies multiplied by 36 transmitting electrode combinations. All numerical tests are performed on a personal computer with a 2.6 GHz main frequency and 28 CPU cores. The serial forward simulation consumes 11.4 h with a memory footprint of 260.7 MB, while the OpenMP parallelized scheme reduces the runtime to 1.1 h at the cost of an increased memory usage of 6.2 GB.

The vertical electrical sounding curves, apparent complex resistivity responses and corresponding relative errors calculated via the finite element method (FEM) and analytical solution are compared in Figure 5. Figure 5a illustrates the real component of apparent complex resistivity derived from the two approaches. The FEM results match the analytical solution well overall, with the maximum relative error controlled below 1.4%. Large relative errors mainly occur at electrode spacings corresponding to the transitional layer, and the relative error rises gradually as the excitation frequency increases (Figure 5c).

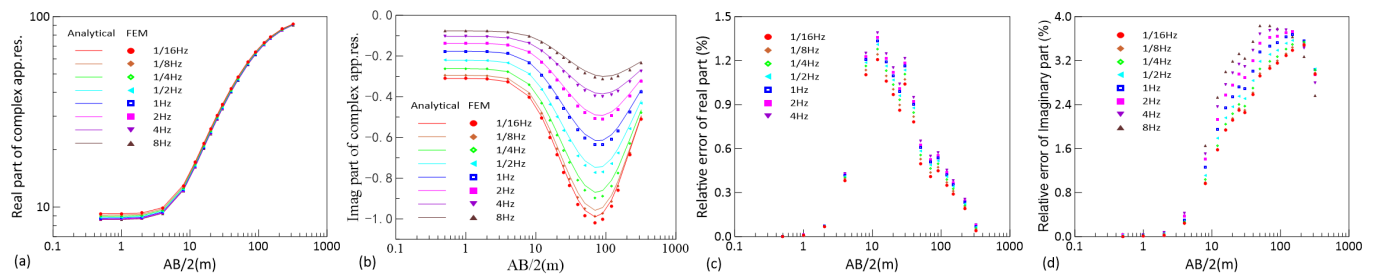


Figure 5. Comparison between finite element numerical solutions and analytical solutions for the three-layer transitional geoelectric model. (a) Real component of apparent complex resistivity; (b) Imaginary component of apparent complex resistivity; (c) Relative error of the real component of apparent complex resistivity; (d) Relative error of the imaginary component of apparent complex resistivity.

Figure 5b presents the imaginary component curves of apparent complex resistivity. The numerical and analytical solutions share identical overall variation trends, yet obvious discrepancies emerge within the transitional layer, where the maximum relative error reaches 3.8% (Figure 5d). For both real and imaginary components of apparent complex resistivity, prominent deviations are concentrated in the transitional zone. Such discrepancies stem fundamentally from different petrophysical interpolation assumptions adopted by the two models: the FEM numerical model implements trilinear continuous variation of properties within each hexahedral element, while the analytical solution only adopts one-dimensional linear variation along the depth direction.

Despite the local deviations in the transitional layer, the generally favorable consistency between numerical and analytical results verifies that the proposed finite element algorithm for continuous medium geoelectric models is accurate and reliable.

We adopt the proposed recursive inversion algorithm to invert apparent electrical sounding curves from two independent datasets: the numerically simulated FEM forward responses and the analytical forward solutions. The inverted apparent Cole-Cole spectral parameter curves are displayed in Figure 6.

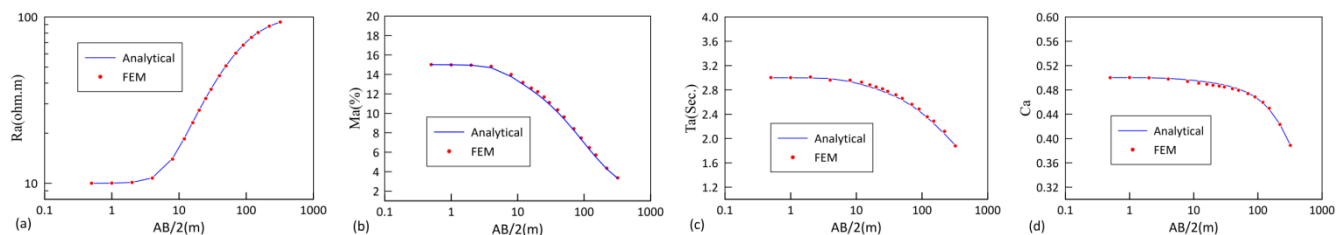


Figure 6. Inversion results of apparent Cole-Cole spectral parameters for the three-layer geoelectric model with a transitional layer (a) Apparent zero-frequency resistivity. (b) Apparent chargeability. (c) Apparent time constant. (d) Apparent frequency exponent.

As illustrated in subplots (a)–(d), the four types of apparent spectral parameters (zero-frequency apparent resistivity, apparent chargeability, apparent time constant and apparent frequency exponent) retrieved from numerical and analytical datasets show excellent consistency. The discrete FEM inversion points almost overlap with the continuous analytical curves across the full range of electrode spacing $AB/2$, which further demonstrates the stability and reliability of the developed recursive inversion approach, even for geoelectric models with continuous transitional layers.

Beyond the consistency of inverted apparent spectral parameters shown in Figure 6, we further investigate the iterative convergence performance of the recursive inversion al-

gorithm. A root-mean-square (RMS) error-based stopping criterion is adopted during inversion: the iterative computation terminates once the average RMS fitting error of apparent complex resistivity between two consecutive iterations drops below $1\text{E-}8$. The convergence curves of inversion under all designed electrode spacings are presented in Figure 7.

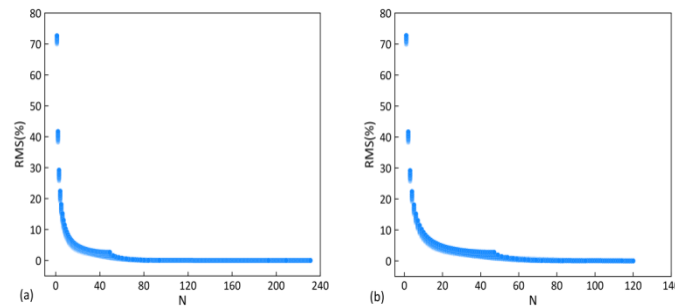


Figure 7. Inversion convergence curves for apparent complex resistivity data of varying electrode spacings. **(a)** Convergence curve for the analytical solution. **(b)** Convergence curve for the numerical solution.

Both the analytical and numerical datasets exhibit similar descending trends and stable convergence behaviors. For the analytical forward dataset, the inversion converges within 49–231 iterations, with converged RMS errors ranging from $6.1\text{E-}7$ to $2.6\text{E-}2$. For the FEM numerical dataset, convergence is achieved after 47–120 iterations, and the final RMS errors fall between $2.4\text{E-}4$ and $2.7\text{E-}2$. All convergence curves show a sharp drop of RMS error at the early iteration stage and then gradually flatten to a stable low-error level. These quantitative convergence results collectively verify the favorable robustness and stability of the proposed recursive inversion algorithm.

7.2. Cube Model with Continuous Frequency-Dependent Properties

To further verify the adaptability of the developed 3-D finite element algorithm for complex localized geoelectric anomalies, a cuboid model is constructed as illustrated in Figure 8a. Continuous linear petrophysical transition zones are arranged around the anomalous body, where all Cole–Cole spectral parameters vary linearly and continuously from the anomalous body to the homogeneous surrounding host rock, and the complete Cole–Cole parameters of the model are listed in Table 1. For numerical simulation, a 24-electrode array is laid horizontally along the X-axis directly above the cuboid anomaly (Figure 8b) with a uniform electrode spacing of 4 m; a symmetrical Schlumberger quadrupole array is adopted for data collection, and the excitation frequencies are defined as 2^j Hz, where the exponent j ranges from -4 to 3 with integer intervals.

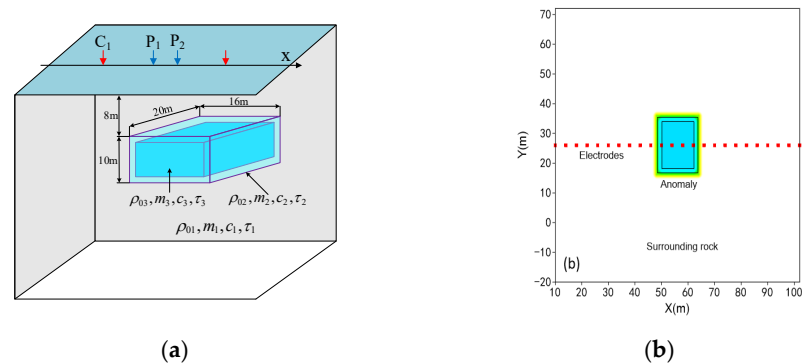


Figure 8. Cuboid geoelectric model. **(a)** 3-D schematic. **(b)** Plan view.

Table 1. Model Parameters.

Parameter No.	$\rho_0 (\Omega \cdot m)$	$m (\%)$	$\tau (s)$	c
1	100.0	1.0	0.2	0.2
2	50.0	5.0	5.0	0.4
3	10.0	10.0	10.0	0.6

Figure 9 presents the pseudo-sections of the real and imaginary components of the apparent complex resistivity for eight different frequencies obtained from the finite element simulation. It can be observed that, with increasing transmission frequency, the variations in the pseudo-sections of the real component are relatively minor, showing almost negligible differences. In contrast, the imaginary component exhibits significant frequency-dependent variations.

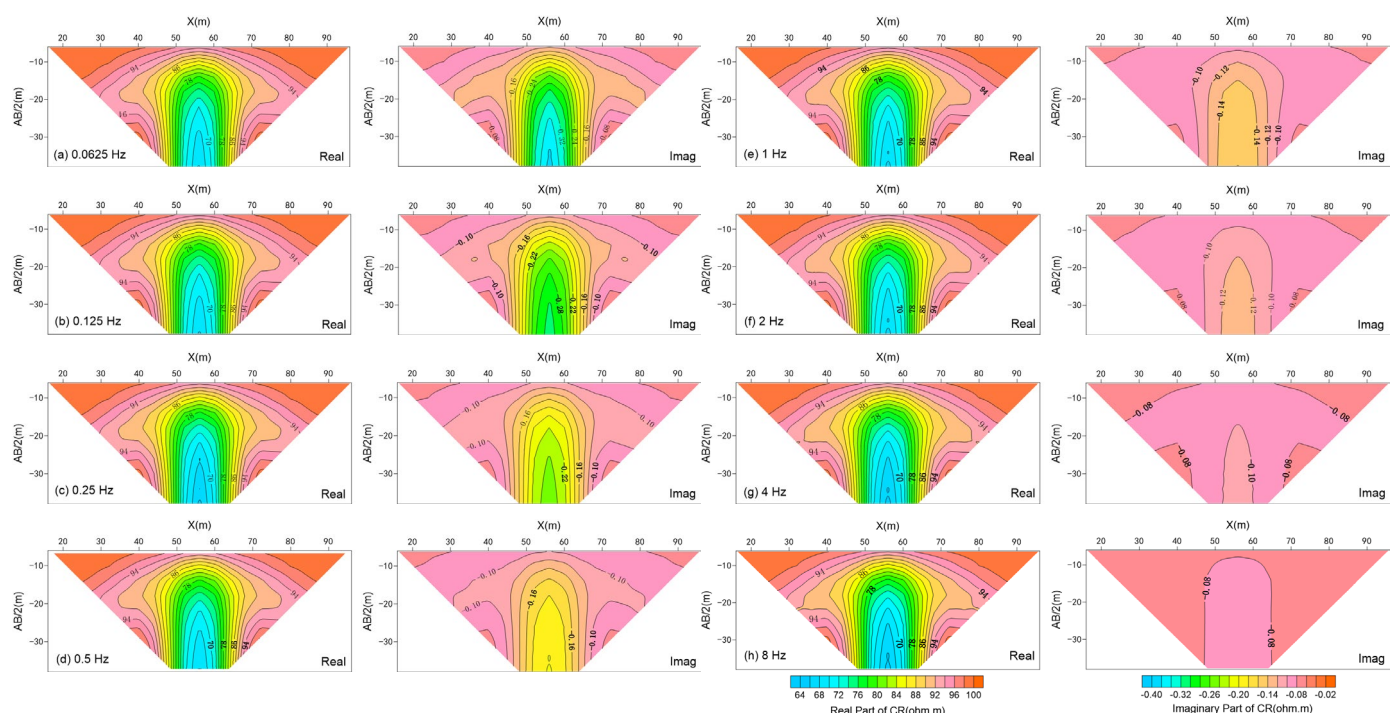


Figure 9. Finite element simulation results of the real (left) and imaginary (right) components of apparent complex resistivity at different frequencies (contrasting-resistivity geoelectric model).

As the transmission frequency increases, the numerical contrasts across the entire pseudo-section gradually decrease, and the anomalous features associated with high polarization progressively become less distinct. This indicates that the spectral induced polarization response is primarily governed by the imaginary component of the apparent complex resistivity and is strongly dependent on the transmitting frequency. Moreover, high transmitting frequencies will cause severe electromagnetic coupling interference, especially in low-resistivity subsurface media, which overwhelms the weak polarization signals of underground anomalous bodies. For most field surveys affected by electromagnetic coupling, low transmission frequency range (0.0625~4 Hz) are preferred. Nevertheless, the optimal excitation frequency should be selected comprehensively based on survey objectives, ambient noise level, electrode geometry and subsurface geoelectric conditions.

Pseudo-section maps of the apparent complex resistivity at eight different frequencies were generated using a multi-frequency recursive inversion algorithm to estimate the apparent Cole–Cole spectral parameters ρ_{0s} , m_s , τ_s and c_s , as shown in Figure 10. The

anomalous body exhibits low-resistivity and high-polarization characteristics. Based on the spectral parameter pseudo-sections, the position and spatial extent of the polarizable body can be inferred.

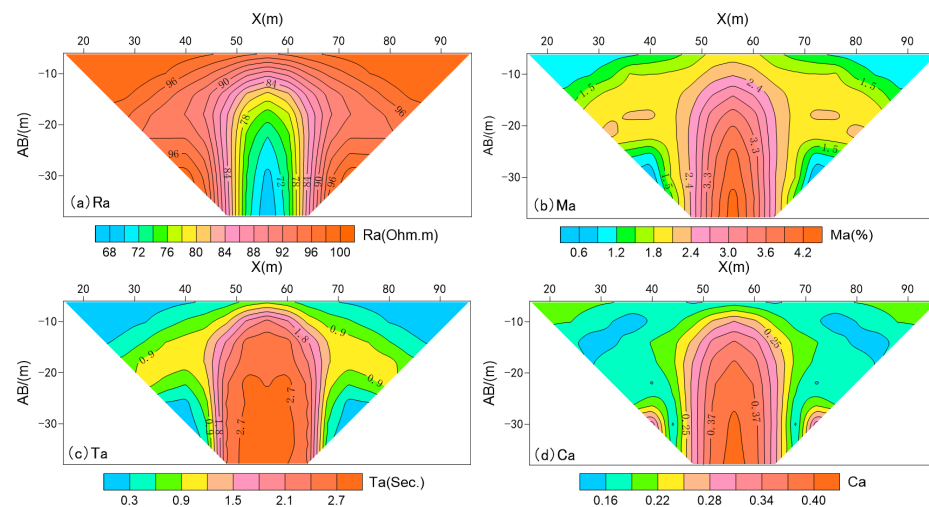


Figure 10. Pseudo-sections of apparent spectral parameters for a cubic anomaly.

The simulation approach proposed in this study provides an effective tool for analyzing the spectral induced polarization (SIP) response characteristics of continuous sub-surface geoelectric models.

To further investigate the frequency-dependent characteristics of induced polarization parameters, the cuboid geoelectric model in Figure 8 is adjusted to a homogeneous half-space background with a zero-frequency resistivity of $100 \Omega\cdot\text{m}$, while all remaining Cole-Cole spectral parameters of the anomalous body stay identical to the original setting. Pseudo-sections of the real and imaginary components of apparent complex resistivity under multiple frequencies are displayed in Figure 11.

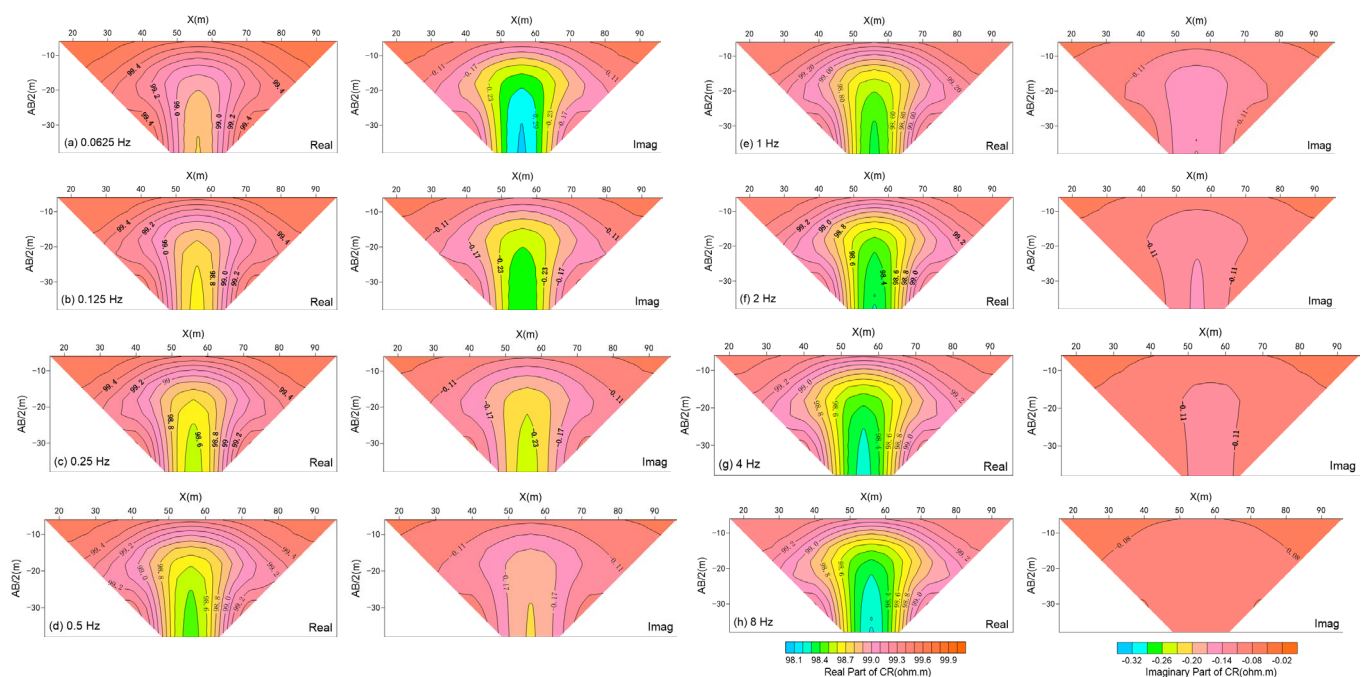


Figure 11. Finite element simulation results of the real (left) and imaginary (right) components of apparent complex resistivity at different frequencies, uniform-resistivity geoelectric model.

The simulation results reveal that even when the anomalous body and surrounding host rock share the identical zero-frequency resistivity, subtle amplitude anomalies can still be observed on the real-component pseudo-sections. This phenomenon proves that the real component of apparent complex resistivity contains weak yet distinguishable induced polarization signals.

Furthermore, an obvious frequency-varying pattern is observed: as the excitation frequency rises, anomalous signatures on the imaginary-component pseudo-sections gradually fade, whereas anomalies on the real-component pseudo-sections become increasingly prominent. This variation demonstrates that induced polarization response redistributes between the real and imaginary components of apparent complex resistivity as frequency changes.

The pseudo-sections of the real and imaginary components of apparent complex resistivity at various frequencies (Figure 11) are further processed to generate extremal amplitude plots varying with excitation frequency, as shown in Figure 12.

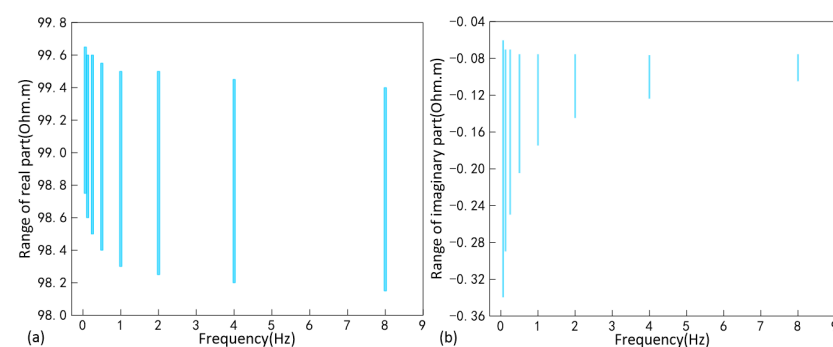


Figure 12. Frequency-dependent variation of the real component (a) and imaginary component (b) of apparent complex resistivity.

The statistical results show two opposite evolutionary trends. For the real component, its extremal amplitude difference (defined as the gap between the maximum and minimum values) gradually rises from 0.9 to 1.25 with growing frequency, while both its maximum and minimum amplitudes generally decline. In contrast, the extremal amplitude difference of the imaginary component decreases continuously as frequency increases. The maximum amplitude of the imaginary component only fluctuates slightly and stabilizes near -0.08 ; meanwhile, its minimum amplitude rises gradually, which drastically narrows the extremal amplitude gap.

These quantitative observations reveal that the induced polarization signals contained in the imaginary component decay rapidly under higher excitation frequencies. This frequency-dependent evolution matches the theoretical dispersion characteristics predicted by the Cole–Cole model.

Recursive inversion is applied to the multi-frequency complex resistivity data in Figure 11, and pseudo-sections of different apparent Cole–Cole spectral parameters are obtained (Figure 13). The overall amplitude of apparent zero-frequency resistivity changes slightly, but its contour distribution can clearly mark the location of the high-polarization anomalous body (Figure 13a). The contour shapes and central anomaly amplitudes of apparent chargeability, apparent time constant and apparent frequency exponent are basically consistent with the forward simulation results in Figure 10. Differences only appear on both sides of the anomalous body, which are preliminarily attributed to the low resistivity of the anomalous body

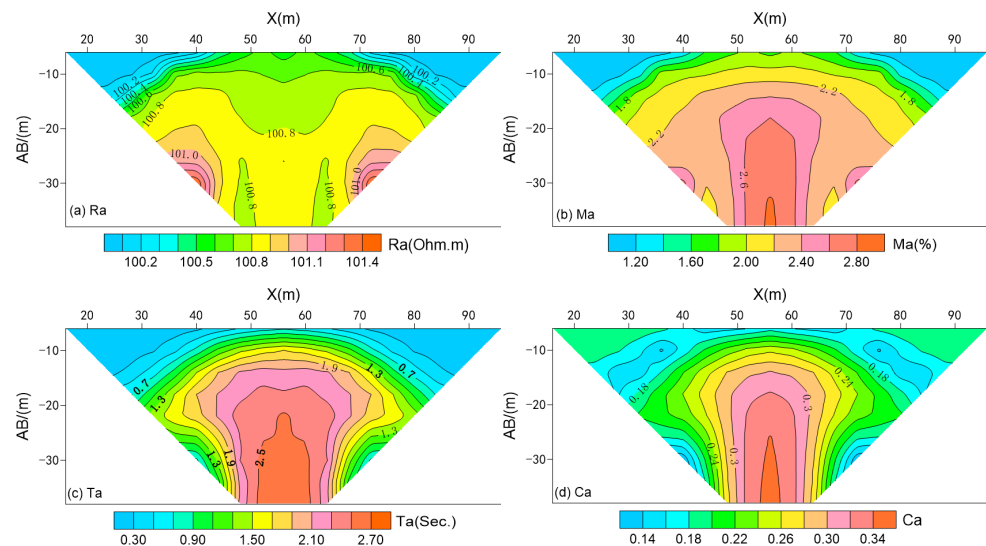


Figure 13. Pseudo-sections of apparent spectral parameters of a cuboid anomaly.

The inversion results further show mutual coupling between rock electrical properties: changes in polarizability will affect the contour shape of apparent zero-frequency resistivity, and resistivity differences will also influence the pseudo-sections of induced polarization parameters such as apparent chargeability, apparent time constant and apparent frequency exponent.

7.3. Sandbox Model

Sandbox physical simulation experiments are widely adopted in geophysical research. To quantify the boundary effect induced by the sandbox wall on measurement results, a sandbox physical model with dimensions of 300 cm × 100 cm × 100 cm is constructed. A horizontal thin low-resistivity high-polarization plate (40 cm × 40 cm × 1 cm) is placed at the sandbox center, with its top surface buried 20 cm below the sandbox upper boundary. The sandbox frame is made of insulating material.

The petrophysical parameters of background sand and the thin anomalous plate are presented in Figure 14. A symmetrical Schlumberger quadrupole sounding array is used for data acquisition. Potential electrodes P_1 and P_2 are fixed on the central axis of the sandbox with a constant spacing $P_1P_2 = 20$ cm. The distance between current electrodes C_1 and C_2 expands symmetrically along the central axis from 40 cm, 60 cm, ..., 300 cm at 20 cm increments. The excitation frequency for signal emission is set as 2^j Hz, where j ranges from -4 to 3 .

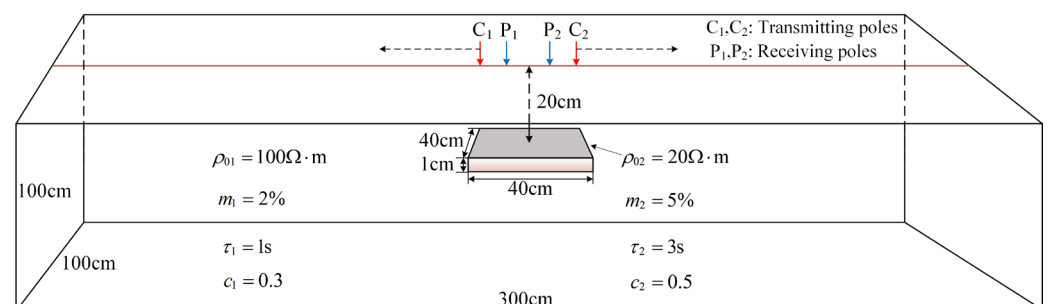


Figure 14. Sandbox geoelectric model.

The simulation results of the sandbox model with the low-resistivity high-polarization thin plate are plotted in Figure 15a. Within the $C_1C_2/2$ range of 20–40 cm, the apparent

complex resistivity at all frequencies presents low-resistivity features, which corresponds to the response of the embedded anomalous thin plate. As the electrode spacing expands, the apparent complex resistivity increases rapidly. This proves that the sandbox enclosure imposes obvious interference on measured data.

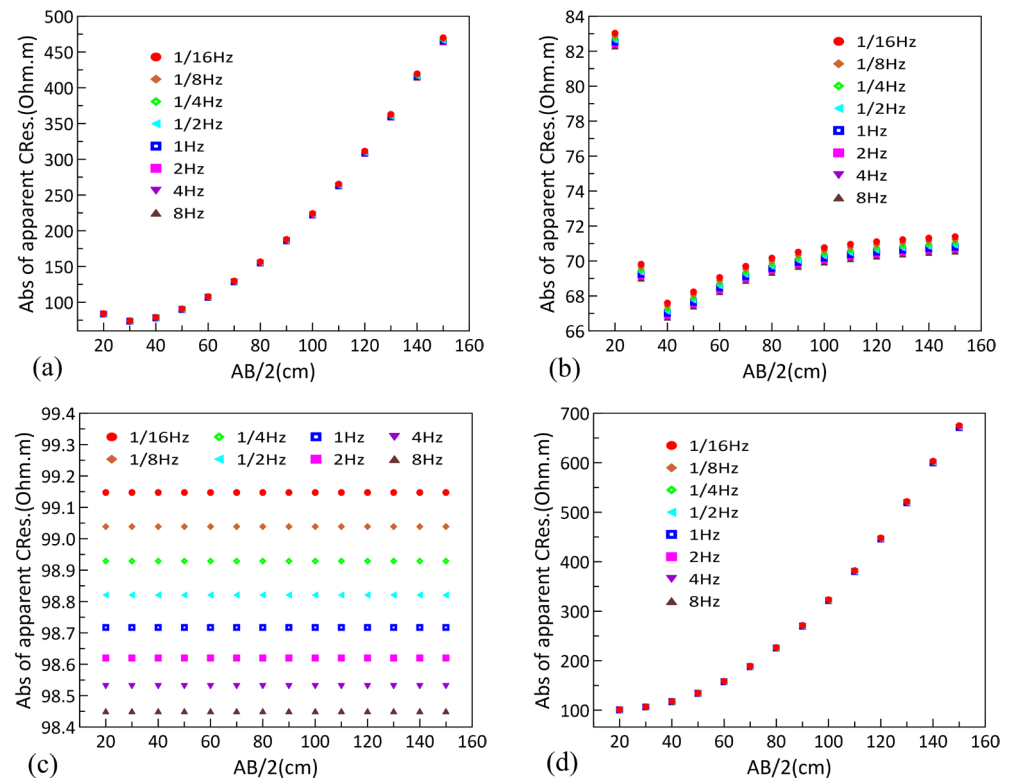


Figure 15. Simulation results of apparent complex resistivity under different conditions: (a) Low-resistivity high-polarization thin plate inside the sandbox; (b) Low-resistivity high-polarization thin plate in homogeneous sand half-space; (c) Pure homogeneous sand half-space model; (d) Empty sandbox model without the anomalous thin plate.

To quantitatively analyze this boundary interference, a control model with the identical thin plate buried in an infinite homogeneous sand half-space is simulated, as shown in Figure 15b. Large discrepancies exist between the half-space results and the sandbox curves in Figure 15a, which verifies that the sandbox boundary exerts a strong influence on simulation responses.

Two extra groups of comparative simulations are carried out for further analysis: a pure homogeneous sand half-space model (Figure 15c) and an empty sandbox model without any anomalous body (Figure 15d). In Figure 15c, the apparent complex resistivity rises as frequency declines, which matches the known frequency dispersion law of induced polarization signals.

In contrast, the data in Figure 15d show that the apparent complex resistivity increases rapidly with larger electrode spacing, while the gaps between different frequency curves remain small. This comparison indicates that the sandbox enclosure is the dominant factor distorting the measured geoelectric response.

To extract spectral parameters from sandbox physical simulation data and mitigate the interference caused by the sandbox boundary, we first invert spectral parameters using the apparent complex resistivity data in Figure 15a,b. The inversion results are shown in Figure 16. The correction formula for spectral parameters is expressed as:

$$P = \frac{P_1}{P_2} P_3 \quad (43)$$

where the parameter P_1 denotes the apparent spectral parameters of the ideal uniform half-space model (free of boundary effects), P_2 denotes the Apparent spectral parameters of the sandbox model without the anomalous body (only boundary effects are present), P_3 denotes the apparent spectral parameters of the sandbox model with the anomalous body (both boundary effects and anomaly signals are present, i.e., the raw measured data), and P denotes the corrected apparent spectral parameters for the sandbox model with the anomalous body. The factor P_1/P_2 acts as a scaling coefficient to remove the boundary-induced distortion from P_3 , recovering the corrected apparent spectral parameter P that would be observed in an infinite half-space. This multiplicative form is intuitive: it normalizes the sandbox response by the known boundary response and then scales it to the ideal half-space response. This correction formula is applicable to boundary effect correction in sandbox and water tank physical simulation experiments.

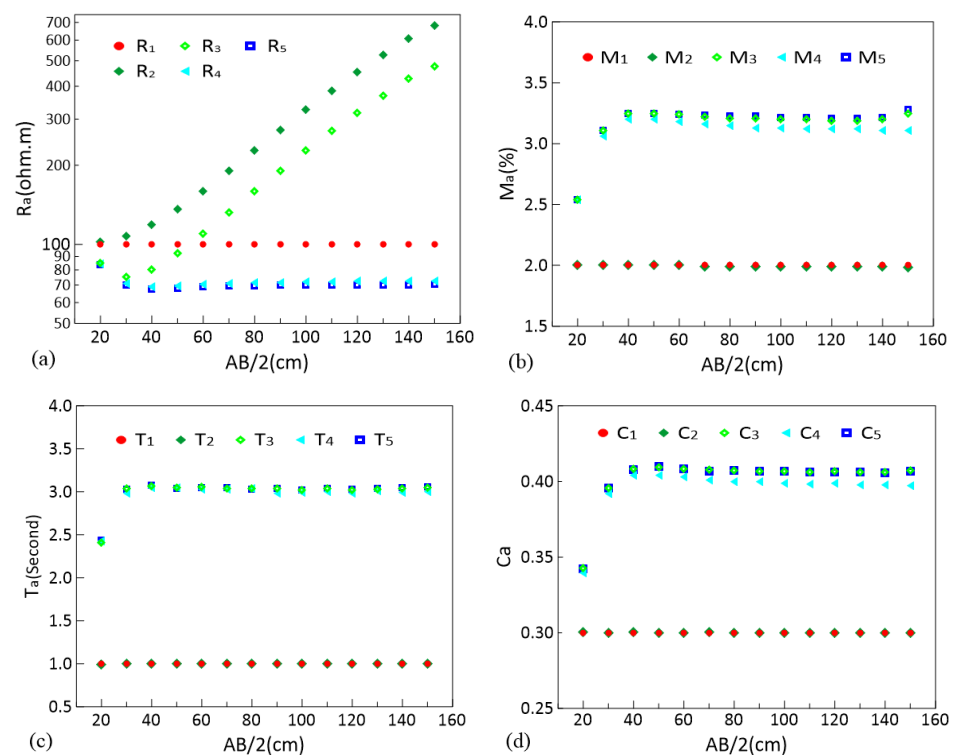


Figure 16. Spectral parameters of sandbox model before and after correction. (a) Apparent zero-frequency resistivity; (b) Apparent chargeability; (c) Apparent time constant; (d) Apparent frequency exponent. Subscripts 1–5 correspond to: 1 spectral parameters of homogeneous half-space; 2 empty sandbox model without anomaly; 3 raw spectral parameters of sandbox model with anomaly; 4 homogeneous half-space model with anomaly; 5 corrected spectral parameters of sandbox model with anomaly.

Figure 16 shows that the sandbox enclosure imposes obvious interference on apparent zero-frequency resistivity for models with an embedded anomalous body. After spectral parameter correction, the scatter points of resistivity nearly coincide with those from the homogeneous half-space model containing the same anomaly. This demonstrates that parameter correction is essential for resistivity interpretation when sandbox physical simulation data are adopted.

In comparison, induced polarization parameters (apparent chargeability, apparent time constant and apparent frequency exponent) barely change before and after correction. It proves that the sandbox boundary exerts negligible interference on these induced polarization parameters.

8. Discussion

The physical properties of subsurface media are jointly controlled by multiple factors including mineral composition, porosity, temperature and pressure, and generally vary continuously in space. In this study, a three-dimensional continuous spectral parameter model is established to characterize subsurface geological structures. The 3D geological domain is discretized into hexahedral elements, and spectral parameters change linearly within each element. This model conforms to the actual heterogeneous characteristics of underground media and reduces approximation errors inherent in traditional stepped block models.

The primary field is analytically calculated based on a homogeneous half-space model, and a layered-earth model can also be adopted for primary field computation. The finite element method is then used to solve the secondary field induced by subsurface anomalous bodies, so as to improve the numerical accuracy of the total complex potential field, especially in the source vicinity. Linear interpolation is adopted within each element to simplify numerical implementation and reduce computational cost.

Three-dimensional spectral induced polarization finite element simulation generates large-scale linear systems with complex coefficients, which brings heavy computational burdens under multi-frequency and multi-source working conditions. To address this problem, an OpenMP parallel computing framework is adopted to distribute computational tasks according to different electrode arrays, effectively accelerating the computation of 3D forward modeling.

The recursive inversion algorithm proposed in this paper does not require manually preset initial model parameters, and spectral parameters can be retrieved using no less than four groups of multi-frequency observed complex resistivity data. This algorithm consumes less computing time and avoids disturbances caused by artificial initial value selection, thus exhibiting stable inversion performance.

This method still has certain limitations. Linear interpolation introduces numerical approximation errors in areas with sharp contrasts in geoelectric properties and abrupt lithological boundaries. In addition, the primary field calculation relies on idealized homogeneous half-space or layered-earth assumptions, which may produce computational deviations when applied to complex geological environments. Quadratic and cubic polynomial enrichment strategies for Crouzeix-Raviart finite elements have been proposed [35], which provides a feasible technical route to further improve the simulation accuracy of the proposed method.

9. Conclusions

This work develops a two-step algorithm for 3D spectral induced polarization (SIP) forward modeling applicable to media with continuous Cole–Cole parameters. A transition-layer geoelectric model is adopted to verify the accuracy of this algorithm. The spectral parameter curves calculated by numerical simulation and analytical solutions match well, which proves that the proposed algorithm can reliably calculate spectral responses in continuous Cole–Cole media.

A 3D continuous electrical transition model is used to systematically analyze the frequency-varying features of the real and imaginary parts of apparent complex resistivity, as

well as the anomaly characteristics of spectral parameters. The results show that this algorithm is an effective tool to compute spectral responses for 3D continuous Cole–Cole models.

For sandbox physical simulation tests, the insulating sandbox wall creates obvious interference on zero-frequency resistivity data. The spectral parameter correction formula proposed in this paper can effectively eliminate such boundary interference.

In addition, the 3D SIP forward modeling method established in this study lays a reliable basis for subsequent research on 3D inversion of continuous geoelectric medium models.

Author Contributions: Conceptualization, H.L. and D.Z.; Methodology, H.L.; Software, H.L. and D.Z.; Validation, H.L., D.Z., Y.Z. and R.C.; Formal analysis, H.L.; Investigation, D.Z. and R.C.; Resources, Y.Z., R.C., T.M.S.A. and C.L.; Data curation, D.Z., Y.Z. and C.L.; Writing—original draft, H.L., Y.Z., R.C. and C.L.; Writing—review and editing, H.L., D.Z., Y.Z., T.M.S.A. and C.L.; Visualization, H.L. and T.M.S.A.; Supervision, D.Z. and T.M.S.A.; Project administration, H.L., Y.Z., R.C., T.M.S.A. and C.L.; Funding acquisition, H.L. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by the National Natural Science Foundation of China (Grant No. 42574099) and the National Science and Technology Major Project for Deep Earth Exploration and Mineral Resource Prospecting of China (Grant No. 2025ZD1005704).

Data Availability Statement: The data presented in this study are available on request from the corresponding author. The data supporting the findings of this study are not publicly available due to permission restrictions.

Conflicts of Interest: The authors declare no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A

Substituting the local coordinate values of each mesh node into Equation (20) yields the integration coefficients of the lower triangular matrix, which are listed as follows.

$$\begin{array}{c}
 \begin{array}{c} \alpha_{11} \\ \alpha_{21} \\ \alpha_{22} \\ \alpha_{31} \\ \alpha_{32} \\ \alpha_{33} \\ \alpha_{41} \\ \alpha_{42} \\ \alpha_{43} \\ \alpha_{44} \\ \alpha_{51} \\ \alpha_{52} \\ \alpha_{53} \\ \alpha_{54} \\ \alpha_{55} \\ \alpha_{61} \\ \alpha_{62} \\ \alpha_{63} \end{array}
 \begin{array}{c} \left| \begin{array}{cccccccc} 9 & 3 & 3 & 9 & 3 & 1 & 1 & 3 \\ 3 & 3 & 3 & 3 & 1 & 1 & 1 & 1 \\ 3 & 9 & 9 & 3 & 1 & 3 & 3 & 1 \\ -3 & -3 & -3 & -3 & -1 & -1 & -1 & -1 \\ -3 & -9 & -9 & -3 & -1 & -3 & -3 & -1 \\ 3 & 9 & 9 & 3 & 1 & 3 & 3 & 1 \\ -9 & -3 & -3 & -9 & -3 & -1 & -1 & -3 \\ -3 & -3 & -3 & -3 & -1 & -1 & -1 & -1 \\ 3 & 3 & 3 & 3 & 1 & 1 & 1 & 1 \\ 9 & 3 & 3 & 9 & 3 & 1 & 1 & 3 \\ 3 & 1 & 1 & 3 & 3 & 1 & 1 & 3 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -3 & -1 & -1 & -3 & -3 & -1 & -1 & -3 \\ 3 & 1 & 1 & 3 & 9 & 3 & 3 & 9 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 3 & 3 & 1 & 1 & 3 & 3 & 1 \\ -1 & -3 & -3 & -1 & -1 & -3 & -3 & -1 \end{array} \right| \end{array}
 \begin{array}{c} \alpha_{64} \\ \alpha_{65} \\ \alpha_{66} \\ \alpha_{71} \\ \alpha_{72} \\ \alpha_{73} \\ \alpha_{74} \\ \alpha_{75} \\ \alpha_{76} \\ \alpha_{77} \\ \alpha_{81} \\ \alpha_{82} \\ \alpha_{83} \\ \alpha_{84} \\ \alpha_{85} \\ \alpha_{86} \\ \alpha_{87} \\ \alpha_{88} \end{array}
 \begin{array}{c} \left| \begin{array}{cccccccc} -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 3 & 3 & 3 & 3 \\ 1 & 3 & 3 & 1 & 3 & 9 & 9 & 3 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -3 & -3 & -1 & -1 & -3 & -3 & -1 \\ 1 & 3 & 3 & 1 & 1 & 3 & 3 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -3 & -3 & -3 & -3 \\ -1 & -3 & -3 & -1 & -3 & -9 & -9 & -3 \\ 1 & 3 & 3 & 1 & 3 & 9 & 9 & 3 \\ -3 & -1 & -1 & -3 & -3 & -1 & -1 & -3 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 3 & 1 & 1 & 3 & 3 & 1 & 1 & 3 \\ -3 & -1 & -1 & -3 & -9 & -3 & -3 & -9 \\ -1 & -1 & -1 & -1 & -3 & -3 & -3 & -3 \\ 1 & 1 & 1 & 1 & 3 & 3 & 3 & 3 \\ 3 & 1 & 1 & 3 & 9 & 3 & 3 & 9 \end{array} \right| \end{array}
 \begin{array}{c} \beta_{11} \\ \beta_{21} \\ \beta_{22} \\ \beta_{31} \\ \beta_{32} \\ \beta_{33} \\ \beta_{41} \\ \beta_{42} \\ \beta_{43} \\ \beta_{44} \\ \beta_{51} \\ \beta_{52} \\ \beta_{53} \\ \beta_{54} \\ \beta_{55} \\ \beta_{61} \\ \beta_{62} \\ \beta_{63} \end{array}
 \begin{array}{c} \left| \begin{array}{cccccccc} 9 & 3 & 1 & 3 & 9 & 3 & 1 & 3 \\ 3 & 3 & 1 & 1 & 3 & 3 & 1 & 1 \\ 3 & 9 & 3 & 1 & 3 & 9 & 3 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 3 & 3 & 1 & 1 & 3 & 3 & 1 \\ 1 & 3 & 9 & 3 & 1 & 3 & 9 & 3 \\ 3 & 1 & 1 & 3 & 3 & 1 & 1 & 3 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 3 & 3 & 1 & 1 & 3 & 3 \\ 3 & 1 & 3 & 9 & 3 & 1 & 3 & 9 \\ -9 & -3 & -1 & -3 & -9 & -3 & -1 & -3 \\ -3 & -3 & -1 & -1 & -3 & -3 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -3 & -1 & -1 & -3 & -3 & -1 & -1 & -3 \\ 9 & 3 & 1 & 3 & 9 & 3 & 1 & 3 \\ -3 & -3 & -1 & -1 & -3 & -3 & -1 & -1 \\ -3 & -9 & -3 & -1 & -3 & -9 & -3 & -1 \\ -1 & -3 & -3 & -1 & -1 & -3 & -3 & -1 \end{array} \right| \end{array}
 \end{array}$$

β_{64}	-1	-1	-1	-1	-1	-1	-1	-1	γ_{11}	9	9	3	3	3	3	1	1	γ_{64}	-1	-1	-1	-1	-1	-1	-1	-1
β_{65}	3	3	1	1	3	3	1	1	γ_{21}	-9	-9	-3	-3	-3	-3	-1	-1	γ_{65}	-3	-3	-1	-1	-9	-9	-3	-3
β_{66}	3	9	3	1	3	9	3	1	γ_{22}	9	9	3	3	3	3	1	1	γ_{66}	3	3	1	1	9	9	3	3
β_{71}	-1	-1	-1	-1	-1	-1	-1	-1	γ_{31}	-3	-3	-3	-3	-1	-1	-1	-1	γ_{71}	-1	-1	-1	-1	-1	-1	-1	-1
β_{72}	-1	-3	-3	-1	-1	-3	-3	-1	γ_{32}	3	3	3	3	1	1	1	1	γ_{72}	1	1	1	1	1	1	1	1
β_{73}	-1	-3	-9	-3	-1	-3	-9	-3	γ_{33}	3	3	9	9	1	1	3	3	γ_{73}	1	1	3	3	1	1	3	3
β_{74}	-1	-1	-3	-3	-1	-1	-3	-3	γ_{41}	3	3	3	3	1	1	1	1	γ_{74}	-1	-1	-3	-3	-1	-1	-3	-3
β_{75}	1	1	1	1	1	1	1	1	γ_{42}	-3	-3	-3	-3	-1	-1	-1	-1	γ_{75}	-1	-1	-1	-1	-3	-3	-3	-3
β_{76}	1	3	3	1	1	3	3	1	γ_{43}	-3	-3	-9	-9	-1	-1	-3	-3	γ_{76}	1	1	1	1	3	3	3	3
β_{77}	1	3	9	3	1	3	9	3	γ_{44}	3	3	9	9	1	1	3	3	γ_{77}	1	1	3	3	3	3	9	9
β_{81}	-3	-1	-1	-3	-3	-1	-1	-3	γ_{51}	3	3	1	1	3	3	1	1	γ_{81}	1	1	1	1	1	1	1	1
β_{82}	-1	-1	-1	-1	-1	-1	-1	-1	γ_{52}	-3	-3	-1	-1	-3	-3	-1	-1	γ_{82}	-1	-1	-1	-1	-1	-1	-1	-1
β_{83}	-1	-1	-3	-3	-1	-1	-3	-3	γ_{53}	-1	-1	-1	-1	-1	-1	-1	-1	γ_{83}	-1	-1	-3	-3	-1	-1	-3	-3
β_{84}	-3	-1	-3	-9	-3	-1	-3	-9	γ_{54}	1	1	1	1	1	1	1	1	γ_{84}	1	1	3	3	1	1	3	3
β_{85}	3	1	1	3	3	1	1	3	γ_{55}	3	3	1	1	9	9	3	3	γ_{85}	1	1	1	1	3	3	3	3
β_{86}	1	1	1	1	1	1	1	1	γ_{61}	-3	-3	-1	-1	-3	-3	-1	-1	γ_{86}	-1	-1	-1	-1	-3	-3	-3	-3
β_{87}	1	1	3	3	1	1	3	3	γ_{62}	3	3	1	1	3	3	1	1	γ_{87}	-1	-1	-3	-3	-3	-3	-9	-9
β_{88}	3	1	3	9	3	1	3	9	γ_{63}	1	1	1	1	1	1	1	1	γ_{88}	1	1	3	3	3	3	9	9

Appendix B

According to [34], the analytical solution of the complex potential at the ground surface for a three-layer model with a transitional middle layer can be expressed as:

$$v(i\omega, r) = \frac{\rho_1(i\omega)I(i\omega)}{2\pi} \left[\frac{1}{r} + 2 \int_0^\infty \frac{\frac{u+1}{u-1} e^{-2\lambda h_1}}{1 - \frac{u+1}{u-1} e^{-2\lambda h_1}} J_0(\lambda r) d\lambda \right] \quad (\text{A1})$$

with

$$u = \frac{\alpha I_1(\xi_1) + K_1(\xi_1)}{\alpha I_0(\xi_1) - K_0(\xi_1)}, \quad \xi_1 = \frac{\lambda \rho_1(i\omega)h}{\rho_2(i\omega) - \rho_1(i\omega)}, \quad \alpha = \frac{K_0(\xi_2) - K_1(\xi_2)}{I_0(\xi_2) + I_1(\xi_2)}, \quad \xi_2 = \frac{\lambda \rho_2(i\omega)h}{\rho_2(i\omega) - \rho_1(i\omega)}$$

where $I(i\omega)$ is the alternating current intensity, $\rho_1(i\omega)$ is the complex resistivity of the top layer, $\rho_2(i\omega)$ is the complex resistivity of the transitional layer, and $\rho_2(i\omega)$ is the complex resistivity of the bottom half-space. r denotes the distance from the receiving point to the transmitting source, and h is the thickness of the transitional layer. J_0 , I_0 , K_0 , I_1 , K_1 , etc., represent Bessel functions of the first kind.

For the integral in Equation (B1), a linear numerical filtering method is adopted [36], such that Equation (B1) can be rewritten as:

$$v(i\omega, r) = \frac{\rho_1(i\omega)I(i\omega)}{2\pi r} \left[1 + 2 \left(\sum_{i=1}^n \frac{\frac{u+1}{u-1} e^{-2\lambda_i h_1}}{1 - \frac{u+1}{u-1} e^{-2\lambda_i h_1}} W_i \right) \right] \quad (\text{A2})$$

where n is the number of filter coefficients, λ_i is the i th sampling point, and W_i is the corresponding weighting coefficient. In this study, the 61-point J_0 filter proposed by Guptasarma and Singh is used, as listed in Table A1.

Table A1. Coefficients of the 61-point J_0 filter.

$\lambda_i = 10^{[a+(i-1)s]} / r, \quad i = 1, 2, \dots, n, \quad a = -5.0825000000, \quad s = 1.16638303862 \times 10^{-1}, \quad n = 61$			
$W_i \quad (i = 1, 2, \dots, n)$			
$3.30220475766 \times 10^{-4}$	$-1.18223623458 \times 10^{-3}$	$2.01879495264 \times 10^{-3}$	$-2.13218719891 \times 10^{-3}$
$1.60839063172 \times 10^{-3}$	$-9.09156346708 \times 10^{-4}$	$4.37889252738 \times 10^{-4}$	$-1.55298878782 \times 10^{-4}$
$7.98411962729 \times 10^{-5}$	$4.37268394072 \times 10^{-6}$	$3.94253441247 \times 10^{-5}$	$4.02675924344 \times 10^{-5}$
$5.66053344653 \times 10^{-5}$	$7.25774926389 \times 10^{-5}$	$9.54412535465 \times 10^{-5}$	$1.24699163157 \times 10^{-4}$
$1.63262166579 \times 10^{-4}$	$2.13477133718 \times 10^{-4}$	$2.79304232173 \times 10^{-4}$	$3.65312787897 \times 10^{-4}$
$4.77899413107 \times 10^{-4}$	$6.25100170825 \times 10^{-4}$	$8.17726956451 \times 10^{-4}$	$1.06961339341 \times 10^{-3}$
$1.39920928148 \times 10^{-3}$	$1.83020380399 \times 10^{-3}$	$2.39417015791 \times 10^{-3}$	$3.13158560774 \times 10^{-3}$
$4.09654426763 \times 10^{-3}$	$5.35807925630 \times 10^{-3}$	$7.00889482693 \times 10^{-3}$	$9.16637526490 \times 10^{-3}$
$1.19891721272 \times 10^{-2}$	$1.56755740646 \times 10^{-2}$	$2.04953856060 \times 10^{-2}$	$2.67778388247 \times 10^{-2}$
$3.49719672729 \times 10^{-2}$	$4.55975312615 \times 10^{-2}$	$5.93498881451 \times 10^{-2}$	$7.69179091244 \times 10^{-2}$
$9.91094769804 \times 10^{-2}$	$1.26166963993 \times 10^{-1}$	$1.57616825575 \times 10^{-1}$	$1.89707800260 \times 10^{-1}$
$2.13804195282 \times 10^{-1}$	$2.08669340316 \times 10^{-1}$	$1.40250562745 \times 10^{-1}$	$-3.65385242807 \times 10^{-2}$
$-2.98004010732 \times 10^{-1}$	$-4.21898149249 \times 10^{-1}$	$5.94373771266 \times 10^{-2}$	$5.29621428353 \times 10^{-1}$
$-4.41362405166 \times 10^{-1}$	$1.90355040550 \times 10^{-1}$	$-6.19966386785 \times 10^{-2}$	$1.87255115744 \times 10^{-2}$
$-5.68736766738 \times 10^{-3}$	$1.68263510609 \times 10^{-3}$	$-4.38587145792 \times 10^{-4}$	$8.59117336292 \times 10^{-5}$
$-9.15853765160 \times 10^{-6}$			

References

1. Vanhala, H.; Peltoniemi, M. A spectral IP study of Finnish ore prospects. *Geophysics* **1992**, *57*, 1545–1555.
2. Slater, L.D.; Lesmes, D. IP interpretation in environmental investigations. *Geophysics* **2002**, *67*, 77–88.
3. Abdel Aal, G.Z.; Slater, L.D.; Atekwana, E.A. Induced-polarization measurements on unconsolidated sediments from a site of active hydrocarbon biodegradation. *Geophysics* **2006**, *71*, H13–H24.
4. Mella, A.; Smeaton, C.M.; Furman, A.; Atekwana, E.A.; Rezanezhad, F.; Van Cappellen, P. Linking spectral induced polarization (SIP) and subsurface microbial processes: Results from sand column incubation experiments. *Environ. Sci. Technol.* **2018**, *52*, 2081–2090.
5. Zohore, U.L.; Kessouri, P.; Deparis, J.; Crampon, M.; Guerin, R.; Jougnot, D. Spectral induced polarization monitoring of toluene biodegradation by *Rhodococcus wratislaviensis* in controlled laboratory conditions. *Geophys. J. Int.* **2026**, *244*, ggaf486. <https://doi.org/10.1093/gji/ggaf486>
6. Naudet, V.; Mainault, A.; Leroy, P.; Florsch, N.; Petersen, J. Spectral induced polarization monitoring of chalcopyrite ore bioleaching: insights from laboratory column experiments. *Geophys. J. Int.* **2026**, *245*, ggag075.
7. Pelton, W.H.; Ward, S.H.; Hallof, P.G.; Sill, W.R.; Nelson, P.H. Mineral discrimination and removal of inductive coupling with multifrequency IP. *Geophysics* **1978**, *43*, 588–609.
8. Nordsiek, S.; Weller, A. A new approach to fitting induced-polarization spectra. *Geophysics* **2008**, *73*, F235–F245.
9. Wong, J. An electrochemical model of the induced-polarization phenomenon in disseminated sulfide ores. *Geophysics* **1979**, *44*, 1245–1265.
10. Dias, C.A. Developments in a model to describe low-frequency electrical polarization of rocks. *Geophysics* **2000**, *65*, 437–451.
11. Soininen, H. The behavior of the apparent resistivity phase spectrum in the case of a polarizable prism in an unpolarizable half-space. *Geophysics* **1985**, *50*, 810–819.
12. Xiong, Z.; Luo, Y.; Wang, S.; Wu, G. Induced-polarization and electromagnetic modeling of a three-dimensional body buried in a two-layer anisotropic earth. *Geophysics* **1986**, *51*, 2235–2246.
13. Yoshioka, K.; Zhdanov, M.S. Three-dimensional nonlinear regularized inversion of induced polarization data based on the Cole–Cole model. *Phys. Earth Planet. Inter.* **2005**, *150*, 29–43. <https://doi.org/10.1016/j.pepi.2004.08.034>
14. Xu, Z.; Zhdanov, M.S. Three-dimensional Cole–Cole model inversion of induced polarization data based on a regularized conjugate gradient method. *IEEE Geosci. Remote Sens. Lett.* **2015**, *12*, 1180–1184.
15. Xi, J.; Liu, Y.; Cui, D. Research on 3D SIP conjugate gradient inversion algorithm with parameter range constraints. *Math. Probl. Eng.* **2021**, *2021*, 6617794. <https://doi.org/10.1155/2021/6617794>

16. Commer, M.; Newman, G.A.; Williams, K.H.; Hubbard, S.S. 3D induced-polarization data inversion for complex resistivity. *Geophysics* **2011**, *76*, F157–F171.
17. Yuval; Oldenburg, D.W. Computation of Cole–Cole parameters from IP data. *Geophysics* **1997**, *62*, 436–448.
18. Routh, P.S.; Oldenburg, D.W. Regularized inversion of spectral IP parameters from complex resistivity data. In Proceedings of the SEG Technical Program Expanded Abstracts, New Orleans, LA, USA, 13–18 September 1998.
19. Loke, M.H.; Chambers, J.E.; Ogilvy, R.D. Inversion of 2D spectral induced polarization imaging data. *Geophys. Prospect.* **2006**, *54*, 287–301.
20. Farias, V.J.D.C.; Maranhao, C.H.D.M.; Rocha, B.R.P.D.; de Andrade, N.d.P.O. Induced polarization forward modelling using finite element method and fractal model. *Appl. Math. Model.* **2010**, *34*, 1849–1860.
21. Farias, V.J.D.C.; Rocha, B.R.P.D.; Rocha, M.P.D.C.D. The use of the fractal model in the interpretation of induced polarization data. *Appl. Math. Model.* **2013**, *37*, 1347–1361. <https://doi.org/10.1016/j.apm.2012.04.002>
22. Kenkel, J.; Hördt, A.; Kemna, A. 2D modelling of induced polarization data with anisotropic complex conductivities. *Near Surf. Geophys.* **2012**, *10*, 533–544. <https://doi.org/10.3997/1873-0604.2012050>
23. Pelton, W.H.; Sill, W.R.; Smith, B.D. Interpretation of complex resistivity and dielectric data: Part I. *Geophys. Trans.* **1983**, *29*, 297–330.
24. Jaggar, S.R.; Fell, P.A. Forward and inverse Cole–Cole modelling in the analysis of frequency-domain electrical impedance data. *Explor. Geophys.* **1988**, *19*, 463–470.
25. Xiang, J.; Jones, N.B.; Cheng, D. Direct inversion of the apparent complex-resistivity spectrum. *Geophysics* **2001**, *66*, 1399–1404.
26. Xu, W.; Ke, S.; Yin, C. Measurement and inversion of complex resistivity spectra for different core samples. In Proceedings of the SEG Technical Program Expanded Abstracts, Denver, CO, USA, 26–31 October 2014.
27. Sant’Ana, T.C.S.; Sampaio, E.E.S. Integrated approach of spectral induced polarization and electromagnetic coupling in exploration geophysics. *IEEE Trans. Geosci. Remote Sens.* **2022**, *60*, 4502409.
28. Cao, Z.; Chang, Y.; Luo, Y. Inversion study of spectral induced polarization based on improved genetic algorithm. *PIERS Online* **2005**, *1*, 266–270.
29. Chen, J.; Kemna, A.; Hubbard, S.S. Comparison between Gauss–Newton and Markov Chain Monte Carlo methods for SIP inversion. *Geophysics* **2008**, *73*, F247–F259.
30. Bérubé, C.L.; Chouteau, M.; Shamsipour, P.; Enkin, R.J.; Olivo, G.R. Bayesian inference of spectral induced polarization parameters. *Comput. Geosci.* **2017**, *105*, 51–64. <https://doi.org/10.1016/j.cageo.2017.05.001>.
31. Lowry, T.; Allen, M.B.; Shive, P.N. Singularity removal: A refinement of resistivity modeling techniques. *Geophysics* **1989**, *54*, 766–774.
32. Xu, S. *Finite Element Method in Geophysics*; Science Press: Beijing, China, 1994.
33. Saad, Y. *Iterative Methods for Sparse Linear Systems*, 2nd ed.; SIAM: Philadelphia, PA, USA, 2003.
34. Mallick, K.; Jain, S.C. Resistivity sounding on a layered transitional earth. *Geophys. Prospect.* **1979**, *27*, 869–875.
35. Dell’Accio, F.; Guessab, A.; Nudo, F. New quadratic and cubic polynomial enrichments of the Crouzeix–Raviart finite element. *Comput. Math. Appl.* **2024**, *170*, 204–212. <https://doi.org/10.1016/j.camwa.2024.06.019>
36. Guptasarma, D.; Singh, B. New digital linear filters for Hankel J0 and J1 transforms. *Geophys. Prospect.* **1997**, *45*, 745–762.

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.