Full-decay spectral modelling of time-domain induced polarization decoupling model and forward meshes

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Direct current (DC) resistivity and induced polarization (IP) geophysical methods are widely used in geophysical near-surface investigations, gaining information about subsurface conductivity structures by injecting electric currents into the ground and measuring electric voltages at different locations. The DC resistivity method provides information about the electrical conductive properties of the subsurface. In contrast, the IP method targets the capacitive characteristics offering additional insight into the physical and electrochemical nature of subsurface materials.

The IP phenomenon has been widely investigated both in time (TDIP) and frequency (FDIP) domains, in the laboratory, or through field studies. The TDIP has been used for many years for disseminated ores and mineral discrimination (e.g. Vanhala and Peltoniemi, 1992; Seigel et al., 1997, 2007). Over the last 20 years significant advancements in IP research have taken place, particularly with respect to the spectral content of the IP signal, which can be applied to engineering and environmental problems, such as the detection of contaminants and old landfills (e.g. Weller et al. 1999; Gazoty et al. 2012; Fiandaca et al., 2015; Johansson et al. 2015), and the derivation of grain size distribution parameters in unconsolidated sediments (e.g. Vanhala et al., 1992, Kemna et al., 2004, 2012).

In the frequency domain, IP phenomena can be represented as a complex conductivity $\sigma^*(\omega)$ that varies with frequency (ω), which can be expressed as:

$$\sigma^*(\omega)=|\sigma(\omega)|e^{i\varphi(\omega)} = \sigma'(\omega) + i\sigma''(\omega) \qquad (1)$$

where * denotes a complex term, $|\sigma(\omega)|$ is the magnitude of conductivity, φ is the phase angle between injected current and measured voltage, $\sigma'(\omega)$ is the real component of conductivity, $\sigma''(\omega)$ is the imaginary component of conductivity, $\omega = 2\pi f$ is the angular frequency representation of frequency f, and $i = \sqrt{-1}$ (Binley, 2015). By neglecting electromagnetic (EM) effects, the complex potential $u^*(\omega) = u'(\omega) + iu''(\omega)$ is linked to the complex conductivity through Poisson's equation:

$$\nabla \cdot \boldsymbol{j}_S^*(\omega,\boldsymbol{r}) = \nabla \cdot [\sigma^*(\omega,r)\boldsymbol{E}^*(\omega,\boldsymbol{r})] \qquad (2)$$

where $\boldsymbol{j}_S^*$ is the applied source current density, $\boldsymbol{r} = (x, y, z)$ is the spatial location, and $\boldsymbol{E}^*(\omega,\boldsymbol{r}) = -\nabla u^*(\omega,\boldsymbol{r})$ is the complex electric field.

In the time domain, Poisson's equation is given as a convolution between the conductivity and the electric field as a function of the time t (e.g. Kemna, 2000):

$$\nabla \cdot j_s(t,r) = \nabla \cdot \left[\int_0^\infty \sigma(t',r) \boldsymbol{E}(t-t',\boldsymbol{r})\, dt' \right] \tag{3}$$

where $\sigma(t)$ is the inverse Laplace transform of $\sigma^*(\omega)$ and $\boldsymbol{E}(t, \boldsymbol{r}) = -\nabla u(t, \boldsymbol{r})$.

As mentioned above, during the last two decades, significant advancements in induced polarization research have taken place, particularly with respect to spectral IP (SIP) and its increasing application in near-surface investigations even if surveys are usually modelled by taking into account only the integral chargeability, thus disregarding spectral content and neglecting the effect of the transmitted waveform, biasing inversion results. In this context, following Fiandaca et al. (2012, 2013)'s approach, EEMverter has been developed to model IP in electric and electromagnetic (EM) data within the same inversion framework and where the forward response is computed in the frequency domain for all dimensionalities, solving the full version of Poisson's equation, and then transformed into the time domain, thus avoiding the time-domain approximation (eq. 3). Here, we will focus only on the galvanic aspects in EEMverter modelling, while the other modelling features of EEMverter, such as EM modelling, time-lapse and joint inversion of galvanic and EM data are treated in Fiandaca a et al. (2024).

From a physical-mathematical point of view, resistivity and IP forward responses are modelled in the frequency domain for a range of frequencies using the finite element method. The responses are then transformed into the time domain for each quadrupole measurement and the transmitted current waveform is applied. In 2-D, the FD forward response assumes an isotropic 2-D distribution of the complex conductivity, neglecting electromagnetic induction. Considering the complex conductivity $\sigma^*(x, z, \omega\,)$ at a given frequency ω with a point source at the origin with (zero-phase) current I, the Poisson's equation can be defined as follow:

$$\frac{\partial}{\partial x}\left(\sigma^* \frac{\delta \sigma^*}{\delta x}\right) + \frac{\partial}{\partial z}\left(\sigma^* \frac{\partial \phi^*}{\partial z}\right) - \lambda^2 \phi^* \sigma^* = -I\delta(x)\delta(z) \tag{4}$$

where ϕ^* is the Fourier-transformed complex potential, λ is the Fourier transformation variable for the assumed strike (y) direction and δ represents the Dirac delta function.

Once the frequency domain potential ϕ^* is computed, the time domain computation is carried out through a cosine/sine transform, solved numerically in terms of Hankel transforms, expressed in terms of Bessel functions of order -1/2 and +1/2, respectively (Johansen and Sørensen, 1979):

$$\frac{1}{\pi}\int_0^\infty f(\omega) \frac{cos}{sin}(\omega t) d\omega = \sqrt{r}\int_0^\infty f_1(\lambda)\lambda J_{\mp 1/2}(\lambda r) d\lambda \tag{5}$$

Where $r = t\sqrt{2\pi}$, $\lambda = \frac{\omega}{\sqrt{2\pi}}$ and $f_1(\lambda) = \frac{1}{\sqrt{\lambda}} f\left(\frac{\lambda}{\sqrt{2\pi}}\right)$.

Finally, the time-domain IP decay is computed as the convolution of the impulse response with the current waveform $i(t)$ between the electrodes, solved as proposed by Fitterman and Anderson (1986) for piecewise linear current waveforms.

EEMverter is implemented in such a way that the inversion parameters are defined on the nodes of the model mesh and migrated to the forward mesh through interpolation (that can be chosen and selected by the user). The spatial decoupling between model and forward meshes allows for defining

the model parameters, e.g., the Cole-Cole (Cole and Cole 1941; Pelton et al. 1978) ones, on several model meshes, one for each inversion parameter, for example.
For each dataset of the inversion process, a distinct forward mesh is defined. The interpolation from model parameters **M** into the values $\mathbf{m}_i$ is expressed through a matrix multiplication:

$$\boldsymbol{m_i} = f_i(\boldsymbol{M}) = \boldsymbol{F_i} \cdot \boldsymbol{M} \quad (6)$$

in which the matrix $\boldsymbol{F_i}$ holds the weights of the interpolation that depends only on the distances between model mesh nodes and the subdivisions of the ith forward mesh (Fiandaca et al., 2024).
As for the forward response, the Jacobian matrix is computed in the frequency domain and then transformed into the time domain. The time-domain Jacobian in the ith forward mesh is computed as:

$$\boldsymbol{J}_{m_i,TD} = \boldsymbol{A} \cdot \boldsymbol{T} \cdot \boldsymbol{J}_{m_i,FD} \quad (7)$$

where the matrix $\boldsymbol{T}$ holds the Hankel coefficients, the matrix $\boldsymbol{A}$ implements the effects of current waveform, gate integration and filters and the frequency-domain Jacobian $\boldsymbol{J}_{m_i,FD}$ is calculated in 1-D through finite difference and in 2-D/3-D using the adjoint method and the chain rule as in Fiandaca et al. (2013) and Madsen et al. (2020), thus allowing to use any parameterization of the IP phenomenon in the inversion:

$$\boldsymbol{J}_{m_i,FD} = \boldsymbol{J}_{\sigma*,i} \cdot \frac{\partial \sigma^*}{\partial_{m_i}} \quad (7)$$

where $\boldsymbol{J}_{\sigma*,i}$ is the Jacobian of the ith forward mesh with respect to the complex conductivity σ^* and $\frac{\partial \sigma^*}{\partial_{m_i}}$ is the partial derivative of the complex conductivity versus the model parameters (Fiandaca et al., 2024).
The Levenberg-Marquardt linearized approach is used for computing the inversion model:

$$\boldsymbol{M}_{n+1,j} = \boldsymbol{M}_{n,j} + \left[\boldsymbol{J}_{M,j}^T \boldsymbol{C}_d^{-1} \boldsymbol{J}_{M,i} + \boldsymbol{R}^T \boldsymbol{C}_{R,}^{-1} \boldsymbol{R}_j + \lambda \boldsymbol{I}\right]^{-1} \cdot \left[\boldsymbol{J}_{M,j}^T \boldsymbol{C}_d^{-1} \cdot \left(\boldsymbol{d} - \boldsymbol{f}_{n,j}\right) + \boldsymbol{R}^T \boldsymbol{C}_{R,j}^{-1} \boldsymbol{R}_j \cdot \boldsymbol{M}_{n,j}\right] \quad (8)$$

where the subscript j indicates that the inversion process can be split in different inversion cycles: in each cycle j it is possible to change the forward computation for each dataset (e.g., from 1-D to 3-D), as well as to insert/remove data/constraints from the objective function (Fiandaca et al., 2023).

However, when using the resistivity and IP method to map subsurface geological structures with complex geometries, 1-D and 2-D inversion schemes are not always sufficient and 3-D modelling and inversion of the data are required. For this reason, EEMverter is also developed for 3-D inversion, following Madsen et al., (2020). To discretize the 3-D problem, a combined triple-grid inversion approach (presented by Günther et al. 2006) is adopted: a coarse tetrahedral mesh is used for the inversion (the model mesh) and two finer discretized tetrahedral meshes (one for the primary potential field and one for the secondary potential field) are used to compute the forward responses, balancing the modelling accuracy, the computational speed and memory usage. The results of the 2-D implementation on synthetic and field data, as well as the 3-D implementation under development, will be presented at the conference.

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