Development and application of 2D magnetotelluric inversion in complex domain

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by

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DECLARATION

This thesis has been composed by me and has not been submitted for any other degree. Except where acknowledgement is made, the work is original.

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ABSTRACT

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The magnetotelluric method is widely used in the investigation of the geo-electric structure of the earth. The field data are traditionally inverted to reveal the subsurface structure solved using regularised iterative inversion techniques. These interpretation schemes effect matrix computations in real domain due to operational simplicity. The speed of convergence of these techniques is controlled by the calculation type and the size of the program or more specifically, size of the matrices used. A common problem encountered when dealing with real matrices in 2D regularised inversion is their huge size. To partly overcome this problem, a new inversion strategy using complex singular value decomposition techniques has been successfully developed. The use of analytical partial derivatives and a variety of problem regularization measures ensure that the scheme is stable and rapidly convergent. In this method, instead of using the Cagniard apparent resistivity and phase, the frequency normalised impedance is adopted as the interpretative data functions for improved model resolution. Sample applications to several synthetic and to field data from Parnaiba Basin in Brazil proved successful and are presented in this thesis. It is also found that the complex form of the data-space and parameter-space eigenvectors contain information on parameter resolution. Suggestions are made for further studies especially of methods of improving parameter resolution in 2D inversion.
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1. INTRODUCTION

The investigation of the earth has appealed to human beings since the dawn of civilization and many methods have been tried as parts of the various scientific disciplines or as non-scientific experiments. Geophysical exploration methods rely upon the measurement of the physical properties of the earth; using invasive or non-invasive techniques. For instance, the investigation of the electrical properties such as resistivity, dielectric permittivity and electrochemical activity requires the use of electric and electromagnetic (EM) methods of geophysics. In all the methods, the response of geological structures to external or internal geophysical excitation is observed and recorded. This response which is in either real or complex domain can be a function of time, frequency, distance or some combination of them. In conventional geophysical data processing some of the real domain data are sometimes transformed into the complex domain by using the Fourier transformation due to the requirements of the method and/or operational simplicity as in the magnetotelluric (MT) method. Beside this, the gathered data may be represented in complex domain by secondary functions using well-known transformations such as the Hilbert transformation in potential field methods (e.g., Nabighian, 1972; Green and Stanley, 1975; Mohan et al., 1982) and some seismic applications (e.g., Taner et al., 1979). In this study focusing in the EM methods, the data of interest data are the MT impedance and its derivatives, hereafter the examples and definitions about modeling will be for EM and especially for the MT methods. To harvest useful information from these data, such as the location or size of the targeted body, requires geophysical interpretation techniques which can be performed under certain assumptions. The simplest one is the one-dimensional (1D) earth model approach which has been very helpful for many years in large scale studies especially as it does not need powerful computer facilities and is operationally simple. As the MT method involved and research investigations expanded from regional studies to local, small-scale investigations especially for natural resources, the 1D interpretation schemes were found to be insufficient to explain the real world. Despite the significant effort to develop the mathematical
basis for two-dimensional (2D) or three-dimensional (3D) earth models for EM methods (e.g., Coggon, 1971) the high computational requirement made any application impractical in the early days. However with the remarkable development of computer technology it has become possible to apply these multi-dimensional interpretations (e.g., Brewit-Taylor, 1976; Wannamaker et al 1985; Sasaki, 1989). However, despite the vast amount of significant research in the area of the 2D MT interpretation methods (Madden and Thompson, 1965; Coggon 1971; Jupp and Vozoff, 1975; Varentsov, 1983; Wannamaker et al., 1985; de Groot-Hedlin and Constable, 1990; Smith and Booker, 1991), there are still some aspects that are worthy of further investigations as highlighted below and form the main topic of this thesis. The interpretation of the geophysical data is done using forward and inversion techniques. Most geophysical processes can be described mathematically and numerical modeling enables us to calculate the observable or measurable data over a given hypothetical earth-type model; this process is called forward modeling and the calculated data are usually called theoretical, synthetic or calculated data (Meju, 1994). Hence, forward theory plays a bridging role in connecting the data we have observed to the physical properties of the earth, or simply these parameters we know or have estimated. Conversely, geophysical inversion can be defined as a process which will allow us to retrieve the parameters we seek from the observable data. The success of the interpretation is measured by comparing the observed and the calculated data or earth response functions (ERF). In this sense the more information the ERF has the better the interpretative results. MT data may be presented in various forms of ERF some of which are the Cagniard (1953) apparent resistivity and impedance phase and tipper information (e.g. Vozoff, 1972); these are simply the normalized form of the MT impedance function. Recent studies have shown that the frequency normalized impedance (FNI) function has enhanced characteristic for 1D and 2D forward solution over classic type ERF (Basokur, 1994; Basokur et al., 1997; Ulugergerli and Meju, 1996, 1997). In this study the FNI will therefore be the interpretative function and the MT data will be presented as the real and the imaginary components of this function. The inverse problem is generally solved using regularized iterative inversion techniques. However, the conventional inverse schemes effect matrix computations in the real domain because
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of operational simplicity. That is, the Jacobian matrix which includes partial derivatives of an objective function with respect to model parameters may be obtained in the complex domain but calculations generally are performed on its real components (see Pedersen and Rasmussen, 1989) due to the availability and extensive developments of real singular value decomposition applications and the symmetry properties of Jacobian matrix. The use of imaginary component as a tag in the Jacobian matrix is a popular way of incorporating it into routine calculations, but such extraneous data would increase the size of the matrix and the calculation time. To partly overcome this problem, a new inversion strategy using FNI and complex singular value decomposition techniques has been developed. Geoelectric inversion in the complex domain is topical (e.g. Parker, 1980 and 1994, pg. 351) and there are still aspects of the method that are not fully resolved. Complex singular value decomposition (Marple, 1987; Klema and Laub, 1980; Forsythe et al., 1977; Lawson and Hanson, 1974) provides an attractive solution to this problem. In this method the data space eigenvectors, U and parameter space eigenvectors, V are computed in the complex domain while the singular values of the problem are real. In order to obtain Jacobian matrix for the 2D MT inversion, an implementation of the reciprocity theory will also be outlined in this chapter. The underlying principles of the methods used in this study are given in various chapters of this report. In the second chapter, the basic equations of the EM theory and definition of the FNI are given. The forward solution for the multi-dimensional subsurface structures is well-known and can only be obtained by means of numerical solution process. The numerical solution to the two-dimensional MT forward problem can be obtained in many ways involving the solution of integral or differential equations. In the third chapter the two-dimensional forward solution for the MT method using differential equations will be summarized. In the fourth chapter, the general theory of the inverse problem is revisited. 1D and 2D MT inversion in complex domain are given in chapter five. However, the 1D application will be kept at theoretical level in this study. Computational development of the proposed method for 2D inversion with a description of the program and the application to synthetic data are presented in the sixth chapter. The first test data are calculated by the use of the forward solution described in the third chapter over the test model in which a simple dike of 1 ohm-m
is embedded in a host medium of 100 ohm-m resistivity. The second test model simulates the simple geoelectric setting of a basin model which consists of a low resistive (10 ohm-m) weathered layer overlying a faulted moderately resistive sediment of 80 ohm-m. Besides the fault zone, the resistivity of which is 20 ohm-m, a low resistivity (5 ohm-m) block over another very highly resistive (10000 ohm-m) one embedded in the sediment furnish the model. The whole group is underlain by crystalline basement of 1000 ohm-m. A weathered uncorformity surface of the basement is simulated by a thin layer of 30 ohm-m. The method is tested to recover the anomalous body from a homogeneous half space starting model which consists of blocks of the same resistivities. It is assumed that the thicknesses and widths of the blocks maybe obtained from either 1D interpretation or other methods. The field data used in this study were collected in Brazil during August 1996 and September 1997, a regional research was conducted across the eastern part of the Parnaiba basin. In the seventh chapter, the regional geology based upon previous research from various sources is summarized and the results with the comparison are presented. The result shows that besides the crystalline basement and some main formations, the electrically conductive zone inside the crust can also be recovered. The location of a fault and crystalline - sediment border are the other outcomes from the inversion. The summary of this study and the conclusions with some recommendations for further research work appear in chapter eight.
2. BASIC ELECTROMAGNETIC THEORY

2.1 Introduction

The general Electromagnetic (EM) theory is outlined in this chapter. EM method is one of the most studied branches of geophysics. Due to the close relation with many other sciences a wealth of research papers on EM methods have been published and there are many books currently available on the subject (e.g. Nabighian, 1988; Zhdanov and Keller, 1994) Instead of giving all the details of the entire theory only the main formulas for Magnetotelluric (MT) method will be presented. All formulas given hereafter are based on the Cartesian coordinate system in which x-axis is positive rightwards and z-axis is positive downwards. Bold letters represent vectors while normal ones are scalars.

In the MT method various components of the EM wave, the source of which may be artificial or natural, are measured on the surface of the earth and used to determine the resistivity structure of the earth. We are interested in the horizontal and vertical components of the magnetic fields and two horizontal components of the electrical fields. The relations between them and the solutions for them are defined by Maxwell equations. Assuming a time variation of the form e^{i\omega t}, the Maxwell equations in frequency domain are

\[ \nabla \times \mathbf{E} = -i\omega \mathbf{B} \]  \hspace{1cm} (2.1)

\[ \nabla \times \mathbf{H} = \mathbf{J} + i\omega \mathbf{D} \]  \hspace{1cm} (2.2)

\[ \nabla \cdot \mathbf{B} = 0 \]  \hspace{1cm} (2.3)

\[ \nabla \cdot \mathbf{D} = \rho' \]  \hspace{1cm} (2.4)
where \( E \) is the electrical field intensity (mV/m), \( H \) is magnetic field intensity (A/m), \( B \) is magnetic induction (nT), \( D \) is dielectric displacement (C/m\(^2\)), \( \rho' \) is electric charge density (C/m\(^3\)), \( J \) is Electric current density (A/m\(^2\)), \( i \) is a complex constant, \( \omega \) is angular frequency equal to \( 2\pi f \) where \( f \) is frequency. Equation (2.1) is the so-called Faraday law and implies that variations of the magnetic field create an electrical field. Equation (2.2) is known as Ampere’s law and indicates that electrical current flow creates a magnetic field. Equation (2.3) shows that the magnetic field is solenoidal. The last equation is called Coulomb’s law.

Maxwell equations do not show any relationship between the behaviour of the EM field and the subsurface structure of the earth or its properties. The constitutive equations fill this gap for the geophysical applications and explain the necessary relations, such as,

\[
J = \sigma E \quad (2.5)
\]

where \( \sigma \) is conductivity (Siemens/m),

\[
D = \varepsilon E \quad (2.6)
\]

where \( \varepsilon \) is dielectric permittivity (F/m) and

\[
B = \mu H. \quad (2.7)
\]

where \( \mu \) is magnetic permeability (H/m).

The physical parameters \( \sigma, \varepsilon \) and \( \mu \) describe the geoelectrical structures for the EM applications in geophysics. According to each different EM method, some of the parameters may be frequency dependent and may not be real in every situation. Therefore, some of them may be defined in complex domain (Keller, 1988). Stratton (1941) showed the dependence of the parameters on frequency for pure metals and dielectrics and discussed the existence of imaginary components of the parameters for sufficiently high frequencies. Fuller and Ward (1970) gave a
review of the theoretical basis for the complex definition of the parameters in some
difficulties in some geophysical applications and the relation between the real and imaginary
components of \( \sigma \) and \( \varepsilon \) through the Hilbert transformation. The common point in
these studies is that the frequency must be high enough to be able to observe that
kind of dependence. In practical applications, to reformulate all equations for the
complex form of the parameters would not be necessary due to the frequency ranges
commonly employed by the methods. Hence, for the sake of simplicity, imaginary
components are obtained using some arbitrary definitions. For example, permittivity
may be taken as imaginary component for the conductivity (Keller, 1988; Bezdova
and Segeth, 1982). Using Maxwell’s constitutive relations, equations (2.1) and (2.2)
can be written in the form

\[ \nabla \times E + i \omega \mu H = 0 \]  
(2.8)

\[ \nabla \times H - \sigma^* E = 0 \]  
(2.9)

where \( \sigma^* \) is the so-called complex conductivity and equal to \( (\sigma + i \omega \varepsilon) \) (Bezdova and
Segeth, 1982). In order to the present basic definitions for MT method the electric
charge density, \( \rho' \) is taken to be zero, \( \varepsilon \) and \( \mu \) are equal to their free-air values (\( \varepsilon_0 = 
8.85 \times 10^{-12} \) F/m, \( \mu_0 = 4\pi \times 10^{-7} \) H/m) and \( \sigma \) is assumed constant in homogeneous
domain so that the wave equations are obtained as follows

\[ \nabla^2 E + k^2 E = 0 \]  
(2.10)

and

\[ \nabla^2 H + k^2 H = 0. \]  
(2.11)

In Equation (2.10) and (2.11) \( k \) is the complex wave number given by

\[ k^2 = -i \omega \mu \sigma^* \]  
(2.12)
The general form of the wave equations are given in Appendix A. In EM prospecting at low frequencies, any magnetic field generated by the displacement current term $i\omega D$ is usually negligible. Removal of $i\omega D$ from Equation (2.2) eliminates the wave nature of the EM field in free space. This result is usually termed the quasi static approximation. At this step the wave equations become the diffusion equation. In the MT method, the use of low frequency range or, namely, quasi-static approximation allows us to neglect the displacement currents and because of this assumption some parameters may either vanish or are defined as constants in the solution sought, that is $\sigma >> \omega^2 \epsilon$ so that $\sigma^* = \sigma$ and $k$ is given as 

$$k^2 = -i\omega \mu \sigma. \quad (2.13)$$

This approximation is equivalent to ignoring the imaginary component of the complex conductivity and this will be used in following sections. Defining

$$a = (\omega \mu \sigma/2)^{1/2} \quad (2.14)$$

the real and the imaginary components of $k$ are now given as

$$k = a (1 - i). \quad (2.15)$$

In the early days of the EM applications in geophysics, the solution for the EM induction over uniform half space was the subject of discussion (e.g., Wait, 1954; Price, 1962; Madden and Nelson, 1963). The main arguments were the source of the EM wave, frequency range in which the solution is valid and effect of spherical shape of the earth. Many researchers reviewed different kinds of source types such as a current sheet parallel to the earth’s surface and an infinitely long straight line, and showed that the solutions for different source types are similar to each other and that the effect of the earth’s shape is negligible (e.g. Madden and
Nelson, 1963; Pirjola, 1982). Following these discussions, solution of diffusion equation over one-dimensional structure for E or H, in the region \(0 < z < \infty\) varying harmonically with time and traveling downward over the homogeneous half space is

\[ E_x \text{ or } H_x = A e^{-i(kz - wt)} \quad (2.16a) \]

where \(A\) is a constant, \(z\) is depth and \(t\) is time. Using the components of \(k\)

\[ E_x = A e^{-iaz} e^{-az} e^{iwt}. \quad (2.16b) \]

In equation (2.16), \(e^{-iaz}\) and \(e^{iwt}\) indicate that the wave has sinusoidal shape as it is a function of \(z\) and \(t\) respectively. The real component \(e^{-az}\) reveals attenuation of EM wave. Accordingly the skin depth, \(\delta\) is defined as a depth where the amplitudes of EM waves decay to \(1/e\) of their initial values at the surface,

\[ \delta = \frac{1}{a} = (\omega\mu\sigma / 2)^{-1/2}. \quad (2.17) \]

2.2 Impedance Relations in One-Dimensional Media

Over 1D media, it is assumed that the derivatives of \(E\) and \(H\) with respect to \(x\)- and \(y\)-axis are zero and variations exist only in the \(z\) direction. Solution of wave equations for \(E\) over the homogeneous half space is given in Equation (2.16). Using the first Maxwell equation,

\[ H_y = -(i\omega\mu)^{-1} \frac{\partial E_x}{\partial z} \quad (2.18) \]

and \(H_y\) can be obtained as

\[ H_y = (k/\omega\mu) A e^{-i(kz - wt)}. \quad (2.19) \]
The EM wave impedance or as it is better known the Cagniard (1953) - Tikhonov (1950) impedance is

\[ Z = \frac{E_x}{H_y} \text{ or } \frac{E_y}{H_x}. \]  \hspace{1cm} (2.20)

Substituting (2.16) and (2.19) into (2.20) yields

\[ Z = \frac{\omega \mu}{k} = \frac{E_x}{H_y} = -\frac{E_y}{H_x}. \]  \hspace{1cm} (2.21)

After slight modification we obtain

\[ Z = (\omega \mu \rho)^{1/2} e^{i\pi/4} \]  \hspace{1cm} (2.22)

where \( \rho \) is the resistivity (the reciprocal of conductivity) of the half space and the exponential term states that the EM impedance has a phase of \( \pi/4 \) over a homogeneous half space. Another useful function introduced by Basokur (1994) is the frequency normalized impedance (FNI) which is given as

\[ Y = (i\omega \mu)^{-1/2} Z. \]  \hspace{1cm} (2.23)

Substituting (2.22) into (2.23) leads to (Basokur, 1994)

\[ Y = (\rho)^{1/2}. \]  \hspace{1cm} (2.24)

The FNI is equal to the square root of resistivity of the homogeneous half space with zero phase. In the case of layered earth, the traditional, Cagniard apparent resistivity and phase of impedance function can be described in terms of the real and imaginary parts of the FNI function (Basokur, 1994), that is:

\[ \rho_a = Y_r^2 + Y_i^2 \]  \hspace{1cm} (2.25)
and

\[ \Phi_Z = \pi/4 + \tan^{-1}(Y_1 / Y_R) \]. \hspace{1cm} (2.26)

Equation (2.25) gives the relation between the FNI and the Cagniard apparent resistivity definitions. It is also possible to obtain other apparent resistivity definitions using the components of the FNI function (see Basokur 1994).

2.2.1 Impedance Relations for N-Layered Earth

Cagniard-Tikhonov type impedance over N layered media was given by Wait (1954) in the interesting form

\[ Z_j = (i \omega \mu / k_j) \tanh(k_j h_j + \tanh^{-1}(k_j / k_{j+1})) \hspace{1cm} j = 1, 2, ..., N \] \hspace{1cm} (2.27)

where \( Z_j \) is the impedance of layer \( j \), \( h_j \) is the thickness of layer \( j \), and \( k_j \) is the propagation constant for the \( j \)-th layer. \( Z_N \) is given in Equation (2.21). In a similar way, the FNI function for N-layered earth is obtained as

\[ Y_j = P_j \tanh(u h_j / P_j + \tanh^{-1}(Y_{j+1} / P_j)) \hspace{1cm} j = 1, 2, ..., N \] \hspace{1cm} (2.28)

where \( Y_j \) is the impedance of layer \( j \), \( P_j \) is the square root of resistivity of layer \( j \), and \( u \) is \((i \omega \mu)^{1/2}\). \( Y_N \) is given by Equation (2.24). The above equation has been programmed by the author as part of initial 1D inversion work (see Appendix B).

2.3 Impedance Relations for Multi-Dimensional Media
The more realistic solution for the typical earth structure is obtained by means of the 2D model in which the resistivity variations occur in the vertical and lateral directions. The horizontal axis along which resistivity does not vary is called the strike direction. This model requires the measurements of each component in orthogonal directions (the principal axes) that are parallel and normal to strike. In practice, $E_z$ measurements are not easy, however, some published accounts of attempts to determine $E_z$ may be found in the literature (e.g., Chave and Filloux, 1985). The relations between $E$ and $H$ in matrix form is

$$
\begin{bmatrix}
E_x \\
E_y
\end{bmatrix} =
\begin{bmatrix}
Z_{xx} & Z_{xy} \\
Z_{yx} & Z_{yy}
\end{bmatrix} \begin{bmatrix}
H_x \\
H_y
\end{bmatrix}
$$

(2.29)

If $E$ is in the strike direction ($E_y$) the measurement is called transverse electric or TE mode. On the other hand, if $H$ is in that direction ($H_y$), it is the transverse magnetic or TM mode (Fig. 2.1). In these definitions the term “Transverse” denotes that the field is transverse to the vertical axis ($z$), not to the horizontal axis, $y$. In Equation (2.29), $Z_{ik}$ is obtained as the ratio of $E_i$ to $H_k$.

![Fig. 2.1 Magnetotelluric polarizations; TE mode (a) and TM mode (b).](image)

The impedance due to $E$- and $H$- polarizations are different depending on the frequency and the location of measurements with respect to the total resistivity discontinuity (O'Brien and Morrison 1967). Over an ideal 1D structure satisfying
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Cagniard's (1953) conditions, \( Z_{xx} \) and \( Z_{yy} \) are zero while \( Z_{xy} \) and \(-Z_{yx}\) are equal to each other.

If the subsurface is 2D, then, \( Z_{xx} \) and \( Z_{yy} \) are zero in the principal direction only (Swift, 1967) while \( Z_{xy} \) and \( Z_{yx} \) have different values. Considering the next step, impedance on the principle axis can be interpreted that is \( Z_{xy} \) and \( Z_{yx} \) take place in the interpretation. Thus, the measurement axis in which impedances are observed and the strike direction are preferred to be the same so that \( Z_{xx} \) and \( Z_{yy} \) are calculated as zero. However, strictly 2-D structures are rare in nature and MT measurement are made in two orthogonal directions which may not be aligned with the (unknown) strike. Suppose our measurement axes \((x,y)\) make an angle \( \Theta \) (measured clockwise from the y-axis) with the true strike, we want to determine our field components in the coordinate rotation matrix for a vector in the (preferred) principal anisotropy axes \((x',y')\) (Fig.4). Let \( R \) be coordinate rotation matrix for a vector in the \((x,y)\) plane given by

\[
R = \begin{bmatrix}
\cos \Theta & \sin \Theta \\
-\sin \Theta & \cos \Theta
\end{bmatrix}
\]  

(2.30)

On rotation of the tensor elements from \((x,y)\) to \((x',y')\) by an angle \( \Theta \) about \( Z \), the rotated impedance tensor becomes (Swift, 1967; Sims and Bostick, 1969)

\[
Z' = R Z R^{-1} .
\]  

(2.31)

By the use of impedance tensors and rotation angle we may define

\[
Z_o = \frac{(Z_{xx} + Z_{yy})\cos 2\Theta}{2} - \frac{(Z_{xx} - Z_{yy})\sin 2\Theta}{2}.
\]  

(2.32)

If the real and imaginary parts of \( Z_o \) are plotted on an Argand diagram for varying \( \Theta \), it is obvious that a 1-D structure will give a single point focus whereas a 2-D
structure will generate a straight line and a 3-D structure will generate an ellipse (Sims and Bostick, 1969).

\[ \Theta = 0.25 \arctan \frac{2 \text{Re}(Z_{xy} + Z_{yx})(Z_{xx} - Z_{yy})}{|Z_{xx} - Z_{yy}|^2 - |Z_{xy} + Z_{yx}|^2} \]  

Fig. 2.2. Rotation of axes by angle $\Theta$
Another method suggested recently (Groom and Bailey 1989; Bahr 1991) is

\[ \Theta_B = 0.5 \ \arctan \ \frac{[S_1, S_2] - [D_1, D_2]}{[S_1, D_1] + [S_2, D_2]} \]  

(2.34)

where

\[ S_1 = Z_{xx} + Z_{yy} \quad S_2 = Z_{xy} + Z_{yx}. \]  

(2.35)

and

\[ D_1 = Z_{xx} - Z_{yy} \quad D_2 = Z_{xy} - Z_{yx}. \]  

(2.36)

and \([\ ]\) defines

\[ [C_1, C_2] = \text{Im} \{C_1, C_2^*\}. \]  

(2.37)

Recent studies, based on the impedance tensor decomposition techniques and the use of synthetic data, have shown that if 2D EM fields over a regional setting are distorted by small scale local (3D) anomalies, the strike direction obtained from (2.33) may not be true (e.g. Groom and Bailey 1989; Bahr 1991). In the case of 3D structures in which resistivity varies in all three directions the elements of the impedance tensor will be different and no mode definition is valid in this situation.
3. NUMERICAL SOLUTION OF THE MAGNETOTELLURIC FORWARD PROBLEM

3.1 Introduction

Analytical solutions for induction in 2D structures exists for simple models such as the dike (Rankin, 1962), the infinite fault (d'Erceville and Kunetz, 1962; Weaver, 1963) and dipping beds (Hvozdora, 1968; Geyer, 1972). Berdichevskiy and Dmitriev (1976) also gave various combinations of the simple structures and the solutions to these models. As previously stated the numerical methods are the only way of calculating the response of complex 2D and 3D earth models. Details of the numerical solution will be presented in this chapter.

The numerical methods for computing the MT responses over arbitrary 2D resistivity structures have been available for years. A number of techniques are discussed in the February, 1971 Geophysics Special Issue on Electromagnetic Scattering. On the contrary, the lack of full analytical solution makes the control of the accuracy of the existing codes hardly possible. However, the analytical solutions for the simple models and the cross-check between various numerical techniques such as integral equation method (e.g. Hohmann, 1971; Parry and Ward, 1971), the transmission surface method (e.g. Madden, 1972) and two differential equation (DE) methods, the finite element method (FEM) (e.g. Coggon 1971; Rijo, 1977) and the finite differences method (FDM) (e.g. Silvester and Haslam, 1972; Brewitt-Taylor and Weaver, 1976) allow the user to choose the method which matches the requirements of a given problem. The comparison of the methods for the different geoelectrical models has also been treated in many papers (e.g. Varentsov, 1983). The main trend in the comparison is in favor of the DE method rather than the integral equations methods over complex geological models. Despite the more mathematical calculation requirement, the FEM has some advantage upon the FDM in which slopes and topography for a complex model can not be handled with ease. However over the simple geoelectric model both FEM and FDM are equivalent to each other.
In the FEM, which is chosen for this study, linear interpolation of the unknown field parallel to strike over triangular subdomains is sought (Wannamaker et al, 1985). The solution is an estimate of the field values parallel to strike at the nodes of the discretized domain. Wannamaker et al, (1985) state that the solution for the total field has a numerical accuracy problem towards low frequencies due to finite length of the computer word and suggested that secondary field solution could overcome this problem. In following section the secondary field formulae (Coggon, 1971; Hohmann, 1988) for the calculation of the responses of arbitrary shaped 2D body embedded in a 1D layered media are outlined. Also the solution of the DE for arbitrary 2D structure and FEM will be summarized without giving full details since they can easily be found in various publications (e.g. Wannamaker et. al, 1986; Silvester, 1990; Huebner and Thornton, 1982).

3.2 Differential Equations for Arbitrary 2D Structures

In chapter 2, the diffusion equations were given as Equations (2.8) and (2.9) for E and H, respectively. Hohmann (1983 and 1988), suggested a solution for the inhomogenous geoelectric model in which the total field calculations are divided

\[ \sigma_0 = 0 \]

Fig. 3.1. General model for a numerical solution (after Hohmann, 1988).
into the primary and the secondary components. In this method, the primary component refers to the field in the case of the lack of the inhomogeneity, that is, the field from the 1D geoelectrical model and the secondary field is the part created by the inhomogeneity. In Fig. 3.1 a simple model consisting of overburden layer of conductivity \( \sigma_1 \), a host rock of conductivity \( \sigma_2 \), a 2-D body of variable conductivity \( \sigma_b \) embedded in the host rock, and a basement of conductivity \( \sigma_3 \).

The primary fields given with subscript \( p \) satisfy the Maxwell equations

\[
\nabla \times \mathbf{E}_p = -i\omega \mu \mathbf{H}_p
\]

(3.1)

and

\[
\nabla \times \mathbf{H}_p = \sigma_n \mathbf{E}_p
\]

(3.2)

where \( \sigma_n \) is the 'normal' (layered-earth) conductivity with the anomalous body not present. The equations for the secondary fields with subscripts \( s \) are

\[
\nabla \times \mathbf{E}_s = -i\omega \mu \mathbf{H}_s
\]

(3.3)

and

\[
\nabla \times \mathbf{H}_s = \sigma_n \mathbf{E}_s + \sigma_a \mathbf{E}
\]

(3.4)

where \( \mathbf{E} \) is total electric field and \( \sigma_a = \sigma - \sigma_n \) is the anomalous conductivity at a point. In Fig. 3.1, \( \sigma_a \) is non zero only in the body where it becomes \( \sigma_a = \sigma_b - \sigma_n \).

The diffusion equation for secondary electrical fields is (Hohmann, 1983)

\[
\nabla^2 \mathbf{E}_s + \nabla \left( \mathbf{E}_s \cdot \nabla \sigma / \sigma \right) - i\omega \mu \sigma \mathbf{E}_s = i\omega \mu \sigma_a \mathbf{E}_p - \nabla \left( \mathbf{E}_p \cdot \nabla \sigma_a / \sigma \right).
\]

(3.5)
Similarly, the secondary magnetic field is written as

\[ \nabla^2 H_s + \sigma (\nabla \times H_s) \times \nabla (1/\sigma) - i \omega \mu_0 \sigma H_s = i \omega \mu_0 \sigma_a E_p - \sigma \nabla (\sigma_a/\sigma) \times E_p. \]  

(3.6)

Equations (3.5) and (3.6) are the DE's to be solved for the secondary E and H fields respectively. The necessary orthogonal components are obtained using Equations (3.1) - (3.4) (Hohmann, 1983, 1988). The general form of diffusion equations based on Hohmann (1983) are given in Appendix A.

### 3.3 Finite Element Method

In the FEM method, the target region is divided into a finite number of triangular subdomains called "finite elements". These subdomains are connected at common nodal points all of which together simulate the entire region. Any continuous function over this region can be approximated by the summations of the polynomials over the subdomains. In the literature, especially in the engineering field, FEM using the Helmholtz equation has wide applications (Zienkiewicz, 1971). Knowing that wave (or in the special case diffusion) equations can be represented in Helmholtz equations family, FEM applications can then be defined in EM method as follows, "Linear interpolation of the unknown field parallel to strike over triangular subdomains is utilized in conjunction with the Galerkin method of basis weighting to derive a system of linear equations which approximates the governing Helmholtz equation" (Wannamaker et. al. 1985). The approximated function, \( F \) from FEM for either of Equations (3.5) or (3.6) can be obtained in operational form,

\[ LF = s \]  

(3.7)

where L and s are the appropriate Helmholtz operator and source. The error in this approximations is
In order to minimize the error, the general method of weighted residuals produces a numerical algorithm by assuming that the inner product between a weighting function and the residual is exactly zero. Selecting weighting function, \( w \) as the function itself, (the Galerkin method), the base equation for the algorithm for \( E_s \) is

\[
\int w[(\nabla^2 + \nabla (\nabla \sigma / \sigma) + k^2) F - (-k^2_a E_p - \nabla (E_p \cdot \nabla \sigma_a / \sigma))] \, dA = 0 \quad (3.9)
\]

and for \( H_s \) is

\[
\int w[(\nabla^2 + \nabla \nabla (1 / \sigma) \sigma + k^2) F - (-k^2_a H_p - \sigma \nabla (\sigma_a / \sigma) x E_p)] \, dA = 0 \quad (3.10)
\]

where \( k^2 = -i \omega \mu \sigma \) and \( k^2_a = -i \omega \mu \sigma_a \). Details of the rest of the calculations for the system equation are given by Wannamaker et. al. (1985) and Rijo (1977). The system of equations to be solved in FEM are of the general form

\[
Gf = s \quad (3.11)
\]

where \( G \) is \( N \times N \) symmetric, sparse, banded and diagonally dominant matrix, and \( N \) is the total number of nodal points in the entire discretized domain. The vector \( f \) is a column vector of \( N \) unknown total values of the function \( F \) at each node of the discretized model. The vector \( s \) is a column vector that contains the source terms. As it was stated before, in this scheme, secondary fields are calculated. Then, for a simple 1D earth model Equation (3.11) becomes

\[
G_p f_p = s \quad (3.12)
\]

where \( p \) indicates primary field. In Equation (3.11) and (3.12), source terms can be defined as
\[ G_f = G_p f_p \]  

(3.13)

remembering the fact that total field is a superposition of the primary and secondary fields, the last equation may be written as follows:

\[ G (f_p + f_s) = G_p f_p \]  

(3.14)

or

\[ G f_s = (G_p - G) f_p \]  

(3.15)

rewriting the last equation with the definition of \( G_f = G - G_p \)

\[ G f_s = -G f_p \]  

(3.16)

where the subscript \( f \) denotes "fictitious" (Rijo, 1977). The entries of \( G_f \) are non-zero only for those nodes within and on the boundaries of the inhomogeneities. Once the solution of the secondary field is obtained, it is added to the primary field yielding the desired total field. The calculated field is either \( E_y \) for TE mode or \( H_y \) for TM mode. The necessary orthogonal component for the impedance calculation can be obtained by the use of Maxwell equations (3.3) and (3.4).

The plane wave 2-Dimensional (PW2D) forward code based on the above formulations and originally developed by Rijo (1977) with modifications by Wannamaker et al., (1985) is adopted in this study. This forward routine has been validated by various workers (see Wannamaker et al., 1985) and is widely used in routine magnetotelluric interpretations (e.g. deGroot-Hedlin and Constable, 1990).
4. GENERALIZED NON-LINEAR INVERSE THEORY

4.1. Introduction

This process of forward modeling is very helpful in experimental design or computation of ERF over assumed or known geoelectrical structures. In real life, there may not be any available information about the true geoelectrical structure. In addition, geoelectrical data are acquired over a range of time, frequency or distance and always contain some components which cannot be reproduced by the use of our simplified mathematical models. One of the main tools for recovering the best geoelectrical model from the geophysical data, acceptable in both geological and physical senses, is inverse theory. This is the set of mathematical and statistical techniques that enable us to find a solution to the interpretational problem especially concerning inaccurate, insufficient and inconsistent data (Jackson, 1972). The solution we seek is usually non-unique. In other words, there will be a number of models whose response will fit the observed data within an acceptable misfit criterion.

In electromagnetic (EM) methods, the model responses are non-linear functions of the appropriate model parameters. The estimation and interpretation of the parameters of a geoelectrical model can be done using linearized or non-linearized inverse techniques. The main types of these solution methods are least squares (e.g. Marquardt-Levenberg and Gauss Newton method) and gradient (e.g. steepest descent and conjugate gradient) methods. Comparison of the methods is the subject of a number of papers. All have advantages and disadvantages but the general trend is in the direction of the least squares method, especially Marquardt-Levenberg (Marquardt, 1963; Levenberg, 1944) method. Following the trend and because of its mathematical robustness, the least squares approach has been chosen for this study.

Before going further into the mathematical basis, the general requirements of the inversion and the interpretation process may be summarized as follows. First,
geological structures should be able to be described by mathematical models, in other words the forward solution is required. All the necessary formulae for the MT method have already been outlined in Chapter 3. Second, the physical specifications or properties characterizing the geological parameters such as resistivity should be known and taken into consideration during the interpretation. Lastly considering the nature of the data, physically and geologically meaningful parameters should be used for the inversion. In other words, to try to solve an inverse problem for which the data do not contain any information will yield a meaningless solution. For instance, in the MT applications if one selects a parameter located deeper than the maximum skin depth the only result would usually be an extremely high or low value that does not fit the geoelectrical model.

As stated previously, the inverse problem of MT interpretation is non-linear but the solution method effectively relies on the linear inversion theory which will not be repeated here. The outlines given in this chapter are based on some books (e.g. Menke, 1984; Meju, 1994) and some papers (e.g. Jackson, 1972; Lines and Treitel, 1984; Oldenburg, 1990) in which the linear inverse theory can also be found. The data and parameter definitions will be given for the MT method which is the subject of this study.

### 4.2 One Dimensional Inversion Theory

The discrete general linear inverse problem reduces to a set of \( M \) equations in \( N \) unknowns. There is generally no unique solution for typical practical problems, but we can find linear combinations of parameters for which restraints are determined (Meju, 1994). Through the chapter bold letters will represent vector and matrices

The restricted earth models are determined by \( N \) free parameters, written as the vector,

\[
P = (p_1, p_2 \ldots p_N)^T
\] (4.1)
where $T$ indicates transpose and the model parameters are resistivities and thickness of the layers resting on a basement. The data values, corresponding to $M$ sample frequencies, are written as the vector

$$ \mathbf{O} = (o(f_1), o(f_2), \ldots, o(f_M))^T $$

(4.2)

here, $o(f_i)$ are the observational data and $f_i$ ($i=1,2,\ldots,M$) are measurement frequencies. The related errors of each observation are given by

$$ \xi = (\xi_1^{-1}, \xi_2^{-1}, \ldots, \xi_M^{-1})^T $$

(4.2)

We have a relation between $\mathbf{P}$ and $o(f_i)$, the so-called forward solution,

$$ o(f_i) = K(f_i, \mathbf{P}) $$

(4.3)

where $K$ is the kernel function. As was stated in Chapter 2 our ERF is FNI and the kernel function is given in equation (2.28). Following Marquardt (1970), non-linear problems can be solved using linear inversion approach. In this method, the relation between parameters and data functions, i.e. the forward solution, is linearized by means of the Taylor Series expansion in which the response variations of any non-linear function for small perturbations of the parameters can be accepted as linear. The first-order Taylor series expansion of $K(f, \mathbf{P})$ is

$$ K(f, \mathbf{P}) = K(f, \mathbf{P}^0) + \sum_{j=1}^{N} \frac{\partial K(f, \mathbf{P}^0)}{\partial \mathbf{P}_j} (\mathbf{P}_j - \mathbf{P}_j^0) + \theta $$

(4.4)

where $\mathbf{P}$ are the perturbed values of $\mathbf{P}^0$ and $\theta$ is the error due to cut-off of the higher degree expansion. Defining the quantity

$$ \Delta \mathbf{P} = \mathbf{P} - \mathbf{P}^0 $$

(4.5)
and neglecting second and higher order derivatives of $K$ we obtain derivatives in matrix from as

$$A_{ij} = \frac{\partial K(f_i, P^0)}{\partial P_j} \quad i=1,2,...,M, \quad j=1,2,...,N. \quad (4.6)$$

Substituting equation (4.5) and (4.6) into equation (4.3) leads to

$$K(f, P) = K(f, P^0) + A \Delta P \quad (4.7)$$

where $K(f, P^0)$ are the estimated data values for $P^0$ which are the estimated parameter values for $P$, the so-called initial guess, and in Equation (4.7) the partial derivatives matrix, $A$ is obtained by the use of $P^0$. According to the Taylor’s theorem $\Delta P$ should be as small as possible, that is $P^0$ and $P$ should be close to each other. In practice, there is usually no available information about the real parameter values. In addition there will always be differences between $o_i$ and predicted $g_i$ due to observation errors (Marquardt, 1970; Menke, 1984). Because of the reasons stated above this discrepancy is called estimation error and during the inversion process one of the targets is to minimize that error which is given by

$$e_i = w_i \left( o(f_i) - K(f_i, P) \right) \quad i=1,2,...,M \quad (4.8)$$

here data weighting ($w_i$) is used for obtaining statically stable solution. Knowing that the observation errors represent the data quality the weighting makes sure that the solution yielded comes from well estimated data. However, there is no standard way of defining the weightings. By the use of observation errors, $\xi_i$ most common ways are $w_i = (1 + o_i/\xi_i)^{-1}$, $w_i = (\log (\xi_i))^{-1}$, $w_i = (\xi_i)^{-2}$ or simply $w_i = \xi_i^{-1}$. In this study, considering the fact that the high technology of the geophysical equipments which records the time series and the robust interpretation methods to calculate the impedances from the time series allow the researcher to deal small observation
errors, the first weighting calculation method is chosen and $W$ will represent the weightings, hereafter. Defining

$$\Delta O = O(f) - K(f,P)$$

(4.9)

substituting (4.7) and (4.9) into (4.8) we have that

$$e = W(\Delta O - A\Delta P).$$

(4.10)

In (4.10) the estimation error is controlled by the unknown quantities, $\Delta P$. Therefore, non-linear inversion, by means of minimizing the estimation error, determines the perturbation or update values for the each parameter rather than parameter itself. The obtained $\Delta P$ value is added to the initial parameters values in to obtain better parameter estimates, i.e.

$$P = P^0 + \Delta P$$

(4.11)

and this can be done in an iterative scheme. In practice this method is repeated until a satisfactory fit between observed and calculated data is obtained.

The minimization can be done in many ways depending on the nature of the problem. The main factor is the relation between the number of parameters, $N$ and the number of the data, $M$. Note that in the case of non-linear inverse problem the parameters sought are the updates, $\Delta P$. In the MT method, the data are generally collected in a large frequency range so that $M$ is usually higher than $N$. In this case the inverse problem is said to be overdetermined and has no exact solution, that is, no zero prediction error for any parameter set. Thus the sought approximate solution can be obtained by minimizing the sum of the errors at all the sampling frequencies. Nevertheless, because of various reasons, the MT data may not have enough information for some part of the parameter set for which the problem becomes ill-conditioned or is said to be under-determined and has infinite range of solutions that can satisfy the data. In general, the method requires more information than the data.
contain, in order to single out a possible parameter set. To be able to generalize the method both cases must be considered and the problem becomes mixed-determined in which a combination of the prediction error and the solution length for each parameter is minimized by the use of Lagrange multipliers (e.g. Menke, 1984)

$$\phi(\Delta P) = e^T e + \beta (\Delta P^T \Delta P + L^2)$$  \hspace{1cm} (4.12)

where $\beta$ is a Lagrange multiplier but will be called damping factor in the next section and $L$ is the bound on the energy of the parameter changes. Note that this process is equivalent to the regularization theory of Tikhonov (Tikhonov and Arsenin, 1977; Twomey, 1977; Tikhonov, 1963) and the above equation can be written as

$$\phi(\Delta P) = (\Delta O - A\Delta P)^T W^2 (\Delta O - A\Delta P) + \beta \Delta P^T \Delta P + \beta L^2$$  \hspace{1cm} (4.13)

or simply

$$\phi(\Delta P) = \Delta O^T W^2 \Delta O - \Delta O^T W^2 A\Delta P - \Delta P^T A^T W^2 \Delta O + \Delta P^T A^T W^2 A\Delta P + \beta \Delta P^T \Delta P + \beta L^2$$  \hspace{1cm} (4.14)

To minimize (4.14), we differentiate $\phi(\Delta P)$ with respect to $\Delta P^T$ and equate the result to zero, viz.:

$$\frac{\partial \phi(\Delta P)}{\partial \Delta P^T} = 0 = 2 A W^2 A^T \Delta P - 2 A^T W^2 \Delta O + 2\beta \Delta P$$  \hspace{1cm} (4.15)

or

$$(A^T W^2 A + \beta I) \Delta P = A^T W^2 \Delta O$$  \hspace{1cm} (4.16)$$
where $I$ is the identity matrix. This equation is called the normal equations. $(A^T W^2 A + \beta I)$ in the left-hand side of equation (4.16) is a square matrix and can be inverted. If we multiply both sides of equation (4.16) by $(A^T W^2 A + \beta I)^{-1}$ we obtain

$$\Delta P = (A^T W^2 A + \beta I)^{-1} A^T W^2 \Delta O.$$  (4.17)

This method is called the Weighted Marquardt (1963) -Levenberg (1944) inversion or weighted, damped least squares inversion method.

Fig.4.1. Behavior of the solutions on error contour (after Marquardt 1963). GN, ML and SD are Gauss-Newton, Marquardt -Levenberg and Steepest Descent methods, respectively.

In equation (4.18), $\beta$ is a positive value between zero and a large number (Marquardt, 1963). If $\beta$ is set to a large number, the solution is similar to the steepest descent method and converges slowly. If $\beta=0$ is selected the solution is equivalent to the Gauss-Newton Method and converges rapidly but it may not lead to a feasible solution. If $\beta$ is given a variable value between zero and one for each
iteration step the solution becomes stable and is the general approach of the Marquardt-Levenberg Method. The choice of $\beta$ is related to the convergence of the solution. The behavior of the solutions can be seen on the error contour map given in Fig. 4.1.

In the case involving complex quantities, the problem can be solved with a simple modification of the theory. The only necessary change is to replace the ordinary transpose with the complex conjugate transpose or Hermitian transpose (Menke, 1984). Then Equation (4.18) becomes

$$\Delta P = (A^H W^2 A + \beta I)^{-1} A^H W^2 \Delta O.$$  \hspace{1cm} (4.18)

Having obtained a general formula for the inversion, the next step should be to find an easy way to calculate the inverse of $(A^H W^2 A + \beta I)$. The typical solution methods are Gauss elimination, LU decomposition or complex singular value decomposition (CSVD). The selection of the method to adopt depends upon the general form of the matrix to be inverted. In this study the CSVD method will be used to calculate the inverse of $(A^H W^2 A + \beta I)$.

### 4.3 Complex Singular Value Decomposition and Matrix Inversion

The formulas given in this section for CSVD applications may be seen in many publications (e.g. Marple, 1987; Klema and Laub, 1980; Forsythe et al., 1977; Lawson and Hanson, 1974). All necessary proofs can also be found in these referred sources. Any non-rectangular complex matrix can easily be inverted by means of the CSVD technique in which the matrix can be factored into a product of three orthogonal matrices. Recalling that the Jacobian matrix, $A$, is a non-rectangular matrix then

$$A = U \Lambda V^H$$ \hspace{1cm} (4.19)
where for rank, $r$ of the system equation, $U$ is the $M \times r$ data space eigenvectors matrix, $V$ is the $r \times r$ parameter space eigenvectors and $\Lambda$ is an $r \times r$ diagonal matrix containing non-zero eigenvalues of $A$. Both $U$ and $V$ are complex while $\Lambda$ is real. The diagonal elements of $\Lambda$ are called the singular values of $A$. Noting that due to orthogonality of $U$ and $V$, $U U^H = V^H V = I$, then the Hermitian transpose and inverse of $A$ are

$$A^H = V \Lambda U^H$$  \hspace{1cm} (4.20)

and

$$A^{-1} = V \Lambda^{-1} U^H.$$  \hspace{1cm} (4.21)

Following Jackson (1972), in Equation (4.18) we may redefine

$$A' = WA$$ \hspace{1cm} (4.22a)

and

$$\Delta O' = W \Delta O$$ \hspace{1cm} (4.22b)

and using (4.20) and (4.21) for $A'$ we obtain (4.18) as

$$\Delta P = (V \Lambda^2 V^H + \beta I)^{-1} V \Lambda U^H \Delta O'$$ \hspace{1cm} (4.23)

or

$$\Delta P = (V (\Lambda^2 + \beta I) V^H)^{-1} V \Lambda U^H \Delta O'.$$ \hspace{1cm} (4.24)

Using orthogonality of $U$ and $V$ and
we have

$$\Delta \mathbf{P} = \mathbf{V} \text{diag}[\lambda_i/(\lambda_i^2 + \beta)] \mathbf{U}^H \Delta \mathbf{O}' .$$  \hspace{1cm} (4.26)

In the last equation, the inverted quantities are non zero so that we have a stable inversion process.

### 4.4 The Evaluation Of The Solution

The inversion may generally be summarized as the finding of $\mathbf{A}^{-1}$ which satisfies the relations between the parameter vector, $\mathbf{P}$ and the vector observation of data, $\mathbf{O}$ in the case of linear inversion. For the sake of simplicity consider linear inversion. Recall that we could only obtain the pseudo inverse (or the Lanczos inverse), $\mathbf{A}_L$ of $\mathbf{A}$ because $\mathbf{A}$ is usually not a square ($m \neq n$) matrix in geophysics applications. After the solution, we obtain estimates of the subsurface parameters, $\mathbf{P}_e$. Equation (4.18) may be re-written for linear case as

$$\mathbf{P}_e = \mathbf{A}_L^{-1} \mathbf{O}$$  \hspace{1cm} (4.27)

this model gives estimated data $\mathbf{K}_e$ and equation (4.27) becomes

$$\mathbf{K}_e = \mathbf{A} \mathbf{P}_e .$$  \hspace{1cm} (4.28)
Substituting (4.27) into (4.28) yields

\[ K_e = A A_L^{-1} O \] (4.29)

and we assume that \( O \equiv K_e \) within acceptable error bounds. From equation (4.29), we can write

\[ A A_L^{-1} = I_K. \] (4.30)

The elements of \( I_K \) give measurement of the data resolution obtained from the inversion. If diagonal elements of \( I_K \) are close to unity the resolution is good. If they are far from unity it means that we could not obtain good enough resolution. We may use a similar approach for the model parameters. If we assume that \( P_e \equiv P \) we may write

\[ P = A_L^{-1} K_e. \] (4.31)

Substituting (4.28) into (4.31) we obtain

\[ P = A_L^{-1} A P_e \] (4.32)

or

\[ I_P = A_L^{-1} A. \] (4.33)

In the last equation, \( A_L^{-1} A \) should be an identity matrix to obtain good resolution for the parameters. \( I_K \) and \( I_P \) are called the information density matrix and the parameter resolution matrix (Jackson, 1972; Wiggins, 1972), respectively. The elements of \( I_P \) give a measure of the closeness of the calculated parameters to the
true parameters. The measure of correlation between parameters is given by the correlation matrix which is an indication of the linear dependence between parameters. The elements of the correlation matrix are given by

\[ [\text{Cor}(p)]_{ij} = [\text{Cov}(p)]_{ij} / \{ [\text{Cov}(p)]_{ii} [\text{Cov}(p)]_{jj} \}^{1/2} \quad i=1,2,\ldots,N, \quad j=1,2,\ldots,N \quad (4.34) \]

where

\[ \text{Cov}(p) = \sigma^2 (A^T A)^{-1} \quad (4.35) \]

and \( \sigma^2 \) is called the variance of the data. \( \text{Cov}(p) \) is a parameter-by-parameter matrix whose \( i \)th diagonal element is the statistical variance of the \( i \)th parameter \( p_i \) and whose off-diagonal elements, the covariance, indicate the correlation between the model parameters. The square roots of the diagonal elements \( \text{Cov}(p) \) are generally referred to as the standard deviations of the least squares parameter estimates and may be used to estimate the bounds of the model parameters (Inman, 1975; Meju, 1994). Having looked at the \( \text{Cov}(p) \) matrix, let us try to see what \( \text{Cor}(p) \) matrix represents. If the value of \( [\text{Cor}(p)]_{jj} \) is near unity, then the parameters \( p_i \) and \( p_j \) are strongly correlated and nearly linearly dependent (Inman, 1975). If the value is close to positive unity a constant quantity for difference between \( p_i \) and \( p_j \) can be obtained. On the other hand, if the value is close to negative unity a constant for sum of \( p_i \) and \( p_j \) can be obtained. If we consider the damped least squares solution, the resolution matrix will not be an identity matrix (e.g. Meju, 1994). We will obtain a bell-curve on its line which has a maximum value at the diagonal of the Resolution matrix (Wiggins, 1972). Note that if SVD components are used \( I_K \) and \( I_p \) are given by \( U^T U \) and \( VV^T \) and are obtained as unity matrix due to their orthogonality and the theory of the SVD technique. For the damped nonlinear solution in the complex domain, the parameter resolution matrix is given by

\[ I_{cp} = (A^H W^2 A + \beta I)^{-1} A^H W^2 A \neq I \quad (4.36) \]
where all parameters are as defined previously. The covariance matrix is then rewritten as

\[
\text{Cov}(p) = (A^H W^2 A)^{-1}.
\]  

(4.37)

One of the most popular topics in inversion is the calculation of parameter bounds. Among the proposed methods the use of most squares techniques (e.g. Meju, 1994) and the covariance matrix (e.g. Inman, 1975) are the common ones. Meju (1994) gives all details of the methods and defines most squares as to extremise the objective function \(P^T b\) subject to the constraint that the residuals \(CHI\) are not greater than some threshold value \(CHI_T\), where \(b\) is the parameter projection vector and \(CHI\) if of optimal least squares solution. Then the solution is given as

\[
\Delta P = (A^H W^2 A + \beta I)^{-1} (A^H W^2 \Delta O + \mu b)
\]

(4.38)

where \(\mu\) is Lagrange multiplier and calculated via

\[
\mu^2 = \pm (CHI_T - CHI_{LS})/( b^T [A^H W^2 A + \beta I]^{-1} b)
\]

(4.39)

\(CHI_T\) usually is set to the number of data or obtained by multiplying the \(CHI\) by a small threshold value such as 1.1 or 1.2. \(b\) is a vector such as \(b = [1,0,0,...,1]^T\) and the 1s show which parameters’ bounds will be obtained.
5. MAGNETOTELLURIC INVERSION IN COMPLEX DOMAIN

5.1. Introduction

As is shown in the previous chapter, the traditional damped least squares inversion method can be performed in the complex domain. In other words, the Jacobian matrix and its inversion involve complex domain calculations. Thus, the updates calculated by using Equation (4.26) are complex. By virtue of the assumption given in Chapter 2 (Equation (2.12)) imaginary parts of the resistivities and updates are ignored and hence real parts of the updates are added up to initial guess values. In this chapter the necessary formulae and algorithms for the 1D and 2D applications will be presented. The source codes of the developed programs are in the attached diskette accompanying this thesis. In the next section the formulae for 1D inversion are given only for the sake of completeness and to define the general calculation procedure for the more interesting 2D inversion in a simple way. Consequently, the results of the 1D modeling will not be analyzed in detail in this study and only simple demonstrative application is presented in Appendix B.

5.2 One Dimensional Magnetotelluric Inversion

Equation (4.26) is the general formula for the inversion process. The first step in the procedure is to construct the appropriate Jacobian matrix, A. The derivatives for each frequency with respect to linear parameters can be obtained via derivatives of nonlinear parameters,

\[ \frac{\partial Y_j}{\partial \log \rho_j} = \rho_j \frac{\partial Y_j}{\partial \rho_j} \]  \hspace{1cm} (5.1)

and
\[ \frac{\partial Y_j}{\partial \log t_j} = t_j \frac{\partial Y_j}{\partial t_j}. \tag{5.2} \]

Equations (5.1) and (5.2) may be thought as a single step calculation to obtain the partial derivatives for the joint inversion of apparent resistivity and phase of impedance. We now require the relevant partial derivatives calculated by means of chain rules, viz.:

\[ \frac{\partial Y_1}{\partial X_j} = \frac{\partial Y_1}{\partial Y_2} \frac{\partial Y_2}{\partial Y_3} \ldots \frac{\partial Y_{j-1}}{\partial Y_j} \frac{\partial Y_j}{\partial X_j} \tag{5.3} \]

where \( X_j \) represents the model parameters \( (P_j = (p_j)^{1/2} \text{ and } t_j) \). The terms in the above equations are given by

\[ \frac{\partial Y_j}{\partial Y_{j+1}} = \text{sech}^2 \left( \frac{u t_j}{P_j} + \tanh^{-1} \left( \frac{Y_{j+1}}{P_j} \right) \right) / (1- \left( \frac{Y_{j+1}}{P_j} \right)^2), \tag{5.4} \]

\[ \frac{\partial Y_j}{\partial P_j} = \frac{(Y_j / P_j) - \text{sech}^2 \left( \frac{u t_j}{P_j} + \tanh^{-1} \left( \frac{Y_{j+1}}{P_j} \right) \right) \left( \frac{u t_j}{P_j} + \frac{Y_{j+1}}{P_j} \right)}{1- \left( \frac{Y_{j+1}}{P_j} \right)^2} \tag{5.5} \]

and

\[ \frac{\partial Y_j}{\partial t_j} = u \text{sech}^2 \left( \frac{u t_j}{P_j} + \tanh^{-1} \left( \frac{Y_{j+1}}{P_j} \right) \right). \tag{5.6} \]

where \( \tanh \) and \( \text{sech} \) indicate hyperbolic tangent and secant functions, respectively. These derivatives are placed in appropriate positions in the Jacobian matrix, i.e.

\[
A = \begin{bmatrix}
\frac{\partial Y(f_1)}{\partial P_1} & \ldots & \frac{\partial Y(f_1)}{\partial P_L} & \frac{\partial Y(f_1)}{\partial t_1} & \ldots & \frac{\partial Y(f_1)}{\partial t_{L-1}} \\
\frac{\partial Y(f_2)}{\partial P_1} & \ldots & \frac{\partial Y(f_2)}{\partial P_L} & \frac{\partial Y(f_2)}{\partial t_1} & \ldots & \frac{\partial Y(f_2)}{\partial t_{L-1}} \\
\vdots \\
\frac{\partial Y(f_M)}{\partial P_1} & \ldots & \frac{\partial Y(f_M)}{\partial P_L} & \frac{\partial Y(f_M)}{\partial t_1} & \ldots & \frac{\partial Y(f_M)}{\partial t_{L-1}} 
end{bmatrix} \tag{5.7}
\]

where \( L \) is the number of layers including the basement.
Once the Jacobian matrix is obtained, the complex U, V and real A matrixes are calculated using complex singular value decomposition theory. Using the non-zero singular values, a set of damping factors is determined. The complex damping factors are of the form

\[ \beta^* = \beta + i\beta \]  \hspace{1cm} (5.8)

but the damping factor can also be real valued as in conventional schemes. In each iteration step, using Equation (4.26), a group of the updates and relevant updated parameters associated with the set of the damping factors are obtained. The best solution among them is selected by using the convergence criteria which is gauged using the measure

\[ \text{CHI}^2 = \frac{1}{2M} \left( Y^o - Y^c \right)^H W^2 \left( Y^o - Y^c \right) \]  \hspace{1cm} (5.9)

where the superscripts o and c denote observed and calculated data respectively. As were defined before Y is the non-logarithmic FNI data and W weights calculated from observational errors. Remember that because of nonlinearity and noise, exact solution (CHI=0) is not possible (Parker, 1984, 1994). During the inversion process, smallest achievable CHI is searched. CHI value generally decreased with each iteration. When a solution is found CHI values between successive iterations become close each other. The fractional decrease, DCHI of the CHI values in successive iterations prevent unnecessary iteration stopping the inversion process.

A 1D inversion program has been developed in FORTRAN language in order to test this method. The flowchart is similar to the one given in Fig. 6.1. The program employs a complex singular value decomposition subroutine, (CSVD, Marple, 1987). The attached floppy diskette contains a source code and test data for the 1D inversion. The programs require observed data, initial parameters and maximum iteration number as input and give updated parameters, CHI and DCHI.
values for all iterations and U, singular values, V and correlation matrix for the last iteration as the output. The program stops when either any of CHI or DCHI reaches predefined limiting value (e.g. $10^{-5}$) or the number of iterations exceeds a predefined value (maximum iteration number). As was stated in introduction 1D modeling will not be analyzed in this study. However, to show the performance of the proposed method, one example of 1D inversion using synthetic data and the inversion results of different methods are given in Appendix B.

5.3 Two Dimensional Magnetotelluric Inversion

In layered-earth inversion, we simply determine the change of resistivity versus depth. Two-dimensional inversion is a much more difficult problem. It is assumed that within a known resistivity structure there is embedded one or more unknown, laterally non-uniform, anomalous domains with constant cross-sections in the y-direction, and of limited extent both in the other horizontal direction and in depth (x-and z-direction, respectively). As is described in Chapter 3, the response of a 2D structure can be calculated via numerical solution using FE method. Basically the relevant equation is

$$Gf = s$$

(5.10)

where $G$ and $s$ are the appropriate Helmholtz operator and source while $f$ is the unknown field ($E_y$ or $H_y$) parallel to strike. The field is computed for each sub-domain.

In practical implementations, it may be useful to choose grid-like blocks corresponding to some subdomains and assume that resistivity is constant in each block which incorporates geoelectric bodies (e.g. Jupp and Vozoff, 1977). Then, in 2D inversion, the block resistivities, $\rho_{ij}$ become the parameters. The Jacobian matrix, $A$ is built up using the derivatives of the fields considered with respect to
the model parameters. Rodi (1976) developed a novel approach for calculating partial derivatives, viz.:

\[ \frac{\partial f}{\partial \rho_{ij}} + \frac{\partial G}{\partial \rho_{ij}} f = 0 \]  

(5.11)

or

\[ \frac{\partial f}{\partial \rho_{ij}} = - \frac{\partial G}{\partial \rho_{ij}} f \]  

(5.12)

where the matrix, \( G \) is already known and the source, \( s \) is assumed to be independent of model parameters. The right hand side of the equation is a column vector and includes new source values. The derivative of \( G \) is calculated numerically. If the matrix decomposition is used for \( G \) the solution of (5.12) can be obtained through a simple process.

Recall that Equation (3.16) and so (5.11) is for the secondary field so that Equation (5.12) would give derivatives with respect to secondary field. Equation (3.15) is also equivalent to Equation (3.16), and so,

\[ G f_s = -(G_p - G)f_p \]  

(5.13)

and

\[ G f_s + G f_p = G_p f_p \]  

(5.14)

From Equation (3.13) it can be seen that the right hand side of the last equation is the source term and is independent of model parameters. Now, the derivatives can be written in terms of primary and secondary fields,

\[ \frac{\partial (f_s + f_p)}{\partial \rho_{ij}} = \frac{\partial G}{\partial \rho_{ij}} (f_s + f_p) \]  

(5.15)
The solution to Equation (5.15) gives derivatives for only one field, either $E_y$ or $H_y$, the other necessary field is calculated by using Maxwell’s equations.

The interpretative ERF used in this study is the FNI function. In early stage of this research, test studies with 2D inversion showed that to employ linear FNI function in inversion is reduce the speed of convergence for the models with large resistivity contrast. The logarithm of complex FNI function is

$$\log Y = (Y_1^2 + Y_2^2)^{1/2} + i \tan^{-1}(Y_1/Y_R) \quad (5.16a)$$

or by virtue of Equation (2.25) and (2.26)

$$\log Y = (\rho_a)^{1/2} + i (\Phi_z - \pi/4) \quad (5.16b)$$

which equivalent to the logarithm of square root of Cagniard apparent resistivity and 45° shifted phase of impedance, and its derivatives are simply

$$\frac{\partial \log Y}{\partial \log \rho_{ij}} = \frac{\partial Y}{\partial \rho_{ij}} \frac{\partial \rho_{ij}}{\partial \rho_{ij}} = \frac{\partial \rho_{ij}}{\partial \rho_{ij}} \frac{\partial Z}{\partial \rho_{ij}} \quad (5.17)$$

and

$$\frac{\partial Z}{\partial \rho_{ij}} = \left( \frac{\partial E}{\partial \rho_{ij}} - Z \frac{\partial H}{\partial \rho_{ij}} / H \right). \quad (5.18)$$

where $Z$ and $Y$ represent surface values of the Cagniard type impedance and FNI, respectively. $E$ and $H$ orthogonal fields for TE or TM mode calculations.

To facilitate comparisons of results in the next sections, the derivatives of the classic ERF Cagniard and phase of impedance are computed in this study as follows

$$\frac{\partial \log \rho_a}{\partial \log \rho_{ij}} = \frac{\partial \rho_{ij}}{\partial \rho_{ij}} \frac{\partial \rho_a}{\partial \rho_{ij}}$$

$$= \frac{\rho_{ij} / \rho_a}{2 / \omega \mu} \Re \left( \frac{\partial Z}{\partial \rho_{ij}} Z^* \right) \quad (5.19)$$
and

\[
\frac{\partial \tan \Phi_Z}{\partial \log \rho_{ij}} = \rho_{ij} \frac{\partial \tan \Phi_Z}{\partial \rho_{ij}} = \rho_{ij} [\text{Im}(\partial Z / \partial \rho_{ij}) - \tan \Phi_Z \text{Re}(\partial Z / \partial \rho_{ij})] / \text{Re}(Z) \quad (5.20)
\]

where star indicates the complex conjugate. The entire calculation is repeated for each parameter, filling in an appropriate column of the Jacobian matrix at a time. Once the Jacobian matrix is obtained, the rest of the inversion process is similar to the method described previously in the 1D case. Note that the convergence criteria (Equation (5.9)) in 2D case is calculated using logarithm of the ERF selected for inversion.
6. PROGRAM DEVELOPMENT AND TESTING

6.1 Introduction

By the use of the formulae and definitions for the 2D inversion highlighted in previous chapters, an inversion program based on the finite element technique has been developed. As was stated before, only the 2D program and interpretation will be presented in this study even though 1D work was also done. Consequently, for the inversion process, the term "parameter" represents the block resistivities unless otherwise stated.

6.2 Implementation of Two-Dimensional Inversion Algorithms

A FORTRAN code (mt2dinv) for the interpretation of 2D MT data has been developed (Fig. 6.1). The main components of the program are as follows: the subroutine PW2D (Rijo, 1977; Wannamaker et al., 1985) is used for the forward solution, the JACOBI subroutine modified from deGroot-Hedlin and Constable (1990) is used for the Jacobian matrix calculations and the CSVD subroutine (Marple, 1987) for the calculation of the complex singular values. In order to handle different ERF (MT data), various input and output subroutines have been added in due course.

In addition to complex domain calculation, the conventional type inversion option in which imaginary part of the Jacobian matrix is used as a tag on to the real part and parameter updates are calculated in the real domain is available.

Some necessary internal parameters such as the maximum number of the iterations, minimum misfit criteria, application and formulation of the type of damping are given in an initialization file and at the beginning of the program any of them, if necessary, may be changed.

Damping factor $\beta$ which may be determined either in real or complex form as in the 1D inversion scheme (Equation (5.9)), can be calculated from three different formulations depending on the data and initial geoelectric model. In each step of the run, help options give the necessary explanations about input prompts (Fig. 6.2).
Fig. 6.1 Flowchart of the program.
The program has three main features. The first feature is the forward calculation which requires a geoelectric model, the sounding locations and the frequencies for ERF from user. The frequencies and selected ERF type for each station will be in the output file. The second option is automatic inversion in which the necessary frequencies are read from the observed data file. All distinct frequencies and a given initial model are used in the inversion process. If any station contains two or more repeat frequencies, the program will use the last sample for this frequency in the modeling process and the output. The last facility is the interactive forward modeling and data comparison. All the necessary frequencies are obtained from observed data file as in the inversion process.

When the program is executed, some information about the storage parameters, maximum size of model, maximum number of frequencies and resistivities and some internal parameters are displayed (see Fig. 6.2). Then the program prompts the user for output header information. If “s” is typed in as input a set-up menu for the internal parameters appears. The next prompt is for the selection of Inversion, Forward or Comparison option. For the inversion and comparison options, the ERF type which are either FNI or only Cagniard apparent resistivity or Cagniard apparent resistivity and Phase or only phase is chosen by the user. This selection is just for the inversion process and, at this stage, there is no dependency to the ERF type of the observed data. Following this definition, the parameter update calculation in either real or complex domain is chosen by the user. The MT mode is about the MT data mode and options are E for TE, M for TM and B for both mode calculations. The initial geoelectrical model (fig 6.3), description of which is given in section 6.3, output file name and the observed data file names are also expected. All observed data from each sounding points are placed in the data file in the order of the sounding points given in the initial geoelectric model. In the case of the joint inversion of TE and TM mode data, first all TE mode and then all TM mode observed data will be located in the same file. It is not necessary to have either common or ordered frequencies for any inversion mode. Sample prompts and necessary inputs are given in Fig. 6.2.

During inversion the actual parameters, calculated parameters and misfit values are displayed for each iteration. The calculated block resistivities with their initial values and the observed and calculated data with misfit information for each sounding points are given in the output file for the inversion and interactive forward comparison modes.
The Program

Chapter 6

sun2.geol:/home/euul> mt2dinv
2 D
\[ M T \]
\[ \text{INV. PROG} \]

MAX. NUMBER FOR;
HORIZONTAL CELLS ; 200
VERTICAL CELLS ; 200
FREQUENCIES (SINGLE MOD); 100
STATIONS (SINGLE MOD); 100
RESISTIVITIES ; 62

DEFAULT PROGRAM PARAMETERS;
SSQST,FSSQST,FSSQ,NSET,ITRS,P MAX KDUM,NSCAL
1.00000E-05 1.00000E-05 0.500000 1 10 3.00000 1 0
DAMP. TYPE R

ENTER SITE TITLE (20A1) OR (S)ETUP DEFAULTS: > test_01

(INVERSION (F)ORWARD (C)OMPAR. OR (H)ELP> i
INVERSION (AND OUTPUT) FUNCTION TYPE >
  FNI..............1
  CAG............2
  CAG+PH.....3
  PH............4
  OUT...........5

1

DP CALCULATIONS IN (R)EAL (C)OMPLEX DOMAIN OR (H)ELP > c
T(E) OR T(M) OR (B)OTH MODE DATA > b

ENTER MODEL-INPUT FILENAME [A20] OR (H)ELP > picos.mod
ENTER OUTPUT-1 FILENAME [A20]: > picos.out

FILE NAME FOR FIELD DATA
FILE FORMAT IS
FREQ, REAL, ER_R, IMAG, ER_I
OR
FREQ, APP.RES, ER_R, PHASE, ER_P

ACCEPTABLE DATA TYPES ARE,
F : FOR FNI DATA
Z : FOR CAGNIARD IMP. DATA
C : FOR CAGNIARD APP. AND PHASE (D)
R : FOR CAGNIARD APP. AND PHASE (R)
M : FOR CSAMT DATA, SAME AS R,(APP TO BE DIVIDED BY 4.)

DATA TYPE MUST BE THE FIRST CHARACTER IN THE
DATA FILE
IT IS ASSUMED THAT ORDER OF DATA IS THE
SAME AS THE ORDER OF THE SOUNDING POINTS
IN THE BOTTOM LINE OF THE INITIAL MODEL
> ?
picosxy.all

Fig. 6.2 Example run for the program. Lower case letters are input (See text for the explanation)
The data space eigenvectors (U), parameter space eigenvectors (V), the singular values of the problem and the parameter correlation matrix are also presented in the same file for only inversion mode. The program also produces a plot file, named plot.inv, in which frequencies, observed data and calculated data for optimal model are given for each station.

6.3. Mesh Design

In order to obtain meaningful numerical solutions to the 2D problem, it is vital to have a good mesh design. The design of a mesh for the geoelectric model for the FEM is a time consuming process, thus, an input model similar to one for the FDM is used in this program (Fig. 6.3). This input is automatically converted to the FEM mesh system and the surface topography, if available, is also smoothed by the program itself. The general rules of the mesh design based on a unit of distance, the skin depth (d), are given as follows (Wannamaker et al, 1985).

1. Element dimensions should not change from one element to the next by more than a factor of 3 to 5.
2. In the vicinity of a change in conductivity of the medium the element dimensions should be approximately d/4 in the medium where the element resides.
3. No single resistivity medium should be less than 3 elements wide or 2 elements thick to fit galvanic components of the field variations.
4. 2 to 3d away from any variation in conductivity the element dimensions may be increased to the order of d of the medium.
5. Vertical element dimensions may be increased approximately exponentially (10,30,100,...) downward from the air-earth interface because of the exponential decay of the fields. The maximum vertical dimensions of an element in the earth should be held 1 to 2d however.
6. The air layer for the TE problem should consist of 7 to 10 element rows increasing exponentially in vertical dimension from the air-earth interface,
7. Vertical mesh boundaries should ideally extend 3 to 6 skin depths away from the nearest 2D structure or 4 to 8 times the height of the inhomogenous structure away.
Fig. 6.3 Sample mesh design (see text for explanations)
8. The bottom mesh boundary should be 3 to 6 skin depths of the background conductivity from the air-earth interface or 4 to 8 times the width of the inhomogenous structure away.

Sample mesh is showed in Fig. 6.3. In the first line, \( N_z \) is the number of the block in the vertical direction while \( N_x \) is for the horizontal direction. \( N_r \) represents the number of the resistivity blocks which construct the geoelectric model including air layer. \( N_a \) is number of the air layer above the surface or the datum level for undulating surface. \( I_r \) controls the fixing option. If it is 0 then the third line in the Fig. 6.3 will be removed and none of the parameter will be fixed during the inversion process. If it is 1 then 0's and 1's in the third line represent fixed and free parameters respectively in the inversion process and must be given in the same order of resistivities (second line of Fig 6.3). The last number of the first line, \( I_o \) is either 0 or 1 which is for displaying the FEM mesh and Jacobian matrix for each iteration. This information is followed by \( N_x \) value for the widths of the blocks. Thickness' are given with the model using the first 10 numerical digits. Alpha-numeric characters, capital and lower cases, represent resistivity blocks. The last two lines in the Fig. 6.3 are number of the stations and their locations in the horizontal direction along the ground surface.

6.4. Application to Synthetic Data

Our first test model is a simple dike of 1 ohm-m embedded in a host medium of 100 ohm-m resistivity. The dike is 500m wide and 1000m thick and is placed 125 m below a flat surface. Observable FNI data are calculated at six sounding points for 12 frequencies between 8192 and 4 Hz as in the ordinary CSAMT (controlled source audio frequency magnetotelluric) experiments. In Fig. 6.4, \( \rho_5 \) represent the dike and \( S_N \) are measurement points. Sample curves show the real (triangular symbol) and the imaginary (box symbol) components of the FNI responses for TE and TM modes of optimal model. Note that the real part of the FNI has the same features as apparent resistivity while the imaginary part represents phase information. As can be seen in Fig 6.4 the data of \( S_N \) 3 have no information about the zone beneath the conductive dike due to the use of high frequencies and this will affect the resolution of this part of the model.
For simple interpretation of the results obtained from the inversion, an initial geoelectric model consisting of 9 blocks each of 50 ohm-m has been chosen (Fig. 6.4). The inversion process has been performed on FNI type data with a maximum limit of 10 iterations and using real type damping factor. For simplicity, the weighting matrix, \( W \) was taken as an identity matrix, \( I \). Fig 6.5 gives part of the output which shows that all but parameter eight have been resolved and the log misfit for this model is 7.12733E-04. The Rightmost two columns are the upper and lower bounds for each parameter. No specific calculation is conducted for these values. Recall that the most squares method requires more iterations in order to find the bounds. In 2D interpretation this is too time consuming.

Fig.6.4. Simple dike model and FNI response for the observable data at the sounding points for 2 and 3. Triangular and squares represent the real and imaginary component of the FNI, respectively. In the model \( \rho_1, \rho_2, \rho_3, \rho_4, \rho_6, \rho_7, \rho_8 \) and \( \rho_9 \) are 100 ohm-m while \( \rho_5 \) is 1 ohm-m.
process to perform. By the use of covariance matrix, the parameter bounds may be obtained but in the case of irrelevant parameter the resulting unrealistic bounds may mislead the interpreter. Meju (private comm., 1997) suggested a non iterative most squares method in which the parameter bounds are obtained from the Jacobian matrix calculated in the last successful iteration. In this present test study, a much simpler method was applied. With the assumption that model parameters usually oscillate when their solutions are close to the real values, their possible values are simply selected during the inversion process according to pre-estimated threshold misfit values. In the program they may also help the user to decide if the model needs more iteration. The recommended process is to invert the model until the upper and lower bounds for all or most of the parameters become different from their calculated values. As an example in Fig. 6.5 none

**LAST MODEL**

<table>
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<th>CODE</th>
<th>FIX(0)</th>
<th>INT. RES</th>
<th>LAST RES.</th>
<th>BOUND.S</th>
</tr>
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<td>50.000</td>
<td>99.996</td>
<td>99.996</td>
</tr>
<tr>
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<td>1</td>
<td>50.000</td>
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</tr>
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<tr>
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</tr>
<tr>
<td>9</td>
<td>1</td>
<td>50.000</td>
<td>106.38</td>
<td>105.57</td>
</tr>
</tbody>
</table>

LOG SSQ FOR INIT. GUESS : 0.331955
LOG SSQ FOR LAST MODEL: 7.12733E-04
FSSQ IN LAST ITR. 2.06145E-02
MODE 1
NO. OF ITER. 10
DAMPING FACTOR CODE 1

Fig. 6.5. The result of the 2D inversion for the dike model.
of the parameters fit this description thus the model could have been inverted more for better resolution.

The interpretation of the complex form of the $V$ matrix from the CSVD given in Fig. 6.6 is similar to the real one. That the resistivities of the top three blocks have been well resolved is indicated by the high values in the first three columns of the $V$ matrix affiliated with the larger singular values. The last singular value is relatively small and this suggests that one parameter has not been resolved or is irrelevant (Jupp and Vozoff, 1975). This is the resistivity of the eighth block which appears as a high value ($0.699, 0.709$) in the last column of the $V$ associated with the smallest singular value. The correlation matrix points out the high correlation between the last three parameters (showed as bold). If any of them has not been resolved this would affect the resolution of the others. This fact is important when interpreting noisy data.

In Fig 6.7 the convergence rate of the method is given, the misfit is plotted without being normalized by the number of the data. Notice that 4 iterations could have been enough for obtaining a similar solution.
PARAMETER EIGENVECTORS:

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| 5   | 0.054| 0.037| 0.000| 0.000| 0.000| 0.000| -0.013| -0.155| -0.968| 0.182| 0.000| 0.000| -0.008| 0.012| -0.002| 0.002
| 6   | 0.031| 0.184| 0.022| 0.215| 0.162| 0.122| 0.069| -0.659| -0.126| -0.619| 0.120| 0.000| 0.034| 0.104| 0.027| 0.106| 0.000| -0.011|
| 7   | -0.018| -0.007| 0.017| -0.003| -0.003| 0.020| -0.101| 0.042| 0.105| -0.025| 0.006| 0.11| -0.579| 0.390| 0.667| -0.196| -0.056| -0.038|
| 8   | -0.002| -0.001| 0.000| 0.000| 0.000| 0.002| 0.000| 0.000| 0.014| -0.001| 0.000| 0.001| 0.000| 0.000| 0.095| -0.009| 0.699| 0.709|
| 9   | -0.018| -0.007| 0.017| 0.003| -0.003| 0.020| 0.101| -0.042| 0.105| -0.025| -0.006| 0.011| 0.579| -0.391| 0.667| -0.197| -0.056| -0.038|

PARAMETER EIGENVALUES:

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Fig. 6.6. Complex form of parameter eigenvalues, eigenvectors and correlation matrix for the inversion of the dike model. Column and row indexes are represent parameters. In each column the values on the right hand side are real component while those on the left hand side are imaginary. Bold numbers in correlation matrix presents the high level correlation between parameters 7,8 and 9.
The second synthetic model selected to test the program is showed in Figure 6.8. The model simulates a simple geoelectric setting of a basin model which consists of a low resistivity (10 ohm-m) confining layer overlying a faulted moderately resistive sediment dry formation of 80 ohm-m. Besides a fault zone of 20 ohm-m, the model contains a low resistivity (5 ohm-m) block over another very highly resistive (10000 ohm-m) block embedded in the sediment. The geological equivalent of these low and high local resistivity structures may be a contaminant plume sourced by desolving gypsum, in an unsaturated aquifer. The whole structure is underlain by a crystalline basement of 1000 ohm-m. An unconformity surface of the basement and a possible paleo weathering zone are simulated by a thin layer of 30 ohm-m.

FNI data are calculated at nine sounding points placed with a spacing of 4 km for 17 frequencies between 8192 and 0.125 Hz. In Figs. 6.9 and 6.10 the pseudo sections show the real and the imaginary components of the FNI responses for TE and TM modes, respectively.
Fig. 6.8 Test model 2: Basin model. Depths are in meters while horizontal distances are in km. Unconformity surface is underlain by 30 meter thick ancient weathered zone.
Fig. 6.9 2D section for the second model. Real (a) and imaginary (b) component of the FNI for TE mode. Horizontal axis distance in Km
The inversion method was tested to see whether it can recover the anomalous bodies starting from a homogeneous half space model. In order to decide the size and thickness of the blocks the following method was applied. The imaginary components of the FNI type data may be used to design the initial guess model. Depending on the resistivity contrasts between the units the zero contours delineate the boundaries. Lack of sufficient contrast results in turning points in the curves. Initially, 5 levels were defined from the pseudo sections and 2 more levels were added to increase the resolution. Sounding points are centered on the separate blocks. The block boundaries in the test model and boundaries of the anomalous regions in the optimum model do not match each other. This disagreement is meant to be the estimation error of the boundaries. The last model which consists of 59 blocks of 50 ohm-m were inverted using both mode MT data. The weighting matrix, W was taken as an identity matrix, I for this test. The program was run for the joint inversion of both modes with a maximum limit of 10 iterations. The geoelectric section obtained from the inversion after 10 iterations is shown in Fig. 6.11. The misfit was reduced from 0.54887 to 0.2446 E-02. In the figure the contours are for 20, 100, 900 ohm-m. The result shows a top confining layer associated with a resistivity in the range of 9.9 - 12.7 ohm-m, the fault zone of 17 - 46 ohm-m, the plume with 8 ohm-m and the crystalline basement characterized by over 900 ohm-m resistivities. On the contrary, the high resistive region under the very conductive plume and thin unconformity layer over the basement were not delineated. The host resistivity around and between the conductive blocks (fault and the plume) near the basement was found higher resistivity (111 - 213 ohm-m) than its real value. The shallow part of the host varies between 55 - 71 ohm-m.

Two other different cases were also investigated but only one type result has been presented here. First one is the mode mixing test in which some of the station TE and TM mode data are switched for lower and higher frequencies and the mixed data are inverted. In real field procedure, the data are usually collected in the NS and EW directions and the true strike may be unknown. As a result, some stations along the profile will be affected by mode mixing (Groom and Bailey, 1989). Although the rotation may help to separate the two MT modes, over 3D complex settings the problem of mode mixing is a difficult to resolve. Using the conventional method
Fig. 6.10 2D section for the second model. Real (a) and imaginary (b) component of the FNI for TM mode. Horizontal axis distance in Km.
involving the inversion of Cagniard apparent resistivity and Phase of impedance, the solution converged very slowly. However, The FNI based method proposed here converged more quickly. The reason for this may be either the function type because the proposed method involves two-stage linearization or the damping factor selection strategy may be more powerful. Recall that although both program used same formula for damping factors calculation. The effect of small or large factor in the update calculation is different.

Fig 6.11 The result of the 2D inversion to basin model. Arrows indicated position of the stations. Calculated block resistivities are given in the center of each block. Contours are 20, 100 and 900 Ohm-m.
7. APPLICATION TO FIELD DATA FROM PARNAIBA BASIN

7.1. Introduction

The Parnaiba Basin in north eastern Brazil (Fig. 7.1) is ellipsoidal in shape and covers an area of approximately 600,000 km² (Almeida et al., 1981). Until recently, there has been no major geophysical effort to examine either the deep structure or the localized features of the basin. Previous work has been of regional scale and most of the major faults and lineaments seen in the recent geological maps have been located using aerial photographs and aeromagnetic studies (Fig. 7.3). However, the existence of some of these inferred structures (e.g. Picos fault) need to be verified on the ground. The necessity for intensive local scale ground follow-up studies is therefore obvious. During the last two decades governmental agencies and some research institutes, one of which is National Observatory in Rio de Janeiro, have conducted some seismic, electromagnetic (EM) and electric regional surveys in parts of the basin (e.g. Cunha 1986; Goes et al., 1993; Arora et al., 1997; Meju et al., 1997).

A major project was jointly undertaken by the National Observatory in Rio de Janeiro and Leicester University to probe the deep structure of this interesting basin using electrical and EM techniques during the period 1993 to 1997. Currently the project has also involved local environmental and groundwater research in some cities of Piauí state (see Meju and Fontes, 1996; Meju et al., 1998). Several MT field data were recorded in 1996 and 1997 across the southeastern margin of the basin and have been inverted as a practical test of the 2D inversion program developed by this author.
Fig. 7.1 1996-97 Parnaiba Project area.
7.2. Geological Setting of Parnaiba Basin

Much of the results of geophysical studies in Parnaiba basin are available in the form of confidential internal company reports (e.g. Cunha and Goes 1989; Goes et al, 1993; Goes, 1991). However some publications (e.g. Meju et al, 1998; Arora et al., 1997) and a few theses (e.g. Cunha, 1986; De Sousa 1996) which refer to these research reports are available in the literature. The geological publications in Brazilian journals generally deal with continental scale studies (e.g. Gomes, 1968) and there are a few relevant publications in international journals (e.g. Soares et al, 1978). The basic review presented here of the geological setting and basement-cover rocks in the study region are based upon these publications and theses.

The Parnaiba basin consists of many sedimentary groups which rest on a crystalline basement (see Fig. 7.2). The basement rocks of the basin consist of quartzites, metamorphosed limestones and schists. Cunha (1986) proposed that there are graben like structures within the basin but the thickness of the sediments (named Riachao and Mirador Formations) filling the suggested graben structures are still unknown.

Serra Grande Group overlie the basement earlier sediments and consists mainly of fluvial sandstones with subordinate siltstones, conglomerates, shales and rare diamicites (Cunha, 1986). This group consists of three formations Ipu, Tiangua and Jaicos. The Ipu Formations which contains middle-coarse grained sandstones and rare siltstones shales, diamicites, shows signs of glacial and fluvioglacial influence, and the approximate thickness is 350m. The Tiangua Formations is extremely micaceous sandstone, with some siltstone and gray shales. The maximum thickness is 200m.

The Jaicos Formation has medium coarse-grained sandstones and pelites with a thickness of approximately 360m. The group was built up by a full transgressive-regressive cycle in the Silurian (Cunha, 1986).

The Serra Grande Group is overlain by the Caninde Group which comprises five formations: Itaim, Pimenteiras, Cabecas, Longa and Poti (Cunha, 1986). The
Fig. 7.2 A geological cross-section thought the south southeastern part of Parnaiba basin (adapted from Cunha, 1986). Fig1 shows the location of the borehole.
Depth (m)

MT Line

Pre-silurien sediments
Itaim Formation is 260m thick and consists of fine whitish sandstones and gray to dark gray shales. The Pimenteiras Formation has dark gray to black shales with fine-grained sandstone bands with a maximum drilled thickness of 320m. The Cabecas Formation contains fine sandstones and is 350 m thick. The Longa Formation is 220m thick, made up of fine - grained sandstones, shales and siltstones. The uppermost formation of this group is the 220m thick Poti formation which also has sandstones with intercalation of shales and siltstones. The group was formed in Devonian and Lower Carboniferous times and the organic rich nature makes it the main target for oil explorations in the basin (Cunha, 1986). These two sedimentary groups in the basin also contain sill intrusions of various ages. The diabase sills do not belong to any class or group.

### 7.2.1. Problems for research

In terms of geophysical research, the generalized geological section (Fig. 7.2) shows gently dipping units which may suggest a simple 2D structure in the region. Large scale photo-geological studies suggest the presence of the Picos fault (Fig. 7.4) However this simplistic geological model has not been verified on the ground using geophysical methods. Among the rare geophysical surveys, airborne magnetic interpretation suggests a more complicated faulted basement (Fig. 7.3). The thickness of the sediments away from the existing boreholes such as F11 in Fig. 7.2 and the location of the sediment - crystalline basement boundary at the basin margin are still unknown and require detailed studies. Besides the delineation of lithological / structural boundaries, Picos area has a groundwater contamination dispersal problem which may possibly be controlled by the Picos fault and local grabens. Due to its high salinity the contaminated part of the aquifer is associated with high conductivity anomalies Meju at al, (1997). Moreover the conductivity contrast between the sedimentary cover rocks and the crystalline basement suggests that EM methods have good potential for structural and lithological mapping in this area. Combined MT and TEM methods were deployed in 1996 and 1997 in Picos area aimed at providing solutions to some of these problems.
Fig. 7.3 Suggested fault zones and lineaments around Picos area based on the interpretations of aeromagnetic data and photo geology (Goes et al, 1993).
7.3. Field Studies

The MT measurements of interest were undertaken at 14 locations along on a 63 km long NW-SE profile extending from Campestre village near Jaicos past Picos to Don Expedito Lopes (Fig. 7.4). The station spacings vary within 1.5 km to 8 km depending on accessibility of the area. The station locations and direction of the line had been chosen to be orthogonal to the suggested trend of main geological features such as Picos fault and the border of the crystalline - sediment units in order to avoid rotation the problem encountered sometimes when selecting the appropriate MT polarization responses to be inverted.

At each station, five field components (two orthogonal, horizontal electric and three orthogonal magnetic) were recorded using an EMI MT system. Coincident- and central- loop mode Transient Electromagnetic (TEM) data were also recorded using Sirotem MK3. The magnetic declination is 23° (West) in the survey area. Ex and Ey measurements in the magnetic North-South (NS) and East-West (EW) directions were done with 50-100m electrode spacings depending on the location of the stations while the TEM data were recorded in the same locations using 50x50m square loop configurations. The data quality is generally good for both methods. In some locations such as close to major settlements or local road control points which have radio transmitters, the noise contamination is too high such that the data is useless.

The recorded time series were analyzed using a software package developed by a commercial company, EMI and converted to classic ERFs within the 125-0.00976 Hz frequency range used in the EMI system. Knowing that the difference between magnetic and geographic north is 23° in northeast Brazil, the magnetic NS and EW directions are assumed as TM and TE modes, respectively, for MT interpretation. The distribution of the MT stations is shown in Fig. 7.4.
Fig. 7.4 Location of the MT stations and the Picos fault.
7.3.1. The field responses

The real earth is inherently heterogeneous and near surface 3D bodies of small sizes are common. Such local 3D bodies affect the electrical fields by means of boundary charges. In the literature there are many descriptions of this phenomena, the more common ones being current channeling or galvanic distortion (Berdichevsky and Dmitriev, 1976; Jiracek, 1990). Galvanic distortion is due to the excess charges built up at a boundary which result in secondary electric fields which add vectorially to the primary electric field (Jiracek, 1990).

The distortion may be observed in three different forms in the MT data (e.g. Groom and Bahr, 1992):
1. For sufficiently high frequencies, deep structures are represented by altered phase.
2. Phase and apparent resistivity curves will be mixed in an arbitrary coordinate system in the case of existing 2D host geometry.
3. Apparent resistivity values are shifted from its true value, a process known as static shift, depending on the contrast in resistivities and sizes of the 3D structures and its host.

The frequency range employed in the MT applications is low enough to allow us to assume that the first effect is negligible.

The second problem is how to overcome the problem of phase mixing and recover regional information in the presence of local geological noise. Using a physical model Bahr (1988) attempted to separate regional and local information by means of tensor decomposition (see also Groom and Bailey, 1989; Groom and Bahr, 1992). In their approach, aided by the assumptions that inductive response is restricted to 1D or 2D bodies and that an inductively small local body of varying conductance is overlying a regional host, the physical model neglects the distortion of the telluric and the magnetic fields by inductively weak bodies. The MT impedance tensors are decomposed into sub matrices. These sub-matrices may be used to minimize or suppress these small-scale scattering effects. Bahr (1991) also showed that this method could be employed only if the data satisfy some
Fig. 7.5 Groom-Bailey (1989) Decomposition of station 06. The graphs on the left
hand side are unconstrained decomposition while those on the right hand side ones
are constrained to 0° strike direction. The observed data (circles), estimated data
(asterisk), and principal axis responses (plus symbol) are presented in the form of
Cagniard apparent resistivity and phase of impedance. Bottom figures show Groom
and Bailey (1989) and Swift (1967) strike direction as plus and cross symbols,
respectively.
conditions. Although the geological setting of the study area has 2D features such as lineaments and Picos fault, the decomposition analysis for the stations indicated no severe scattering problem and suits the requirements of the decomposition based on the physical model. In order to demonstrate the decomposition, 2 sounding data for stations 06 and 08 are given in Fig. 7.5 and 7.6, respectively. These soundings were selected according to their closeness to major structures. In both figures, the observed data (circle symbols), estimated data (asterisk symbol) and principal axis response (plus symbol) are presented in the form of Cagniard apparent resistivity and phase of impedance. The bottom figures show the Groom and Baily (1989) and Swift (1967) strike directions. The left side of the figures display the unconstrained decomposition while in the right side the strike constrained to 0°. As expected, the strike directions in both figures vary from -15° to 15°. This also is the general trend in the other stations. To enable us obtain corrected responses, the strike direction corresponding with the known geological trend of Picos fault, was selected as 0°. Note however that the angle between the magnetic north and the fault axis is around 85° but the angle is selected as 0° in our coordinate framework in order to compare the observed and estimated data and make it comparable with unconstrained data. In general, neither estimated data nor the principal axis response is different from the observed data and no improvement is observed in any data. The reason for this may be that the decomposition method requires certain conditions such as strong 2D host and weak 3D scattered source for the data. In the light of these results and the scope of this study it is decided that the decomposition process is not necessary.

The last effect results in a vertical, parallel shift in log - log plotted apparent resistivity curves. The shift is independent of frequency and can generally be defined as a constant quantity for the apparent resistivity data. It is accepted that there is no static shift problem on the phase of impedance (Jones, 1983). The theoretical details of this effect can be seen in many papers (e.g. Groom and Bahr, 1992; Jiracek, 1990; Jones, 1983).

There are several papers dealing with static removal (e.g. Jones, 1983) but none has been proven to work in every geological environment (Groom and Bahr, 1992). Among the known methods, the use of independent measurements (e.g. Andrieux and Wightman, 1984; Sternberg et al, 1988) has been chosen for this
Fig. 7.6. Groom-Bailey (1989) Decomposition of station 08. Left graphs are unconstrained decomposition while right side ones are constrained to 0° strike direction. Symbols are the same as fig. 7.5.
study. Sternberg et al (1988) showed that Central-loop TEM data recorded in the same location with MT data could be used to remove this shift from the apparent curves. In their method, TEM apparent resistivity and time values are transformed to equivalent MT apparent resistivities and frequencies using simple constant scale factors (see also Meju 1996). Recently, Meju (1997) has drawn attention to the necessity of both central- and coincident-loop, TEM measurements due to their similarities with the MT modes TE and TM. In his approach the central loop mode TEM data generally is related to TE mode MT data while the coincident mode is similar to the TM mode. This is the approach adopted in the current study.

Having obtained the ERFs, the Cagniard apparent resistivity and the impedance phase data are displayed together with TEM data and for each station, the static shift values for both TE and TM modes are determined by visual trial-and-error method on the computer screen. The data used in the inversion as FNI components were determined from corrected Cagniard apparent resistivity and phase of impedance by the program itself.

7.4. Two Dimensional Inversion of Field Data

Identification of target geological features such as Picos fault or basement-cover rock contact require the use of multi dimensional modeling schemes for a realistic interpretation of the data. Following a similar procedure to that described in the previous chapter the 2D non-linear inversion of the data via complex domain calculations was performed to derive a 2D resistivity structure of the area. Initial geoelectrical model consisted of 61 blocks each of 100 ohm-m. The model was inverted with a maximum of 5 iterations. After the first step, comparison of observed and calculated data values for each station led to changes of some block locations and dimensions. Then the inversion was performed on the corrected model. This process was repeated 2 times and the last model is accepted to be the best possible solution to the data. Appendix C contains the comparison of the observed and calculated data for the last geo-electric model. In Fig. 7.7 a section based on 2D interpretation shows that the crystalline units (1), the eastern segment
Fig. 7.7 The Geo-electric section obtained from 2D inversion of MT data. Stars show the location of the station. Depth axis contains two parts 0 - 4 km and 4 to 30 km and each part is scaled linearly.
of the line, and basement were delineated clearly. However the depths found are
different from those proposed by the previous workers (e.g. Cunha, 1986; Goes et
al., 1993). Diabase sill and dike are known to outcrop in the area (see also Fig. 7.2).
The resistive surfical layer (2a) to the west is thus in agreement with the geology.
Layering (2b) observed in the resistivity distribution correlates with geological
model of alternating sandy and shallow formations (Fig. 7.2) Pimenteiras (red unit)
and Jaicos (two yellow units). Jaicos possibly show zonation with resistive upper
zone suggesting dry conditions and the bottom moderately resistive zone that may
be saturated with groundwater. Two subgrabens (3a and b) are suggested in
agreement with that seen elsewhere (Fontes et al, 1997). A conductive zone is found
around 3 km depth at about 43 km east. This may be related to small size horst and
graben structures rooted in the basement or a geothermal plume in the Jaicos
Formation.

The Picos fault (4) is detected and extends vertically into basement. This
may have acted as an impermeable barrier to groundwater flow leading to
concentration of salt to the east. In addition to local features, there seems to be a
electrically conductive zone (5) around 15 km within the lower crust (6). Interestingly Vitorello et al., (1997) presented evidence for the existence of a deep
conductive zone within the basement beneath the southern part of Brazil and Nesbitt
(1993) stated that the middle portion of the continental crust (13 to 20 km) is often
anomalously electrically conductive in comparison to the upper crust and this
anomaly may have been caused by the presence of crustal fluids or existence of
graphite at this depth. There still is no clear evidence about the real source of the
anomaly in this zone but the presence of fluids trapped in a ductile zone is favoured
by this author.

In Fig 7.3 aeromagnetic studies offer some geo-electric features. Palmeiras -
Sao Juliao Lineament extending in a SW to NE direction maps out the surface of
the crystalline base. The edges of the lineament may be associated with the units 1
and 7 in Fig 7.7.
8. CONCLUSIONS AND SUGGESTIONS FOR FURTHER WORK

8.1 Conclusions

In the course of this study, a computer program and to some extent a new approach for the interpretation of 2D Magnetotelluric (MT) data was developed and applied to synthetic and field data sets. The main conclusions of this study are summarized below.

1. An effective program has been developed for interpreting the magnetotelluric Frequency Normalised Impedance (FNI) response function by means of complex domain calculations. The conventional way is that Jacobian matrices for apparent resistivity and phase are calculated separately and placed in a real matrix sequentially. Then the rest of the calculations are performed on the real matrix. The adopted complex calculation method for the inversion techniques has helped to reduce the size of the program by replacing big size real matrices with smaller size complex ones.

   It was found that the FNI response functions offer somewhat improved sensitivity to structure over the Cagniard-type responses but further work is required to fully evaluate this aspect of the response function. Comparative studies have also shown that the inversion of the logarithm of the FNI function is similar to the joint inversion of the logarithm of square root of Cagniard apparent resistivity and 45° - shifted phase of the MT impedance. The FNI approach is thus an interesting alternative to the conventional joint inversion of Cagniard apparent resistivity and phase of impedance.

2. The forward routine used in this study is the well-known Plane - wave 2D (PW2D) finite element code of Rijo (1977). Its validation has been the subject of
many papers and is used widely in MT interpretation (e.g. Wannamaker et al., 1986; Fischer et al., 1992).

3. The Jacobian calculation routine (JACOBI) used in this study is modified from deGroot-Hedlin and Constable (1990). It may be useful to evaluate the validity of the modified routine with a different calculation type (e.g. DeLugao and Wannamaker, 1996).

4. The performance of the program has been tested on several different synthetic models two of which are presented in Chapter 6. The speed of convergence and resolution for the parameters generally are same as the ones in the conventional methods of inversion. However it is observed that for complex models, there is a slight advantage in favour of the method proposed in this study. The advantage may be explained in terms of obtaining a model with better misfit. In the some case of interpretation of real data, the proposed method produced a model with smaller misfit value. But this conclusion is based upon preliminary results from restricted test models and methodology followed and may be deceiving. The final decision requires much work to be done.

5. The interpretation of field data from Parnaiba basin yielded geologically meaningful results. The main sedimentary sequences, grabens, faults and basement were delineated clearly. The grabens were previously suggested from aeromagnetic study and show up as two electrically conductive steep zones at around 2.5 km depth. The present study shows that the Picos fault is a major structure that extends vertically into the crystalline basement. The deeper laterally extensive conductor at 15 km depth may be caused by the presence of fluids trapped in the middle crust in agreement with studies in other continents (e.g. Nesbitt, 1993).

8.2. Suggestions For Further Developments
The subsurface structure is often complex in true field situations and data presentation is one of the main and useful steps of MT interpretations. During the early stage of this study various earth response function (ERF) have been compared and mathematical models have been used to analyze some conventional and alternative MT responses over 2D resistivity structures of general exploration interest. It was seen that besides the use of new functions, new apparent resistivity definitions may also help the user during the interpretation and field studies (Spies and Eggers, 1986; Basokur, 1994; Ulugergerli and Meju, 1996). With the FNI type ERF, shorter period MT field recordings will be enough to determine basement depth and resistivity; and since the alternative apparent resistivity values such as Schmucker (1970) type apparent resistivity definition obtained easily using FNI components approach the true resistivity of subsurface structures (Ulugergerli and Meju, 1996; Basokur et al. 1997), it is envisaged that there will be considerable reductions in the time required to construct an optimal interpretative model using existing modeling procedures.

Some important points which either have not been completed due to time constraints or are necessary to be made clear for users are outlined below;

1. Because of static shift correction technique, the data used in this study were obtained from the Cagniard apparent resistivity and phase of impedance. If the phase has been corrected (reduced to first or fourth quadrant) there may be a sign change in the imaginary component of the FNI data and this will affect the data resolution. To be able to get rid of this problem, the data for inversion should directly be calculated from the impedance tensor itself.

2. Static shift may be incorporated in the inversion process as a parameter (e.g. deGroot - Hedlin 1991). To do this, we simply need to re-state the original inverse problem described in this study as follows: since static shift is a site dependent factor, we may denote it as site gain vector, g_s. All site gains are assumed as real number. In log domain, this is additive to the undisturbed field data Y_un so that the resultant shifted data, Y_s, is described by
Conclusions

Chapter 8

\[
\log (Y_s) = \log(Y_{un}) + g_s
\]

where \(Y_{un}\) calculated FNI data. Because \(g_s\) is a real vector, this equation will only affect the real components of \(\log(Y_{un})\) which is square root of the apparent resistivity (see Equation (5.16)). For Jacobian calculation, \(\log(Y_{un})\) is replace with \(\log(Y)\) in Equation (5.17). The inversion problem is therefore stated as minimizing the error for 2D case,

\[
e = W (\log (Y_{obs}) - \log(Y_s))
\]

where \(o_j\) and \(K(f_1.P)\) are replaced by \(\log(Y_{obs})\) and \(\log(Y_s)\), respectively, in Equation (4.8). Note that since the relation between \(\log (Y_s)\) and \(g_s\) linear function, derivatives with respect to \(g_s\) are independent of the particular model and need only be calculated once (deGroot-Hedlin, 1991). The rest of the calculation will be same as before and site gains will take place in the inversion as parameter.

3. The effect of noise was tested in the present study using synthetic data obtained from same routine (PW2D) and contaminated with noise by means of both a method described in the Appendix B and at some sounding points switching TE and TM mode data for some frequencies. It would be worthwhile to use a different routine for forward calculation and a random number generator or a gaussian noise to contaminate synthetic data up to about 10% as common in modern field observations. For field data, it is recommended that the most squares algorithm (Equation (4.48)) should be implemented in the program.

4 a. The program is currently set up to handle 61 blocks (maximum of 200 x 200 cells in the finite element set up). This limitation was placed by the existing computational platform. As an extension of the current work, it is recommended to adapt the program onto a powerful computer that will allow the use of a large number of finely discretized blocks so that conventional smoothness constraints (e.g. deGroot-Hedlin and Constable, 1990) can be applied effectively. That way, the
program can be tested against the conventional smoothness-constrained 2D inversion programs (e.g. deGroot-Hedlin and Constable, 1990; deLugao and Wannamaker, 1996).

4 b. Alternatively, and the preferred approach would be to allow the size of the resistivity blocks in the inversion. Thus block sizes will be model parameters (e.g. Rodi, 1976).

5. Application of this method to the complex parametric inverse is recommended. Preliminary indicators are that with the help of the complex form of $U$ and $V$ SVD matrices, the resolution of the model parameters may be explained better than with the real parameter eigenvectors. It is therefore recommended that further work be done on understanding the CSVD process and interpreting the resulting matrices and singular values.

6. Early stage of this study and accompanied works, it has been observed that magnetotelluric methods can be employed to trace shallow 2D structures by the use of imaginary component of FNI or, equivalently, phase of impedance (Ulugegerli and Meju, 1996; Meju et al. 1996; Meju et al. 1998). Vertical resolution (i.e. thickness of the layer and the depth of basement) depends upon frequency range while horizontal resolution (i.e. location of the fault zones) requires dense spatial sampling in MT surveys over complex 2D structures.
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References


APPENDIX A

A.1 Solution of Electromagnetic Wave Equations for Arbitrary 2D Structures

Following the Hohmann's (1983 and 1988) notation general solutions for $E$ and $H$ are given in this Appendix. Fig. 3.1 shows a simple model. In order to simulate source for secondary fields, additional to the model an external current source, $J_p$ at the earth surface is considered. Due to attenuation in the earth only low frequencies are of interest, so displacement currents can be ignored. Furthermore, the effect of conductivity changes usually predominate the effect of magnetic permeability changes, so we set $\mu = \mu_0$ everywhere. If displacement currents are neglected, the coupled space and frequency dependence of the electric and magnetic fields is described by Maxwell's equations. Equation (2.1) and (2.2) can be written as

$$\nabla \times E = -i \omega \mu H \quad (A.1)$$

and

$$\nabla \times H = \sigma E + J_p. \quad (A.2)$$

Taking the curl of Equation (A.1) and substituting Equation (A.2) into this equation yields a vector diffusion equation for electric field:

$$\nabla \cdot \nabla \times E + i \omega \mu \sigma E = -i \omega \mu J_p. \quad (A.3)$$

Similarly, in Equation (A.2) dividing both side of the equation by $\sigma$, taking the curl and substituting equation (A.1) into it yields a diffusion equation for the magnetic field:
\[ \nabla \times (\nabla \times \mathbf{H} / \sigma) + iw\mu \mathbf{H} = \nabla \times (\mathbf{J}_p / \sigma). \]  \hfill (A.4)

Applying the vector identity

\[ \nabla \times \nabla \times \mathbf{A} = - \nabla^2 \mathbf{A} + \nabla (\nabla \cdot \mathbf{A}) \]  \hfill (A.5)

equation (A.3) becomes

\[-\nabla^2 \mathbf{E} + \nabla (\nabla \cdot \mathbf{E}) + iw\mu \sigma \mathbf{E} = - iw\mu \mathbf{J}_p. \]  \hfill (A.6)

Taking the divergence of Equation (A.2) yields

\[ \nabla \cdot (\sigma \mathbf{E}) = \sigma \nabla \cdot \mathbf{E} + \nabla \sigma \cdot \mathbf{E} = - \nabla \cdot \mathbf{J}_p. \]  \hfill (A.7)

so that

\[ \nabla \cdot \mathbf{E} = (1 / \sigma) (-\nabla \sigma \cdot \mathbf{E} - \nabla \cdot \mathbf{J}_p) \]

Substituting \((\nabla \cdot \mathbf{E})\) into Equation (A.6) we have

\[ \nabla^2 \mathbf{E} + \nabla (\mathbf{E} \cdot \nabla / \sigma) - iw\mu \sigma \mathbf{E} = iw\mu \mathbf{J}_p - (1 / \sigma) \nabla (\nabla \cdot \mathbf{J}_p) \]  \hfill (A.8)

assuming that the source is in a region of homogeneous conductivity.

Using the identity

\[ \nabla \times \phi \mathbf{A} = \phi \nabla \mathbf{A} - \mathbf{A} \nabla \phi \]  \hfill (A.9)

Equation (A.4) can be rewritten as:

\[-\nabla^2 \mathbf{H} + \nabla (\nabla \cdot \mathbf{H}) - \sigma (\nabla \times \mathbf{H}) \times \nabla (1 / \sigma) + iw\mu \sigma \mathbf{H} = \nabla \times \mathbf{J}_p. \]  \hfill (A.10)
substituting Equation (2.7) into (2.3) and taking divergence of Equation (2.3),

\[ \nabla \cdot \mathbf{H} = 0 \quad \text{(A.11)} \]

Equation (A.10) can be written

\[ \nabla^2 \mathbf{H} + \sigma (\nabla \times \mathbf{H}) \times \nabla (1 / \sigma) - i \omega \mu \sigma \mathbf{H} = - \nabla \times \mathbf{J}_p. \quad \text{(A.12)} \]

Equations (A.8) and (A.12) are general equations for the total \( \mathbf{E} \) and \( \mathbf{H} \) which are valid at every point. The primary field, which would apply everywhere if the body were absent, satisfy the equations. The primary fields given with subscript \( \text{p} \) satisfy the Maxwell equations

\[ \nabla \times \mathbf{E}_p = - i \omega \mu \mathbf{H}_p \quad \text{(A.13)} \]

and

\[ \nabla \times \mathbf{H}_p = \sigma_n \mathbf{E}_p + \mathbf{J}_p. \quad \text{(A.14)} \]

where \( \sigma_n \) is the ‘normal’ (layered-earth) conductivity with the anomalous body not present. The equations for the secondary fields with subscripts \( \text{s} \) are

\[ \nabla \times \mathbf{E}_s = - i \omega \mu \mathbf{H}_s \quad \text{(A.15)} \]

and

\[ \nabla \times \mathbf{H}_s = \sigma \mathbf{E}_s + \sigma_a \mathbf{E}_p \quad \text{(A.16)} \]

or
\[ \nabla \times \mathbf{H}_S = \sigma_a \mathbf{E}_S + \mathbf{J}_S \quad \text{(A.17)} \]

where \( \mathbf{J}_S = \sigma_a \mathbf{E} \), \( \mathbf{E} \) is total electric field and \( \sigma_a = \sigma - \sigma_n \) is the anomalous conductivity at a point. In Fig. 3.1, \( \sigma_a \) is non zero only in the body where it becomes \( \sigma_a = \sigma_b - \sigma_n \). The quantity \( \mathbf{J}_S \) is equivalent (scattering) current that replaces the body and is the source of secondary field. Comparing the Equations (A.15) and (A.17) with Equations (A.13) and (A.14), shows that differential equations for \( \mathbf{E}_S \) is the same for \( \mathbf{E} \) in Equation (A.8) with \( \mathbf{J}_p \) replaced by \( \sigma_a \mathbf{E}_p \) i.e.,

\[ \nabla^2 \mathbf{E}_S + \nabla (\mathbf{E}_S \cdot \nabla \sigma/\sigma) - i\omega \mu \sigma \mathbf{E}_S = i\omega \mu \sigma_a \mathbf{E}_p - \nabla (\mathbf{E}_p \cdot \nabla \sigma_a/\sigma). \quad \text{(A.18)} \]

Since \( (\nabla \cdot \mathbf{E}_p) \) is zero in the body, which is the only place \( \sigma_a \) is non zero. Similarly, using Equation (A.7), the secondary magnetic field is written as

\[ \nabla^2 \mathbf{H}_S + \sigma (\nabla \times \mathbf{H}_S) \times \nabla (1/\sigma) - i\omega \mu \sigma \mathbf{H}_S = i\omega \mu \sigma_a \mathbf{H}_p - \sigma \nabla (\sigma_a/\sigma) \times \mathbf{E}_p. \quad \text{(A.19)} \]

Notice that the source of \( \mathbf{E}_S \) in Equation (A.18) are currents and charges in the volume and on the surface of the body, respectively, where \( \sigma_a \) and \( \nabla \sigma_a \) are nonzero. The source of \( \mathbf{H}_S \) in Equation (A.19) are volume and surface currents in and on the body (Hohmann, 1983 and 1988).
APPENDIX B

B.1 One Dimensional Inversion

Three computer programs have been developed in FORTRAN. The main structure and output subroutine in these programs have been modified from Arnason and Hersir (1980). A flowchart of the inversion scheme is shown in Figure 6.1. The first program (P1) is for the conventional method which takes imaginary components as augmenting data in Jacobian matrix. The second program (P2) deals with complex domain calculations and employs a complex singular value decomposition subroutine (CSVD, Marple, 1987). Both programs use linear form of FNI while parameters are logarithmic. In order to test and compare the results third program, P3 in which P2 is modified to handle logarithm of FNI also prepared. The solution for ΔP given by CSVD application is complex. Although it is possible to employ complex model parameter in this type of calculations, for the sake of simplicity real type model parameters have been chosen in this study (layer conductivity and thickness) and hence the real components of ΔP are employed for updating the parameters.

For stability of the solution three different checks are used;

a) None of the parameter is allowed to change by more than a factor of 10 (1.0 in logarithmic space) in any iteration step. In other words the magnitude of ΔP_l is kept smaller than 1.0.

b) The RMS value of ΔP are also kept less than 1.0 in each iteration.

c) Following the Jackson and Matsu’ura (1985)’s notation, Equation (4.11) can be written as

\[ P^l = P^0 + b \Delta P \]  \hspace{1cm} (B.1)

The factor b scales the step sizes (Jackson and Matsu’ura, 1985). Its value is set to be between zero and one, depending on the problem. It has been found by trial-and-
error using synthetic data as 0.2 for three programs and held fixed during the inversion steps.

A set of damping factors in increasing order of magnitude is calculated in each iteration step. Starting from the smallest factor each of them is used to obtain a set of updates until achieving better convergence. The convergence in the programs is gauged using Equation (5.9). note that Hermitic transpose H becomes normal transpose for P1 and Y is replaced with log(Y) for P3. All programs require observed data and initial parameters as input and give the updated parameters, CHI and DCHI values for all iterations and U, $\Lambda$, V and correlation matrix for last iteration as the output. The DCHI value is fractional decrease of the CHI values in successive iterations.

\textbf{B.2 Application to Synthetic Data}

The programs have been tested on various models and the results are encouraging. The test model is a conductive layer of resistivity 10 ohm-m and thickness 50m embedded in a host of resistivity 100 ohm-m at a depth of 250m. The real and imaginary components of FNI data are calculated for 12 frequencies between 8192 and 4 Hz as in common CSAMT (controlled source audio frequency magnetotelluric) experiments by using 2D forward routine. Calculated data scattered minimum three percent. Scattering constant, scr is calculated for each impedance sample,

$$scr = 1 - 0.1 \sin \left( \frac{2\pi i}{(0.3) imax} \right) \quad i = 1, 2, \ldots, imax$$  \hspace{1cm} (B.2)

with a condition scr > 0.03. In (B.2) imax is taken as number of frequencies. error is obtained as

$$err = Y_{un} (1 - scr)$$  \hspace{1cm} (B.3)

where $Y_{un}$ is undisturbed FNI value. The observable $Y_{obs}$ value is
\[ Y_{\text{obs}} = Y_{\text{un}} + \text{err} \]  \hspace{1cm} (B.4)

The weighting matrix was calculated as described previously by the use of \text{err} values. The observable values used are given in Table B.1.

Table B.1. The observable values used in the inversion. \text{YR} and \text{YI} are the real and imaginary components of FNI, respectively. \text{err} shows related errors for the components.

<table>
<thead>
<tr>
<th>Frequencies</th>
<th>\text{YR}</th>
<th>\text{YRerr}</th>
<th>\text{YI}</th>
<th>\text{YIerr}</th>
</tr>
</thead>
<tbody>
<tr>
<td>8192.0</td>
<td>10.7861</td>
<td>1.5698</td>
<td>0.1846</td>
<td>0.3686</td>
</tr>
<tr>
<td>4096.0</td>
<td>9.4409</td>
<td>1.0821</td>
<td>0.2123</td>
<td>0.4217</td>
</tr>
<tr>
<td>2048.0</td>
<td>8.9577</td>
<td>2.1377</td>
<td>0.1035</td>
<td>0.4426</td>
</tr>
<tr>
<td>1024.0</td>
<td>10.9262</td>
<td>0.9266</td>
<td>0.2122</td>
<td>0.3823</td>
</tr>
<tr>
<td>512.0</td>
<td>10.9545</td>
<td>0.9290</td>
<td>1.0593</td>
<td>0.0898</td>
</tr>
<tr>
<td>256.0</td>
<td>8.3612</td>
<td>1.9954</td>
<td>1.5659</td>
<td>0.3737</td>
</tr>
<tr>
<td>128.0</td>
<td>7.6782</td>
<td>0.8800</td>
<td>1.3993</td>
<td>0.1604</td>
</tr>
<tr>
<td>64.0</td>
<td>8.0585</td>
<td>1.1728</td>
<td>0.8085</td>
<td>0.1177</td>
</tr>
<tr>
<td>32.0</td>
<td>7.2290</td>
<td>0.2951</td>
<td>0.2578</td>
<td>0.4080</td>
</tr>
<tr>
<td>16.0</td>
<td>6.7189</td>
<td>1.8061</td>
<td>-0.3770</td>
<td>0.1013</td>
</tr>
<tr>
<td>8.0</td>
<td>8.1370</td>
<td>0.2279</td>
<td>-0.4786</td>
<td>0.3943</td>
</tr>
<tr>
<td>4.0</td>
<td>9.0139</td>
<td>1.1257</td>
<td>-0.7900</td>
<td>0.0987</td>
</tr>
</tbody>
</table>

The initial model parameters used in the inversion were a 100 ohm-m half-space with boundaries at depths of 100, 200m. All the programs have been run with a maximum limit of 50 iterations. All of them completed maximum iteration.

The results are presented as FNI components in Figure B.1. In Figure B.1, upper curves are the real components of the FNI while the lower ones are imaginary.
The final fit in the curves and the closeness of the estimated models to the original model are generally good. All methods but P2(I) locate the conductive layers in correct depth. When different initial guess with deeper or shallower boundaries is selected P1 gave similar solution but P2(I), and P3 failed. P2(C) and P2(R) depending on the initial guess either produced similar result or calculated thickness of conductor larger or thinner.

Table B.2. Recovered parameters for test model. R, C and I indicate real, complex and imaginary type damping factor. Real type damping factor is employed for P3. CHI value of Initial guess for P3 is 2.0171

<table>
<thead>
<tr>
<th>Init. G.</th>
<th>( \rho_1 )</th>
<th>( \rho_2 )</th>
<th>( \rho_3 )</th>
<th>( t_1 )</th>
<th>( t_2 )</th>
<th>CHI</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1</td>
<td>99.72</td>
<td>3.05</td>
<td>88.06</td>
<td>247.73</td>
<td>12.19</td>
<td>0.4329</td>
</tr>
<tr>
<td>P2 (R)</td>
<td>98.3</td>
<td>5.52</td>
<td>87.17</td>
<td>252.15</td>
<td>18.38</td>
<td>0.4745</td>
</tr>
<tr>
<td>P2 (I)</td>
<td>96.01</td>
<td>72.55</td>
<td>73.8</td>
<td>72.11</td>
<td>28.50</td>
<td>0.9176</td>
</tr>
<tr>
<td>P2 (C)</td>
<td>98.39</td>
<td>14.52</td>
<td>87.38</td>
<td>237.72</td>
<td>55.44</td>
<td>0.4748</td>
</tr>
<tr>
<td>P3</td>
<td>97.57</td>
<td>3.06</td>
<td>86.35</td>
<td>253.15</td>
<td>11.44</td>
<td>1.3172</td>
</tr>
</tbody>
</table>

It should be mentioned that program P2 is more sensitive to the initial guess and damping factor type than P1 is. Calculated perturbations in P2 vary in a large scale depending on the damping factors. In order to search the best updates in each iterations a number of different damping factors are used, to stabilize the variations and to avoid the local minimums during the iterations the factor \( b \) should be selected as a small number. Although it makes the convergence slower, but ensure the better solutions.
Figure B.1. Upper curve is the real component of the FNI while the lower one is imaginary. The symbols o, +, ~, x, *, and - indicate observed data, calculated data from P1, P2(R), P2(I), P2(C) and P3 respectively.
APPENDIX C

The Comparison of the Observed and Calculated Data

The observed (●) and the calculated (x) data are presented in the form of real and imaginary component of the FNI. Both are presented in different scale to be able to show the small variations in the data. Error bars are normalized data errors which were used in the inversion as weights (see section 4.2).
Station: Brejo do Tucona
Location: 01
Lon. = 07.00.816
Lat. = 41.42.715
Alt. = 430m

Station: Angical (Portelandia)
Location: 02
Lon. = 07.02.627
Lat. = 42.02.627
Alt. = 306m

TE Mode

TM Mode

Frequency (Hz)
Station: Gameleira
Location: 03
Lon. = 07.05.46
Lat. = 41.34.26
Alt. = 205m

Station: Angico Branco
Location: 04
Lon. = 07.06.054
Lat. = 42.32.801
Alt. = 235m

TE Mode

TM Mode

Frequency (Hz)
Station: Torroes
Location: 05
Lon. = 07.07.681
Lat. = 41.31.404
Alt. = 251 m

Station: Pitombeiras
Location: 06
Lon. = 07.09.90
Lat. = 42.30.36
Alt. = 235 m
Station: Dengoso
Location: 07
Lon. = 07.09.859
Lat. = 41.28.730
Alt. = 120m

Station: Bugi
Location: 08
Lon. = 07.10.86
Lat. = 42.26.46
Alt. = 150m
Station: Barreiros
Location: 09
Lon. = 07.14.726
Lat. = 41.22.234
Alt. = 330m

Station: Veados
Location: 10
Lon. = 07.13.38
Lat. = 42.23.70
Alt. = 210m
Station: Imbuzeiro
Location: 11
Lon. = 07.17.100
Lat. = 41.17.880
Alt. = 390m

Station: Capim
Location: 12
Lon. = 07.19.713
Lat. = 42.13.552
Alt. = 390m
Station: Carnaubeiras
Location: 13
Lon. = 07.20.255
Lat. = 41.09.296
Alt. = 248m

Station: Imbuzeiro Cavado
Location: 14
Lon. = 07.23.255
Lat. = 42.07.110
Alt. = 208m