

A MAGNETOTELLURIC STUDY IN THE MOINE THRUST REGION OF
NORTHERN SCOTLAND

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DECLARATION

I hereby declare that the work presented in this thesis is my own unless otherwise stated in the text and that the thesis has been composed by myself.

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ABSTRACT

The initial objective of this study was the determination of the lateral variation in electrical structure of the crust and upper mantle across the Moine Thrust region of Northern Scotland. To this effect Magnetotelluric measurements were made along a profile in the Moine Thrust region of Northern Scotland between National Grid references 21279243 and 27188943 in the frequency range 780 Hz. To 0.1 Hz. using the then recently developed Short Period Audio-Magnetotelluric (S.P.A.M.) system.

The data were supplemented by that of Mbipom (1980) in the frequency range 0.05 Hz. TO 0.0012 Hz. from along a nearby profile.

The data were processed in the frequency domain. The bias on the data was estimated using the four impedance tensor element estimators.

The processed resistivity and phase data were modelled using a Hedgehog algorithm and two-dimensional modelling was conducted using a biased linear estimation algorithm extended by the author.

Contrary to the lateral variation of conductivity expected as a result of the structures revealed by the offshore Moine and Outer Isles Seismic Traverse reflection profile and of combined electromagnetic and seismic reflection studies in the Eastern United States Of America there was no evidence in this study of an electrical Moine Thrust structure. Moreover no common features were observed in the electrical models and the results of geological, gravity and aeromagnetic studies. A resistive structure of not less than 1×10^4 ohm-metres was found at National Grid Reference 23939160 with a possible extension as far eastwards as National Grid Reference 25279021. More intensive field observations are required for the verification and elaboration of this model structure.

The two-dimensional models yield a resistivity profile similar to that proposed by Hjelt (1987) for cold crusts.

The determination of the two-dimensional electrical model led the author to investigate and modify a two-dimensional magnetotelluric inversion method using singular value truncation and ridge regression methods iteratively. This development itself became the major objective and probably the most significant part of the study.

A computer programme was written to invert the two-dimensional Magnetotelluric data. Novel block boundary parameters were used and parametric errors were calculated using a linear approximation. Three experimental inversions were conducted and it was found that:

- (1) The procedure improved the fit between the model response and the data when the initial model consisted of a section of collated one-dimensional models.
- (2) The novel block boundary technique improved convergence for a given number of model resistivity blocks.
- (3) With the models used at least ten iterations would be required for convergence.

The inversion procedure used a two-dimensional finite difference forward modelling algorithm due to Brewitt-Taylor and Weaver and this was modified. A method for calculating derivatives was extended by use of a series to account for non-linearity in the finite interval over which the derivative was required. The computation time for the derivatives was reduced to a minimum of 0.065 of that for the original algorithm in the case of a 1800 node finite difference mesh.

The above routines have been further developed and applied in the current Magnetotelluric research in the Department Of Geophysics at the University Of Edinburgh.

CHAPTER I

INTRODUCTION

1.1. THE INITIAL OBJECTIVES.

The initial objective of this study was the determination of the lateral conductivity structure of the crust and upper mantle in the Moine Thrust region of Northern Scotland. This required an electrical method capable of resolving conductivity structures to depths exceeding 20 Kms. in the crust. One such available procedure which did not require large transmitter arrays was the Magnetotelluric Method, (Kaufman and Keller 1981). This method utilizes natural electromagnetic fields with frequencies extending from a few kilohertz to milihertz and the fact that conductivity structures below the surface of the earth being subject to electromagnetic induction, affect measured surface electric and magnetic fields. Earth response functions derived from these fields thus allow models of the conductivity structures to be calculated.

1.2 THE MODIFICATION OF THE OBJECTIVES.

Magnetotelluric data were collected particularly in the area where the Moine Thrust is evident at the surface, and also at sites having a greater geographical separation to the east of this area. One-dimensional modelling of the data suggested that the Moine Thrust could not be readily identified and that contrary to expectation the area with the most variable electrical conductivity structure lay in the eastern area where data of only moderate quality could be collected. This was due to undesirable electromagnetic noise from high voltage transmission lines and hydro-electric plants.

Since one-dimensional modelling could not accurately be applied to a region with observed large lateral conductivity variations within the length of one skin depth, it was apparent that at least two-dimensional modelling would be required. This led the author to examine a two-dimensional inversion scheme utilizing biased linear estimation and to its development to the extent that it constitutes a major part of this study. Following the inversion of the field data further study of the inversion scheme was undertaken. This resulted in the modification

of the forward finite difference two-dimensional modelling algorithm in a novel way which resulted in a considerable reduction of computer run time.

1.3 THE STRUCTURE OF THE THESIS.

Following the introductory comments of this chapter and an account of general Magnetotelluric theory in Chapter II the contents of this thesis are grouped into two parts related to the modification of the initial project objectives. Chapters III, IV and V are primarily concerned with the regional study. The second and principal part of this thesis (Chapters VI, VII and VIII) is concerned with the two-dimensional inversion theory and its application to the data used in the regional study. This part also contains in Chapter VII the additional inversion studies which were tested but not applied to the regional data. Finally Chapter IX summarises the conclusions of the study and contains suggestions for further work.

1.4 THE KNOWN GEOLOGY AND GEOPHYSICS OF THE STUDY REGION.

The Moine Thrust Region consists of a Lewisian Foreland to the north-west and a Moinian Hinterland to the south-east. The Foreland consists of two parts. To the west of Assynt is found the Scourian type area which has been extensively intruded with dykes (2400 Ma. TO 2200 Ma. Watson (1983)) having a north-west south-east trend. To the north and south of Assynt lies the later Laxfordian Complexes (2400 Ma. TO 2200 Ma. Watson (1983)). The Moines to the east of the Thrust, which at the surface dips eastwards at approximately 15° , consist largely of siliceous granulites. In north-eastern Sutherland migmatitic and granitic complexes are found while the eastern coastal regions are characterized by old red sandstone and younger rocks. The Hinterland is also characterized by a number of Lewisian inliers and igneous intrusions. Of the intrusions the Rogart, Grudie, Fearn, and Migdale granites are in the region of the study and are generally considered to be the Newer Granites (435 Ma. TO 390 Ma. (Brown 1983)). To the south lies the early (550 Ma. TO 450 Ma. (Brown 1983)) Carn Chunneag and Glen Dessary complexes. Within Assynt and within the vicinity of the study region are found the Loch Borrolan and Loch Ailsh intrusives (426 Ma. TO 434 Ma. (Van Breemen ET. AL. 1979)) of the alkaline suite of the north-west Highlands.

The Hinterland is thought to have overthrust the Foreland by possibly up to 100 Kms. (Elliott and Johnson (1980)). Various models have been

proposed to represent the thrusting including those of Soper and Barber (1982) who considered the deep structures and Elliott and Johnson (1980) who considered the shallow structure with the use of balanced cross-sections.

Sweit (1972) proposed that the existence of sedimentary rocks overlying part of the Lewisian Foreland may imply that this region formed the western subtidal margin of the Proto-Atlantic or Iapetus Suture. According to Cook ET. AL. (1979) and Cook ET. AL. (1981) the Appalachian system may have formed the eastern boundary of the Iapetus Suture. However there are a number of alternative theories concerning the location of the Iapetus Suture in Britain (Kennedy (1979)).

The entire structure in the Moine Thrust region has been compared with the Appalachian structure of North America (Barton (1978)). The more recent COCORP seismic study has been compared by Brewer and Smythe (1981) with the results of the M.O.I.S.T. seismic study (Section 1.5.3) conducted across the supposed offshore extension of the Moine Thrust (Figure 1.3). The seismic reflectors were compared and found to be similar. Greenhouse and Bailey (1981) and Thompson ET. AL. (1983) considered a geomagnetic variation study and reaffirmed an over-thrusting model for the Appalachians.

1.5 MISCELLANEOUS STUDIES AND CONCEPTS.

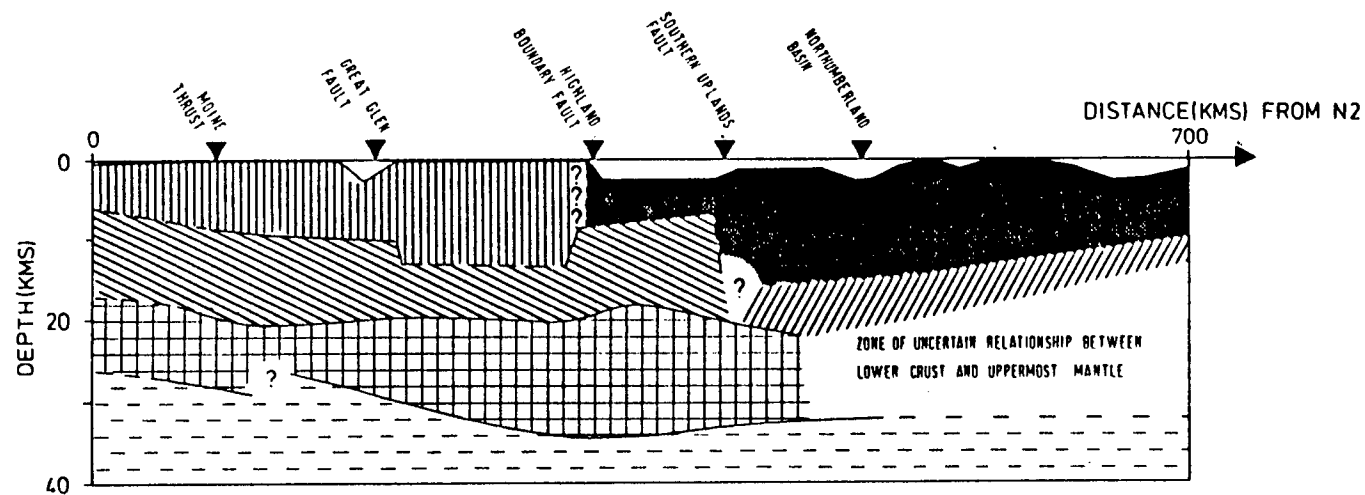
We collect here for convenience a series of studies and concepts referred to at regular intervals throughout the thesis.

1.5.1. THE LITHOSPHERIC SEISMIC PROFILE OF BRITAIN.

The Lithospheric Seismic Profile Of Britain (LISPB) was conducted with large shot spacings by Bamford ET. AL. (1978). The profile extended from Northern Scotland into Northern England. A generalised seismic velocity structure for Scotland derived from the results of this study is shown in Figure (1.1).

1.5.2 THE MODEL OF SOPER AND BARBER.

The model was constructed from existing geological and geophysical observations by Soper and Barber (1982). Since their model shown in Figure (1.2) was proposed at the time of initiation of this study it was used as a basis for the site locations of the Magnetotelluric profile discussed in this thesis.



KEY

- Superficial layer
- Caledonian belt metamorphics (61-62 km/s)
- Lower Palaeozoic (5.8-6.0 km/s)
- Pre-Caledonian basement (~6.4 km/s)

- Pre-Caledonian basement (~6.3 km/s)
- Lower crust (~7 km/s)
- Upper mantle (~8 km/s)
- ? Uncertain structure

FIGURE 1.1. THE LISP IV. SEISMIC PROFILE. SCHEMATIC CROSS-SECTION THROUGH THE CRUST AND UPPERMOST MANTLE OF NORTHERN BRITAIN.

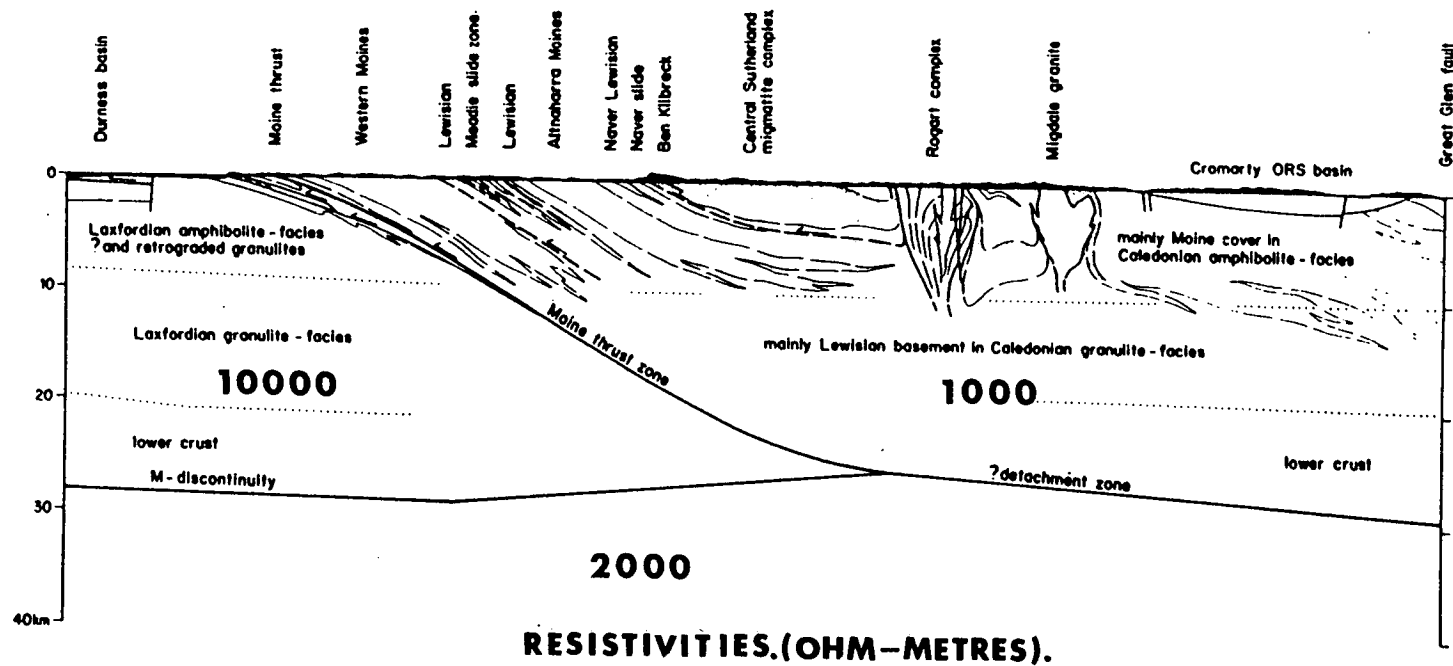


FIGURE 1.2. THE MOINE THRUST MODEL OF SOPER AND BARBER (1981) WITH ADDITIONAL RESISTIVITIES USED TO DERIVE A POSSIBLE REGIONAL MAGNETOTELLURIC RESPONSE.

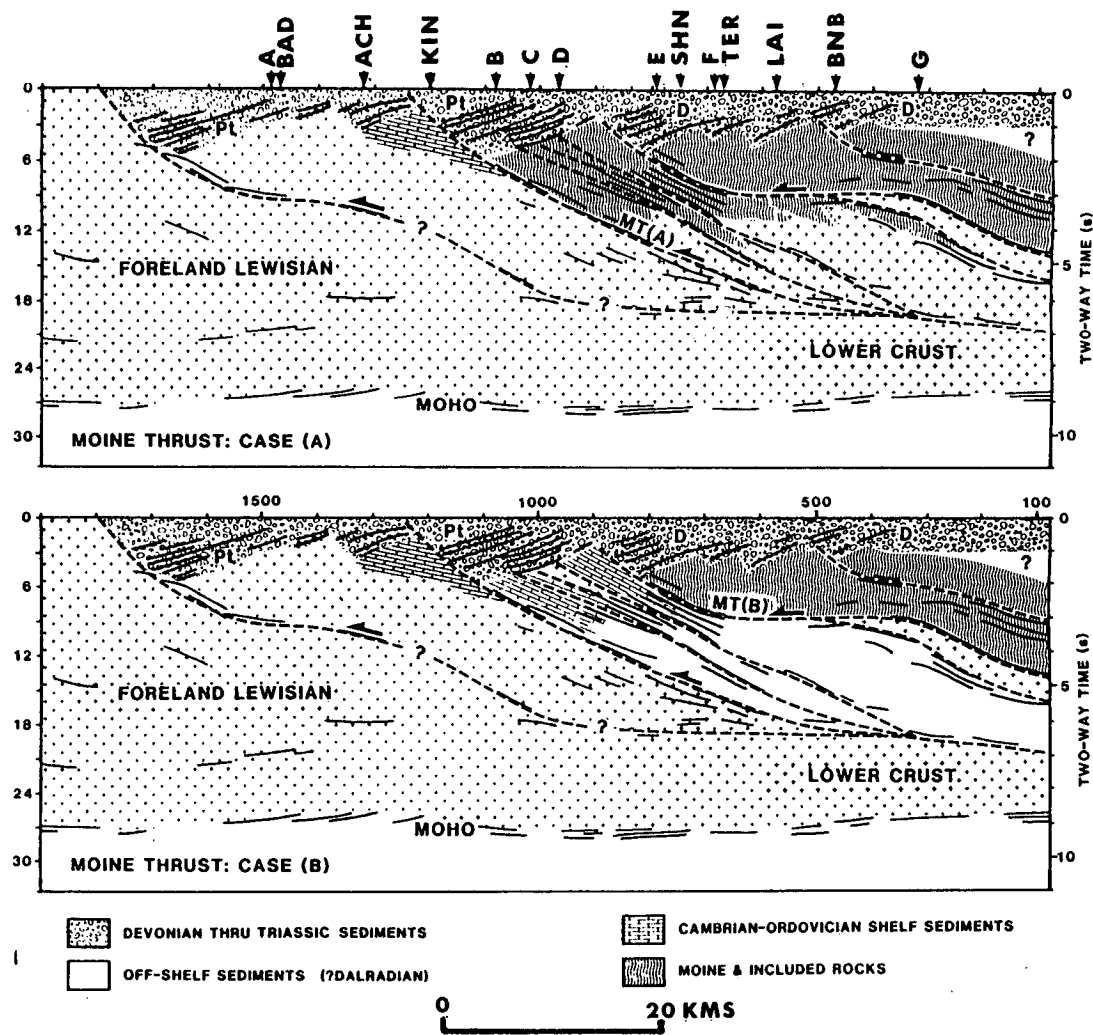


FIGURE 1.3. THE M.O.I.S.T. B.I.R.P.S. SEISMIC SECTION AS INTERPRETED BY BREWER AND SMYTHE, (1984).
CASE (B) IMPLIES CLOSER SIMILARITIES IN THE GEOLOGICAL DEVELOPMENT OF THE APPALACHIANS AND
THE CALDONIDES THAN CASE (A). (BREWER AND SMYTHE (1984)).

1.5.3 THE MOINE AND OUTER ISLES TRAVERSE OF THE BRITISH INSTITUTIONS REFLECTION PROFILING SYNDICATE.

The Moine and Outer Isles Traverse (M.O.I.S.T.) was undertaken commercially along the profile indicated in Map (1) for the British Institutions Reflection Profiling Syndicate (B.I.R.P.S.) after the Magnetotelluric fieldwork for this study had been completed. An interpretation of the M.O.I.S.T. data was published by Brewer and Smythe (1981) who detected two possible signatures of an offshore extension of the Moine Thrust (Figure 1.3).

1.5.4. THE SEISMIC PROFILE OF THE CONSORTIUM FOR CONTINENTAL REFLECTION PROFILING.

The seismic profile of the Consortium For Reflection Profiling (COCORP) was conducted in the southern Appalachians of the United States Of America (Cook ET. AL. 1979, Cook ET. AL. 1981). The structure in this region was considered by Brewer and Smythe (1984) to be a continuation of the Moine Thrust structure of (Figure 1.4).

1.5.5. THE LAW OF ARCHIE.

The conductivity of many rocks may be attributed to the presence of electrolytes within their porous structure. The law of Archie (1942) relates the conductivity of the saturated porous rock σ_R with that of the electrolyte σ_E and the porosity of the rock η as below:

$$\sigma_R = \alpha \sigma_E \eta^\beta$$

where β and α are constants with $1 < \beta < 2$.

1.5.5 THE SEMICONDUCTION IN HEATED ROCKS.

Many materials which constitute the crust of the Earth possess filled valence bands (Kittel 1962). At high temperatures these materials may exhibit semiconduction. For intrinsic semiconductors the conductivity σ_i is related to the temperature T as below:

$$\sigma_i \propto T^{3/2} e^{-E_g/2kT}$$

where E_g is the forbidden energy gap between the filled valence band and the conduction band for the semiconductor.

However impurities affect the value of E_g substantially so that the value of σ_i is unknown unless the impurities and their concentrations are known. We may be able to account for conductivity at depth where high temperatures are found by semiconduction. However since no maximum

value for E_G is known we are unable to show that high resistivities cannot be found at depth where high temperatures are found.

CHAPTER II

THE THEORY OF THE MAGNETOTELLURIC METHOD

2.1 THE ELECTROMAGNETIC SOURCE FIELD FOR MAGNETOTELLURIC SOUNDINGS

The sources of the electromagnetic disturbances (Bleil 1964, Matsushita and Campbell 1967, Orr 1973) used in Magnetotelluric Sounding are located in the Magnetosphere for frequencies below approximately 0.2 Hz. and in the Earth Ionosphere Cavity for the higher frequencies above approximately 0.2 Hz. The frequency spectrum for the disturbances is shown in Figure (2.1).

In the Magnetosphere which results from the interaction of the Solar Wind with the permanent geomagnetic field there exists a plasma. This has the properties of a gas but since the conductivity of the plasma is large, it remains frozen to the geomagnetic field lines. Hence disturbances in the plasma result in disturbances of the geomagnetic field.

Assuming a uniform magnetic field the plasma may support transverse Alfvén waves and compressional Fast waves. Further, assuming that the plasma exerts a pressure a further slow wave is introduced which corresponds to an acoustic wave.

The classification of the electromagnetic disturbances is found in Table (2.1). The Pc5, Pc4 and Pc3 events and possibly some Pc2 events are due to standing Alfvén waves. The Pc4 events are associated with the reflection of hydromagnetic wave packets from the ends of the geomagnetic field lines which act as wave guides. The Pi1 and Pi2 events generally occur at night and are found in the Auroral zone. The Pi2 events may be associated with the vibrations of the last closed field line near the midnight meridian in high latitudes or with the ringing of the Plasmapause in middle latitudes.

The excitation of the modes may be effected by Kelvin-Helmholtz instability at the Magnetosphere-Solar Wind boundary, by fluctuations in the Solar Wind or by wave particle interactions as in the case of the Pc1 disturbances.

The higher frequency disturbances above approximately 0.2 Hz. are due to electrical storms. The disturbance propagates in the Earth-Ionosphere cavity. The cavity also allows the establishment of

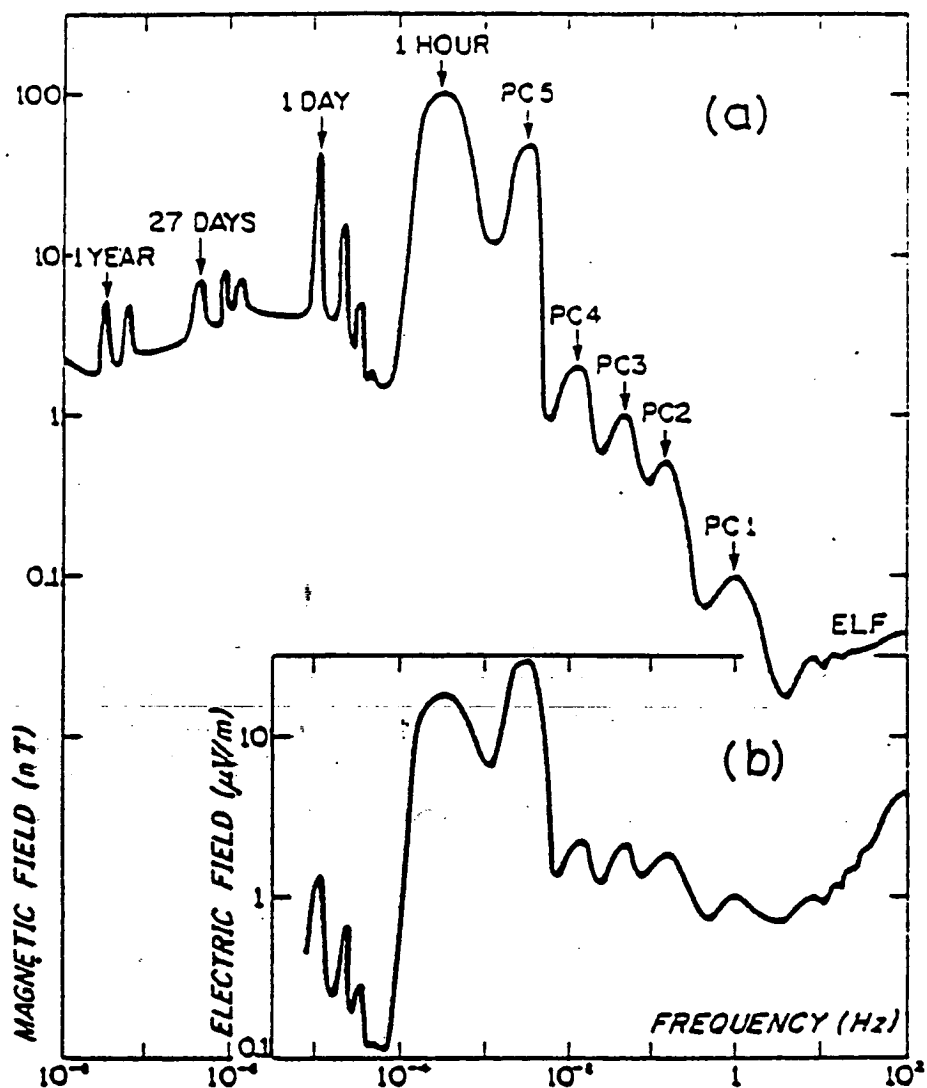


FIGURE 2.1. THE FREQUENCY SPECTRUM FOR THE ELECTROMAGNETIC DISTURBANCES.
 (A) THE MAGNETIC FIELD.
 (B) THE TELLURIC FIELD ASSUMING A 20 OHM-METRE HALF SPACE.

DESCRIPTION	DISTURBANCE	PERIODICITY (SECONDS)
Pc1	CONTINUOUS	0.2 TO 5.0
Pc2	CONTINUOUS	5.0 TO 10
Pc3	CONTINUOUS	10 TO 45
Pc4	CONTINUOUS	45 TO 150
Pc5	CONTINUOUS	150 TO 600
Pi1	IRREGULAR	1.0 TO 40
Pi2	IRREGULAR	40 TO 150

TABLE 2.1. THE NATURAL ELECTROMAGNETIC DISTURBANCE DEFINITIONS.

resonances.

The remote location of these sources of the electromagnetic disturbances allows the assumption of the incidence of plane electromagnetic waves at the surface of the Earth.

2.2 THE ELECTRICAL HALF SPACE

Let us assume that the electromagnetic waves arriving at the surface of the Earth are plane . As is customary in magnetotellurics we shall assume that the electromagnetic waves arriving at the surface of the earth are normally incident upon that surface. If the skin depth (see below) of the electromagnetic waves in the Earth is small compared with the dimensions of the Earth we may model the situation as plane waves arriving normally on a half -space . Let the surface of the half-space lie in the x-y plane and z represent the depth. Then from Maxwells equations :

$$\text{div } \underline{D} = \rho$$

1

$$\text{div } \underline{B} = 0$$

2

$$\text{Curl } \underline{H} = \underline{J} + \frac{\partial \underline{D}}{\partial t}$$

3

$$\text{Curl } \underline{E} = - \frac{\partial \underline{B}}{\partial t}$$

4

We may obtain for media homogeneous in μ and ϵ ;

$$\frac{\partial^2 E_x}{\partial z^2} = i \omega \mu \sigma E_x$$

5

where σ is the conductivity of the half space . This expression has been obtained under the assumptions that $\partial/\partial t = j\omega$ and that the displacement current has been neglected ($\sigma \gg \omega\epsilon$). This is often true at the frequencies used in electromagnetic induction studies (less than 1000 Hz.) and with the Earth resistivities encountered (greater than 10 ohm-metres.). The associated magnetic field is given by :

$$H_x = 0$$

6

$$\frac{\partial E_x}{\partial z} = j \omega \mu H_y$$

7

$$H_z = 0$$

8

We require some frequency invariant parameter to represent the electrical conductivity of the half-space. The driving point impedance (viewed downwards from the surface) is given by :

$$Z_{xy} = E_x / H_y = (1+j) \sqrt{\frac{\omega \mu}{2\sigma}}$$

9

The apparent resistivity is defined by :

$$S_A = \frac{1}{\omega \mu} Z_{xy} Z_{xy}^*$$

10

The phase is defined by :

$$\phi = \text{Arg } Z_{\text{ex}} \quad 11$$

Thus for a half space we find that :

$$\delta_A = 1/\omega \quad 12$$

$$\phi = \pi/4 \quad 13$$

The skin depth in the medium is defined as the distance over which electric field falls to $1/e$ of its initial value. In a homogeneous medium the skin depth w is given by :

$$\delta = \sqrt{\frac{2}{\omega \mu \sigma}} \quad 14$$

2.3 THE LAYERED EARTH MODEL.

Consider now the half-space replaced by a stack of N homogeneous conductivity layers as in the case of a layered earth characterized by

$1, k_2, \dots, k_n$. where :

$$k_n^2 = -j\omega\mu\sigma_n \quad 15$$

TH.

Let the field at depth z in the n layer be given by:

$$E_x = A_n e^{j k_n z} + B_n e^{-j k_n z} \quad 16$$

TH.

Let the impedance as viewed downwards from the n interface be Z_n .

Since the tangential electric and magnetic fields are continuous across boundaries we may apply (7) and (16) to obtain:

$$Z_n = \frac{\omega\mu [A_n e^{j k_n h} + B_n e^{-j k_n h}]}{k_n [A_n e^{j k_n h} - B_n e^{-j k_n h}]} \quad 17$$

TH.

Similarly at the $(n-1)$ interface we obtain:

$$Z_{n-1} = \frac{\omega\mu [A_n + B_n]}{k_n [A_n - B_n]} \quad 18$$

Where $h = z_n - z_{n-1}$

From (17) and (18) we obtain the following recursion formula:

$$Z_{n-1} = -\frac{\omega\mu}{k_n} \coth \left[\coth^{-1} \left[\frac{-k_n Z_n}{\omega\mu} \right] - j k_n h_n \right] \quad 19$$

The deepest layer in the stack is assumed to be the half space with an impedance Z_n given by (9).

Details of the application of (19) in a Hedgehog modelling programme are given in Section (5.1.1).

2.4 THE TWO-DIMENSIONAL CASE

In the two-dimensional case we assume that the properties of the half space previously considered vary with x and z but are invariant with y . Let the term E-Polarization refer to the case when $E_x \neq 0$, $E_y = 0$ and $E_z = 0$ and H-Polarization refer to the case when $H_x \neq 0$, $H_y = 0$ and $H_z = 0$. Maxwell's equations (1 TO 4) decouple into two sets of equations. The expressions for E-Polarization are :

$$\frac{\partial^2 E_x}{\partial y^2} + \frac{\partial^2 E_x}{\partial z^2} = j\omega\mu\omega E_x \quad 20$$

$$H_x = 0 \quad 21$$

$$\frac{\partial E_x}{\partial z} = j\omega\mu H_y \quad 22$$

$$\frac{\partial E_x}{\partial y} = j\omega\mu H_z \quad 23$$

In the case of H-Polarization we account for the structural conductivity gradients :

$$\frac{\partial^2 H_x}{\partial y^2} + \frac{\partial^2 H_x}{\partial z^2} - \frac{1}{\omega} \left[\frac{\partial \omega}{\partial y} \frac{\partial H_x}{\partial y} + \frac{\partial \omega}{\partial z} \frac{\partial H_x}{\partial z} \right] - j\omega\mu\omega H_x = 0 \quad 24$$

$$E_x = 0 \quad 25$$

$$\frac{\partial H_x}{\partial z} = \omega E_y \quad 26$$

$$\frac{\partial H_x}{\partial y} = -\omega E_z \quad 27$$

Kron (1944) and Madden (1965) have likened the two-dimensional case to that of an electrical transmission surface. This may in turn be approximated by a two-dimensional lumped circuit (Brewitt-Taylor and Johns 1980). The transmission surface is characterized by series impedance Z per unit length and shunt admittance Y per unit length so that :

$$\text{grad } V = -ZI \quad 28$$

$$\text{div } I = YV \quad 29$$

After some manipulation we obtain the following analogue :

$$\frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} - \frac{1}{Z} \left[\frac{\partial Z}{\partial y} \frac{\partial V}{\partial y} + \frac{\partial Z}{\partial z} \frac{\partial V}{\partial z} \right] + ZYV = 0 \quad 30$$

$$\frac{\partial V}{\partial y} = -ZI_y \quad 31$$

$$\frac{\partial V}{\partial z} = -ZI_z \quad 32$$

Comparing (30), (31) and (32) with (20), (22) and (23) we have the analogue for E-polarization where, $V=E_x$, $I_y=H_y$, $Z=i\omega\mu$ and $Y=\sigma$ with μ invariant with position for example. Comparing (30), (31) and (32) with (24), (26) and (27) we have the analogue for H-polarization where $V=H_x$, $I_y=-E_y$, $I_z=E_z$, $Z=\sigma$ and $Y=-i\omega\mu$ for example. The expressions (30), (31) and (32) also give an analogue for the one-dimensional case.

2.5 THE FINITE DIFFERENCE REPRESENTATION

In general the solution of the two-dimensional problem requires the use of numerical methods. Two common methods are the finite-difference and finite-element methods. The finite-difference method (Brewitt-Taylor and Weaver 1976, Brewitt-Taylor and Johns 1976) was used for the purposes of this investigation and is described below.

A mesh of nodes is laid over the region of interest. Each grid square is assigned a conductivity at its centre whereas the field values are calculated at the nodes. The mesh lines form divisions between regions of different conductivity, as shown in Figure (2.2).

2.5.1 E-POLARIZATION AND H-POLARIZATION.

Consider the case of E-Polarization described in Figure (1.2).

Using central difference formulae to second order we obtain a finite difference expression for (20) of the form :

$$\frac{2}{K_m + K_{m-1}} \left[\frac{E_{m+1/2, n}}{K_m} + \frac{E_{m-1/2, n}}{K_{m-1}} \right] + \frac{2}{K_n + K_{n-1}} \left[\frac{E_{m, n+1}}{K_n} + \frac{E_{m, n-1}}{K_{n-1}} \right] = j\omega\mu \langle \sigma \rangle E_{mn} + \left[\frac{2}{K_m K_{m-1}} + \frac{2}{K_n K_{n-1}} \right] E_{mn} \quad 33$$

Where the conductivity has been averaged in orthogonal directions to give $\langle \sigma \rangle$ as :

$$\langle \sigma \rangle = \frac{K_{m-1} K_n \sigma_{m-1/2, n-1/2} + K_{m-1} K_n \sigma_{m-1/2, n+1/2} + K_m K_{n-1} \sigma_{m+1/2, n-1/2} + K_m K_{n-1} \sigma_{m+1/2, n+1/2}}{[K_{m-1} + K_m][K_{n-1} + K_n]} \quad 34$$

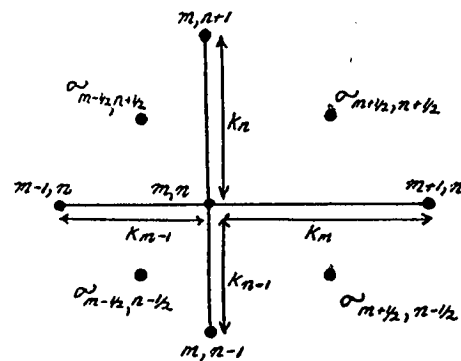
The surface value of the magnetic field is obtained from (20) and (22). At a surface node m, q the expression for the electric field is expanded upwards and downwards in a Taylor series to produce after some algebra:

$$B_y = \frac{j K_q K_{q-1}}{\omega [K_q + K_{q-1}]} \left[\frac{E_{mq+1}}{K_q^2} - \frac{E_{mq-1}}{K_{q-1}^2} \right] - \left[\frac{1}{K_q^2} - \frac{1}{K_{q-1}^2} + j \frac{\omega \mu \sigma_{mq+1/2}}{2} \right] E_{mq} \quad 35$$

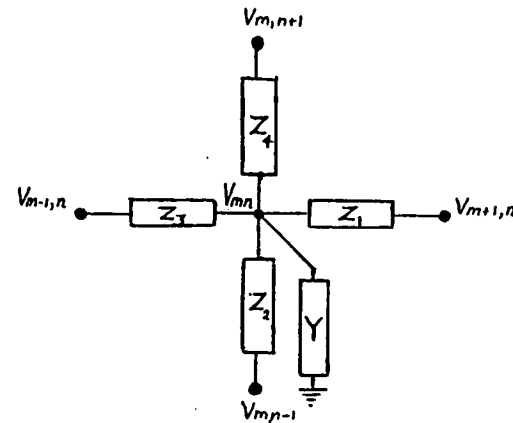
Now consider the case of H-Polarization. The use of the central difference formulae to second order in conjunction with equation (24)

yields:

$$\frac{1}{K_m + K_{m-1}} \left[\left[\frac{2S_{mn}}{K_m} + \left(\frac{\partial S}{\partial y} \right)_{mn} \right] B_{m+1/2, n} + \left[\frac{2S_{mn}}{K_{m-1}} - \left(\frac{\partial S}{\partial y} \right)_{mn} \right] B_{m-1/2, n} \right] + \frac{1}{K_n + K_{n-1}} \left[\left[\frac{2S_{mn}}{K_n} + \left(\frac{\partial S}{\partial z} \right)_{mn} \right] B_{m, n+1/2} + \left[\frac{2S_{mn}}{K_{n-1}} - \left(\frac{\partial S}{\partial z} \right)_{mn} \right] B_{m, n-1/2} \right] = \left[\frac{2S_{mn}}{K_m K_{m-1}} + \frac{2S_{mn}}{K_n K_{n-1}} + j\omega\mu \right] B_{mn} \quad 36$$



PARAMETER DEFINITIONS



LUMPED CIRCUIT ANALOGUE REPRESENTING THE BREWITT-TAYLOR WEAVER EQUATIONS FOR A LIMITED RANGE OF MODELS

LUMPED CIRCUIT EQUIVALENCES. E-POLARIZATION.	LUMPED CIRCUIT EQUIVALENCES. H-POLARIZATION.
$Z_1 = \frac{2}{K_m (K_m + K_{m-1})}$	$Z_1 = \frac{2}{(K_m + K_{m-1})} \left[\frac{\langle S \rangle}{K_m} + \left(\frac{S_{m,n} - S_{m,n-1}}{K_m + K_{m-1}} \right) \right]$
$Z_2 = \frac{2}{K_{n-1} (K_n + K_{n-1})}$	$Z_2 = \frac{2}{(K_n + K_{n-1})} \left[\frac{\langle S \rangle}{K_{n-1}} - \left(\frac{S_{m,n} - S_{m,n-1}}{K_n + K_{n-1}} \right) \right]$
$Z_3 = \frac{2}{K_{m-1} (K_m + K_{m-1})}$	$Z_3 = \frac{2}{(K_m + K_{m-1})} \left[\frac{\langle S \rangle}{K_{m-1}} - \left(\frac{S_{m,n} - S_{m,n-1}}{K_m + K_{m-1}} \right) \right]$
$Z_4 = \frac{2}{K_n (K_n + K_{n-1})}$	$Z_4 = \frac{2}{(K_n + K_{n-1})} \left[\frac{\langle S \rangle}{K_n} + \left(\frac{S_{m,n} - S_{m,n-1}}{K_n + K_{n-1}} \right) \right]$
$Y = i\omega\mu \langle \sigma \rangle$	$Y = i\omega\mu$
$\langle \sigma \rangle = \frac{K_{m-1}K_n \sigma_{m-1/2,n-1/2} + K_{m-1}K_n \sigma_{m-1/2,n+1/2} + K_m K_{n-1} \sigma_{m+1/2,n-1/2} + K_m K_n \sigma_{m+1/2,n+1/2}}{(K_m + K_{m-1})(K_n + K_{n-1})}$	$\langle S \rangle = \frac{K_{m-1}K_n S_{m-1/2,n} + K_{m-1}K_n S_{m+1/2,n} + K_m K_{n-1} S_{m,n-1/2} + K_m K_n S_{m,n+1/2}}{(K_m + K_{m-1})(K_n + K_{n-1})}$

FIGURE 2.2. THE FINITE DIFFERENCE MESH. THE CIRCUIT ANALOGUE.

The resistivities are averaged using an expression similar to (35) and the expressions for $(\partial\rho/\partial y)_{mn}$, $(\partial\rho/\partial z)_{mn}$ are obtained to first order from the appropriate central difference formulae.

The surface electric field is obtained by expanding the expression for B_{m1} downwards by means of a Taylor series. By assuming that the surface nodes are located inside the region of varying conductivity we obtain $(\partial\rho/\partial z)_{mn}=0$. Then from (24) and (26) we conclude that:

$$E_y = \frac{S[B_{m1} - \mu H]}{\mu K_1} - j \frac{K_1 \omega \mu H}{2} \quad 37$$

where H is the magnetic field strength at the surface.

2.5.2 AN ELECTRIC CIRCUIT ANALOGUE.

We may now exploit the lumped circuit analogue of (30), (31) and (32). We note that for a structure such as that shown in Figure (1.2) :

$$\frac{V_{mn1}}{Z_1} + \frac{V_{mn-1}}{Z_2} + \frac{V_{m-1n}}{Z_3} + \frac{V_{m,n+1}}{Z_4} = \left[\frac{1}{Z_1} + \frac{1}{Z_2} + \frac{1}{Z_3} + \frac{1}{Z_4} + Y \right] V_{mn} \quad 38$$

This expression is seen to be similar to both (33) for the E-Polarization and (36) for the H-Polarization under certain circumstances. The necessary equivalences to obtain similarity are found in Figure (1.2).

The simultaneous solution of such a set of simultaneous equations involves a sparse coefficient matrix with no more than five coefficients per row as compared with seven coefficients per row for the finite element equations where triangular elements are used. The Brewitt-Taylor and Weaver program uses a sparse matrix inversion procedure due to Zollenkopf. In this procedure only non-zero elements are processed to produce an inverse in terms of left and right-hand factors.

2.6 THE ROTATION OF THE IMPEDANCE TENSOR

In general the electric and magnetic field vectors above a conductivity structure are related by the impedance tensor Z where:

$$\underline{\underline{Z}} \underline{\underline{H}} = \underline{\underline{E}} \quad 39$$

Let $\underline{\underline{E'}}$ and $\underline{\underline{H'}}$ be the electric and magnetic fields measured in the rotated frame of reference and let $\underline{\underline{Z'}}$ be the corresponding impedance tensor such that:

$$\underline{\underline{Z'}} \underline{\underline{H'}} = \underline{\underline{E'}} \quad 40$$

Then if R is a rotation matrix we have:

$$Z' = R Z R^{-1} \quad 41$$

In the general three-dimensional case (Sims and Bostick 1969, Hermance 1973) the elements of Z' are as below:

$$Z'_{xx} = \left[\frac{Z_{xx} + Z_{yy}}{2} \right] - Z_0 \left[\theta + \pi/4 \right] \quad 42$$

$$Z'_{yy} = \left[\frac{Z_{xx} + Z_{yy}}{2} \right] + Z_0 \left[\theta + \pi/4 \right] \quad 43$$

$$Z'_{xy} = \left[\frac{Z_{xy} - Z_{yx}}{2} \right] + Z_0 \left[\theta \right] \quad 44$$

$$Z'_{yx} = \left[\frac{Z_{yx} - Z_{xy}}{2} \right] + Z_0 \left[\theta \right] \quad 45$$

Where Z_0 is given by:

$$Z_0 = \left[\frac{Z_{xy} + Z_{yx}}{2} \right] \cos 2\theta - \left[\frac{Z_{xx} - Z_{yy}}{2} \right] \sin 2\theta \quad 46A$$

and θ is the angle through which the frame of reference is rotated.

In the two-dimensional case the E-Polarization and H-Polarization equations decouple into two independent sets as shown so that $Z_{xx} = Z_{yy} = 0$. Furthermore in the one-dimensional case we have in addition $Z_{xy} = -Z_{yx}$.

2.6.1 THE DIMENSIONALITY INDICATORS.

A convenient index of dimensionality is given by the skew S where :

$$S = \frac{|Z_{xx} + Z_{yy}|}{|Z_{xy} - Z_{yx}|} \quad 46B$$

where the conductivity structure of the earth is one or two-dimensional when $S=0$ (section 1.4) whereas for three dimensional conductivity structures S is finite.

2.7 THE ESTIMATION OF THE IMPEDANCE MATRIX

Consider measurements of the parameters E_x , H_x , E_y and H_y where:

$$\begin{bmatrix} H_{x1} & H_{y1} \\ H_{x2} & H_{y2} \end{bmatrix} \begin{bmatrix} Z_{xx} \\ Z_{xy} \end{bmatrix} = \begin{bmatrix} E_{x1} \\ E_{x2} \end{bmatrix} + \begin{bmatrix} \mathcal{E}_1 \\ \mathcal{E}_2 \end{bmatrix} \quad 47$$

On condition that the polarizations of the two source fields differ, that is $\det H \neq 0$ we may estimate z_{xx} and z_{xy} .

Define the squared error as ψ for n such equations (Sims and Bostick 1969, Hermance 1973). Then we have:

$$\psi = \sum_{i=1}^n \left[E_{xi} - Z_{xx} H_{xi} - Z_{xy} H_{yi} \right] \left[E_{xi}^* - Z_{xx}^* H_{xi}^* - Z_{xy}^* H_{yi} \right] \quad 48$$

Differentiating ψ with respect to real and imaginary parts and setting :

$$d\psi/d\mathcal{R}\{Z_{xx}\} = d\psi/d\mathcal{I}\{Z_{xx}\} = 0 \quad 49$$

We obtain :

$$\sum E_{xi} H_{xi}^* = Z_{xx} \sum H_{xi} H_{xi}^* + Z_{xy} \sum H_{yi} H_{xi}^* \quad 50$$

$$\sum E_{xi} H_{yi}^* = Z_{xx} \sum H_{xi} H_{yi}^* + Z_{xy} \sum H_{yi} H_{yi}^* \quad 51$$

The noise on E_x may be minimised by the simultaneous solution of (50) and (51) as below :

$$\langle E_x H_x^* \rangle = Z_{xx} \langle H_x H_x^* \rangle + Z_{xy} \langle H_y H_x^* \rangle \quad 52$$

$$\langle E_x H_y^* \rangle = Z_{xx} \langle H_x H_y^* \rangle + Z_{xy} \langle H_y H_y^* \rangle \quad 53$$

where the mean values have been taken.

Using a similar method we obtain :

$$E_x E_x^* = Z_{xx} \langle H_x E_x^* \rangle + Z_{xy} \langle H_y E_x^* \rangle \quad 54$$

$$E_x E_y^* = Z_{xx} \langle H_x E_y^* \rangle + Z_{xy} \langle H_y E_y^* \rangle \quad 55$$

Equations (52 TO 55) yield six estimates for z_{xy} as below :

$$\langle Z_{xy} \rangle = \frac{\langle H_x E_x^* \rangle \langle E_x E_y^* \rangle - \langle H_x E_y^* \rangle \langle E_x E_x^* \rangle}{\langle H_x E_x^* \rangle \langle H_y E_y^* \rangle - \langle H_x E_y^* \rangle \langle H_y E_x^* \rangle} \quad 56$$

$$\langle Z_{xy} \rangle = \frac{\langle H_x E_x^* \rangle \langle E_x H_y^* \rangle - \langle H_x H_y^* \rangle \langle E_x E_x^* \rangle}{\langle H_x E_x^* \rangle \langle H_y H_x^* \rangle - \langle H_x H_y^* \rangle \langle H_y E_x^* \rangle} \quad 57$$

$$\langle Z_{xy} \rangle = \frac{\langle H_x E_y^* \rangle \langle E_x H_y^* \rangle - \langle H_x H_y^* \rangle \langle E_x E_x^* \rangle}{\langle H_x E_x^* \rangle \langle H_y H_y^* \rangle - \langle H_x H_y^* \rangle \langle H_y E_x^* \rangle} \quad 58$$

$$\langle Z_{xy} \rangle = \frac{\langle H_x E_x^* \rangle \langle E_x H_y^* \rangle - \langle H_x H_y^* \rangle \langle E_x E_y^* \rangle}{\langle H_x E_y^* \rangle \langle H_y H_x^* \rangle - \langle H_x H_y^* \rangle \langle H_y E_y^* \rangle} \quad 59$$

$$\langle Z_{xy} \rangle = \frac{\langle H_x E_y^* \rangle \langle E_x H_y^* \rangle - \langle H_x H_y^* \rangle \langle E_x E_x^* \rangle}{\langle H_x E_y^* \rangle \langle H_y H_y^* \rangle - \langle H_x H_y^* \rangle \langle H_y E_y^* \rangle} \quad 60$$

$$\langle Z_{xy} \rangle = \frac{\langle H_x H_x^* \rangle \langle E_x H_y^* \rangle - \langle H_x H_y^* \rangle \langle E_x H_x^* \rangle}{\langle H_x H_x^* \rangle \langle H_y H_y^* \rangle - \langle H_x H_y^* \rangle \langle H_y H_x^* \rangle} \quad 61$$

The fields are usually assumed to be slowly varying functions of frequency (although this may not always be true as in the case near vertical conductivity boundaries) so that the mean $\langle A_i B_j^* \rangle$ represents the cross-power spectrum between A_i and B_j at some centre frequency.

In a one-dimensional situation where the fields are highly unpolarized estimates (58) and (59) become unstable since $\langle E_x E_y^* \rangle$, $\langle E_x H_x^* \rangle$, $\langle E_y H_y^* \rangle$ and $\langle H_x H_y^* \rangle$ tend to zero.

2.8 THE EFFECTS OF RANDOM NOISE UPON THE Z ESTIMATES

Let X_C be a measured electric or magnetic field component so that :

$$X_C = X_{CS} + X_{Cn} \quad 62$$

where X_{CS} is the signal and X_{Cn} is the noise. Assume for simplicity (Sims and Bostick 1969) a one-dimensional model where we may decompose the signal as below :

$$E_x \neq 0 \quad H_y \neq 0 \quad \langle E_x E_x^* \rangle \neq 0 \quad \langle H_y H_y^* \rangle \neq 0 \quad \langle E_x H_y^* \rangle \neq 0$$

Also

$$E_y \neq 0 \quad H_x \neq 0 \quad \langle E_y E_y^* \rangle \neq 0 \quad \langle H_x H_x^* \rangle \neq 0 \quad \langle E_y H_x^* \rangle \neq 0$$

But where

$$\langle E_x E_y^* \rangle \rightarrow 0 \quad \langle H_y H_x^* \rangle \rightarrow 0$$

Under these conditions we have in addition :

$$\langle E_x E_y^* \rangle \rightarrow 0 \quad \langle E_x H_x^* \rangle \rightarrow 0 \quad \langle E_y H_y^* \rangle \rightarrow 0 \quad \langle H_x H_y^* \rangle \rightarrow 0$$

Equations (58) and (59) then yield :

$$\langle Z_{xy} \rangle \rightarrow \langle E_x E_x^* \rangle / \langle H_y E_x^* \rangle \quad 63$$

$$\langle Z_{xy} \rangle \rightarrow \langle E_x H_y^* \rangle / \langle H_y H_y^* \rangle \quad 64$$

Utilizing (62) we obtain the cross-power and autopower spectra expressions below :

$$\langle E_x E_x^* \rangle = \langle E_{xs} E_{xs}^* \rangle + \langle E_{xn} E_{xn}^* \rangle \quad 65$$

$$\langle H_y H_y^* \rangle = \langle H_{ys} H_{ys}^* \rangle + \langle H_{yn} H_{yn}^* \rangle \quad 66$$

$$\langle E_x H_y^* \rangle = \langle E_{xs} H_{ys}^* \rangle + \langle E_{xs} H_{yn}^* \rangle + \langle E_{xn} H_{ys}^* \rangle + \langle E_{xn} H_{yn}^* \rangle \quad 67$$

$$\langle H_y E_x^* \rangle = \langle H_{ys} E_{xs}^* \rangle + \langle H_{ys} E_{xn}^* \rangle + \langle H_{yn} E_{xs}^* \rangle + \langle H_{yn} E_{xn}^* \rangle \quad 68$$

Let us assume that the noise signals are random, that is they are uncorrelated with either the signal or with themselves. In this case (67) and (68) yield :

$$\langle E_x H_y^* \rangle = \langle H_y E_x^* \rangle = \langle E_{xs} H_{ys}^* \rangle \quad 69$$

Under these conditions (63) yields :

$$\langle Z_{xy} \rangle = Z_{xy} \left[1 + \frac{\langle E_{xn} E_{xn}^* \rangle}{\langle E_{xs} E_{xs}^* \rangle} \right] \quad 70$$

Similarly (64) yields :

$$\langle Z_{xy} \rangle = Z_{xy} / \left[1 + \frac{\langle H_{yn} H_{yn}^* \rangle}{\langle H_{ys} H_{ys}^* \rangle} \right] \quad 71$$

It is thus seen that the noise effectively biases the Z estimates. This fact was used in this study to assess the reliability of the data before modelling was undertaken.

2.9 THE COHERENCE FUNCTIONS

Let $s(t)$ and $u(t)$ be two series and let $S(\omega)$ and $U(\omega)$ be their respective Fourier transforms. Then the coherence between $s(t)$ and $u(t)$ is given by c_{su} where :

$$C_{su}^2 = \frac{\langle S(\omega) U^*(\omega) \rangle \langle S(\omega) U^*(\omega) \rangle}{\langle S(\omega) S^*(\omega) \rangle \langle U(\omega) U^*(\omega) \rangle} \quad 72$$

The index yields $C_{su}=1$ for perfectly correlated signals and $C_{su}=0$; for totally uncorrelated signals.

Now consider the signal $s(t)$ to be a linear combination of $u(t)$ and $v(t)$ as below:

$$S(\omega) = Z_u(\omega) U(\omega) + Z_v(\omega) V(\omega) \quad 73$$

The expected value of $S(\omega)$ is given by :

$$\langle S(\omega) \rangle = \langle Z_u(\omega) U(\omega) \rangle + \langle Z_v(\omega) V(\omega) \rangle \quad 74$$

Define the Predicted Coherency between $S(\omega)$ and $\langle S(\omega) \rangle$ as below :

$$C_{ss}^2 = \frac{|\langle Z_u \rangle \langle S(\omega) U^*(\omega) \rangle + \langle Z_v \rangle \langle S(\omega) V^*(\omega) \rangle|^2}{\langle S(\omega) S^*(\omega) \rangle [\langle Z_u \rangle \langle Z_u^* \rangle \langle U(\omega) U^*(\omega) \rangle + \langle Z_v \rangle \langle Z_v^* \rangle \langle V(\omega) V^*(\omega) \rangle + 2 \Re \{ \langle Z_u \rangle \langle Z_v^* \rangle \langle U(\omega) V^*(\omega) \rangle \}]} \quad 75$$

The effect of noise upon the coherence may be envisaged by writing :

$$S(t) = S_s(t) + S_n(t) \quad 76$$

$$u(t) = u_s(t) + u_n(t) \quad 77$$

where s_s and u_s are noise free signals and s_n and u_n represent the random noise. If s_n and u_n are uncorrelated and independent of the signals then we obtain :

$$C_{su}^2 = \frac{S_s(\omega) S_s^*(\omega) U_s(\omega) U_s^*(\omega)}{[S_s(\omega) S_s^*(\omega) + S_n(\omega) S_n^*(\omega)] [U_s(\omega) U_s^*(\omega) + U_n(\omega) U_n^*(\omega)]} \quad 78$$

Thus we obtain a coherence C_{su}^2 where $C_{su}^2 < 1$.

2.10 THE ESTIMATION OF THE POWER SPECTRA

Define the cross-correlation function of two transient signals $x(t)$ and $y(t)$ as $p_{xy}(\tau)$ where :

$$p_{xy}(\tau) = \int_{-\infty}^{+\infty} x(t) y(t+\tau) dt \quad 79$$

The Fourier transform of $p_{xy}(\tau)$ is known as the cross-energy density function $P_{xy}(\omega)$ where :

$$P_{xy}(\omega) = \int_{-\infty}^{+\infty} p_{xy}(\tau) e^{j\omega\tau} d\tau \quad 80$$

Let us assume that we may represent $y(t+\tau)$ by the expression below :

$$y(t+\tau) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} Y(\omega) e^{j\omega(t+\tau)} d\omega \quad 81$$

Then from (79) we may obtain :

$$p_{xy}(\tau) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} Y(\omega) \left[\int_{-\infty}^{+\infty} x(t) e^{j\omega t} dt \right] e^{j\omega\tau} d\omega \quad 82$$

Hence we obtain the cross-energy density function of $x(t)$ and $y(t)$ as

$$P_{xy}(\omega) = X^*(\omega) Y(\omega) \quad 83$$

where $X(\omega)$ and $Y(\omega)$ are the Fourier transforms of $x(t)$ and $y(t)$ respectively.

When considering stationary random processes we may define the cross-correlation function as :

$$p_{xy}(\tau) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-T/2}^{+T/2} x(t) y(t+\tau) dt \quad 84$$

The Fourier transform of (84) produces the cross-power spectrum :

$$P_{xy}(\omega) = \int_{-\infty}^{+\infty} p_{xy}(\tau) e^{-j\omega\tau} d\tau \quad 85$$

In practice it is not possible to calculate numerically a Fourier transform over the range $-\infty$ TO $+\infty$ and it is customary to take the transform of $x(t)$ over a window of duration t as below :

$$X(\omega) = \int_{-T/2}^{+T/2} x(t) e^{-j\omega t} dt \quad 86$$

However the window modulates $x(t)$ in the time domain to produce sidebands characterized by the sinc function. These sidebands which are generally described as leakage may be reduced by using a tapered window of some description defined by $w(t)$. Then we have :

$$X(\omega) = \int_{-T'}^{+T'} x(t) w(t) e^{-j\omega t} dt \quad 87$$

where T' is taken to be sufficiently large to cover the range where $w(t) \neq 0$. The cosine taper window was used in this study. As we only

use ratios of the Fourier transforms it is not necessary to correct for the effect of the window taper used.

CHAPTER III

THE INSTRUMENTATION

3. THE INSTRUMENTATION.

This chapter describes a set of active filters used in conjunction with the N.E.R.C. Geologger and the E.C.A. CM11E magnetic sensors. The resultant Magnetotelluric system was designed by the author with a pass-band extending from 0.4 Hz. TO 100 Hz.

In addition the Short Period Automatic Magnetotelluric (S.P.A.M.) system is also described.

3.1 THE NEED FOR A NON-AUTOMATIC LONG PERIOD RECORDING SYSTEM

During September 1981, the S.P.A.M. system of Dawes described in section (3.5) was completed and first used in the Travale region of Italy in a program of research undertaken as part of the E.E.C. Geothermal Project. The system was theoretically capable of automatically selecting Magnetotelluric events on a real-time basis in the frequency range 780 Hz. TO 0.01 Hz. which was divided into four adjacent bands. Approximately seventy sets of five component Magnetotelluric events could be recorded on a magnetic tape for each band. When the measurements in one band had been completed the measurements in another band could commence. It was found however that whereas event recording for each of the first two highest frequency bands took approximately one hour each, it took approximately three hours to record data from the third band covering the frequency range 6.0 Hz. TO 0.25 Hz.

It was realized that a digital tape recorder such as the N.E.R.C. Geologger digitising at the rate of 1 Hz. could be operated continuously for more than six hours before the magnetic tape had to be replaced. Such a system need not actually select events, but record all magnetic and telluric variations, the tape later being analysed in the laboratory in a fraction of the actual recording time. Furthermore the system could be operated without attention on a continuous basis while higher frequency data were being recorded with the S.P.A.M. system.

In the Moine Thrust region the crustal rocks were expected to have resistivities in the range 10^2 TO 10^4 ohm-metres. Thus electromagnetic

fields of frequencies from 0.25 Hz. TO 0.01 Hz. could penetrate to depths greater than the crustal thickness of approximately 30 Km. and data in this frequency range could constrain the range of possible structures at the base of the eventual crustal model.

3.2 THE GENERAL DESIGN

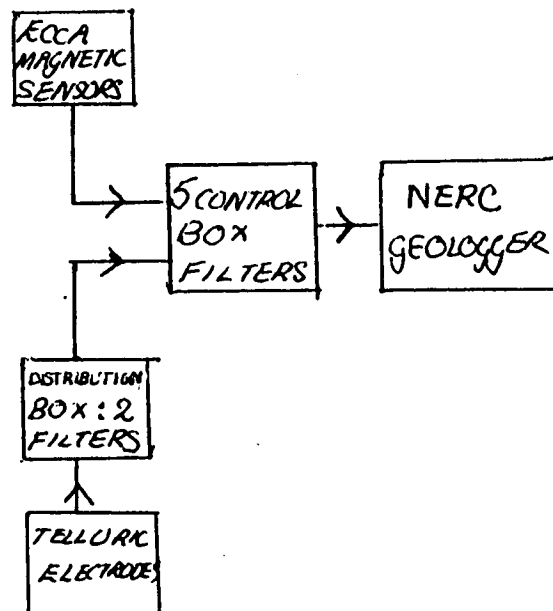
The author was required to formalize the specification of a set of five matched bandpass filters and also to design and test these filters. The filters were required for use in conjunction with the N.E.R.C. Geologger and E.C.A. CM11E magnetic sensors. An additional pair of matched filters was required for use with the telluric electrodes having a contact resistance of not more than 10 kilohms.

The principal requirement of the design of the five matched filters was the production of an anti-aliasing high-frequency cut-off. Since the N.E.R.C. Geologger was to be used with its maximum digitising rate of 1 Hz., the voltage transmission of the filters at the Nyquist frequency (0.5 Hz.) was to be not less than 20 db. below that at the band centre. In addition the flat transmission region was to extend as close to the 0.25 Hz. cut-off as possible. The requisite sharp curvature of the response function in the cut-off region thus necessitated the use of circuits which were less than critically damped and it was also necessary that the band edge ringing and overshoot characteristics of the circuit were not excessive. A three pole Butterworth-Optimum-L (Papoulis (1958), Kuo (1966)) Transition filter met the above requirements with minimum circuit complexity and is described in section (3.3) and shown in Figure (3.1).

The lower frequency -3db. point was thought to be of less importance at the time of design and was effected by two passive R-C circuits. The complete circuit thus assumed an assymetric transmission characteristic.

The telluric signal amplifiers were designed to be used with a cross electrode configuration with the common earth electrode at the centre of the cross. This configuration unlike the L configuration does not allow the appearance of any variation in the earth electrode potential as coherent signals in the two orthogonal telluric directions.

The principal requirements of the design for the telluric signal filters were that they should provide a high input impedance of approximately 1 megohm. and D.C. decoupling for the electrodes so that any electrochemical potential between the electrodes would not saturate the subsequent amplifiers. Suppression of 50 Hz. and low frequency noise was effected by a passive R-C bandpass configuration.



THE CONTROL BOX FILTERS

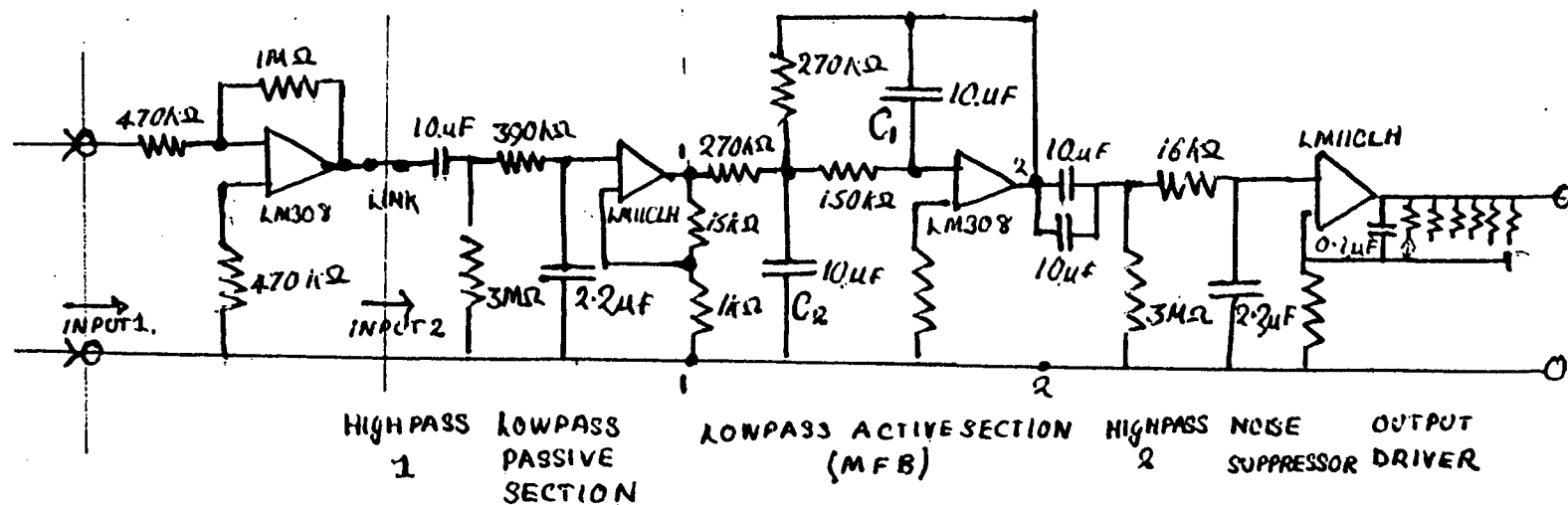
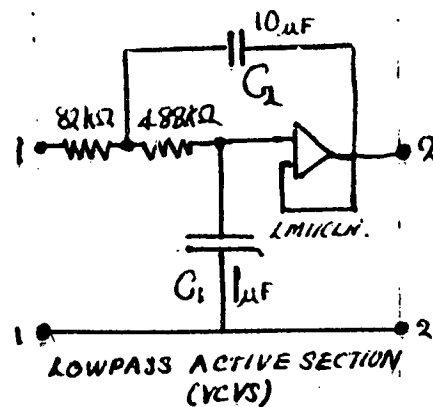


FIGURE 2.1. THE BAND IV SYSTEM FILTERS.

The required passband gains for the five matched filters were in the range from 10 TO 1000, with an additional gain of 10 for the telluric signal filters. With a Geologger dynamic range of ± 10 volts in 5 millivolt digitising steps, this allowed the recording of magnetic signals in the range $\pm 0.1 \times 10^{-13}$ tesla TO $\pm 20 \times 10^{-8}$ tesla and telluric signals in the range 5 microvolts (determined by circuit noise) to 100 millivolts. These ranges were considered suitable for recording signals arising from Pc2, Pc3 and Pc4 magnetic disturbances (section 1.1).

3.3 THE CIRCUIT DESCRIPTION

3.3.1 THE CONTROL BOX CIRCUIT

The assymetric all-pole bandpass characteristic was realized using a lowpass monotonic Butterworth-Optimum-L transition filter in conjunction with a passive high-pass filter. The two complex poles of the transition filter required an active two pole stage. The actual section was of the Multiple Loop Feedback (M.F.B.) type, but the printed circuit board was furnished with Sallen Key Voltage Controlled Voltage Source (V.C.V.S.) connections so that the cut-off could be improved without excessive ratios of $C_1:C_2$ of capacitance in the M.F.B. circuit (Figure 3.1). The transitional lowpass filter was designed graphically with a maximum ratio $C_1:C_2$ of 10 : 1. The single real pole of the transition filter was combined with a real pole of the high-pass filter to form a passive band-pass filter. This passive section preceded the under-damped active section to reduce the possibility of spikes on the input signal reaching and causing saturation at the active section itself. The remaining pole of the high-pass filter was located at the output of the active section and a lowpass L-section with a high cut-off frequency added to suppress high frequency noise before final amplification at the variable gain output stage.

Most of the amplifiers were used in the voltage follower configuration. This was necessary in order to realize sufficiently high input impedances and high gains for the low frequency filters, without the necessity of using high value resistors in the inverting configurations or additional operational amplifiers. Even so with the values of resistors used, moisture and stray capacity affected the circuit performance and thorough varnishing and screening precautions had to be taken. Although R-C product multiplication of 15 or more may be achieved at the expense of circuit gain this technique was not used

in this circuit since the relevant configurations showed little advantage in terms of noise over the high resistance circuits.

It was realized that near 0.2 Hz. there would be little signal. In an attempt to enhance the amplification in this region, the band edge peak of the active section was increased in gain by decreasing the damping. However in practice this led to excessive spike noise at the output and so this approach was abandoned.

3.3.2 THE DISTRIBUTION BOX CIRCUIT

The telluric pre-amplifiers and filters were designed to be used with a cross configuration of electrodes with a central earth. The currents utilized two voltage follower configurations with high input impedances driving a differential amplifier configuration a passive filter section and an output stage. When used with the LM11CLH operational amplifier the circuit proved unsatisfactorily noisy and was temporarily abandoned in favour of the use of two Keithley Model 155 microvoltmeter chopper amplifiers.

A similar circuit was later constructed by Dawes who used the OP-07 operational amplifier which had become available and this circuit was sufficiently quiet for use as a telluric preamplifier.

The Keithley microvoltmeter chopper amplifiers were D.C. decoupled from the electrodes with a high-pass passive R-C section to prevent saturation of the amplifiers by constant electrode potential differences. The amplifiers were used with an L electrode configuration.

A discrete component chopper amplifier circuit based upon the Keithley microvoltmeter circuit but incorporating LM11CLH operational amplifiers yielded similar noise levels to those of the microvoltmeter amplifiers. However they were abandoned in favour of the simplicity of the circuit incorporating the OP-07 operational amplifiers.

3.4 THE CALIBRATION

The calibration of the system was carried out using a spectrum analyser. The five control-box amplifiers were tested for comparable responses as were the responses of the telluric amplifiers. The frequency responses of both sets of amplifiers were obtained independently and these responses together with the published CM11E magnetic sensor response curves were used to obtain the total magnetic and telluric responses. It should be noted that a more satisfactory method of obtaining the total responses would have been by direct

measurement but accurate facilities were not locally available for the magnetic responses, and so such a procedure was similarly not used for the telluric responses.

The noise levels for the system were obtained by loading the inputs with suitable resistors and digitally recording the noise with the N.E.R.C. Geologger. The total noise for the magnetic channels was deduced using these measurements in conjunction with the published data for the CM11E magnetic sensors. Direct measurements of the noise on the magnetic channels was again impractical.

3.5 THE SHORT PERIOD AUTOMATIC MAGNETOTELLURIC (S.P.A.M) SYSTEM

The Short Period Automatic Magnetotelluric (S.P.A.M) system was designed by Dawes to automatically select windows on a real time basis in the field. In this way only good quality data need be recorded.

The S.P.A.M. system recorded data in three bands; 780 Hz. TO 20 Hz. and 30 Hz. TO 1 Hz. and 4 Hz. TO 0.125 Hz. and a fourth band which was not used 0.3 Hz. TO 0.01 Hz. The signal was initially amplified and optionally applied to 50 Hz. and 150 Hz. notch filters to reduce the affects of noise from electrical supply lines. The signal was then applied to anti-aliasing band-pass filters which could select signals in the above frequency ranges. After further programmable amplification the Z,D,H,E and N signals were sequentially sampled and converted from analogue to digital form for in-field computing purposes and written to tape for further analysis.

Each window was sampled at 512 points in the time-domain. The input voltage into the analogue to digital converter was adjusted using the programmable amplifier by decreasing the gain to suitable levels at the beginning of each window. After the window had been converted to digital form the computer analysed the data in the time domain to ensure that :

- (1) The signals had not saturated the equipment.
- (2) The signals contained no spikes.
- (3) The mean of the modulus of the signal amplitude exceeded a given minimum.

On condition that the signals met the above criteria the Fourier transform of the data was taken at 256 frequencies and the data averaged into approximately ten frequency bands.

The data was then analysed in the frequency domain to ensure that:

- (1) The minimum coherencies for the orthogonal measurement directions exceeded a given minimum.
- (2) The number of frequency bands with coherencies satisfying (1) per window exceeded a given minimum.

If any of the above criteria were not met then the time-series data already written to tape was over-written by that of the next window analysed.

CHAPTER IV

THE DATA ACQUISITION AND ANALYSIS

4.1 THE PROFILE LOCATION.

The data for this study were collected in the region of the Moine Thrust (Map 1). A profile line orthogonal to the line of the Thrust was adopted with a high linear density of sites between sites B and F where it was believed the Moine Thrust structure may exist. The objective was to extend the data set of Mbipom (1980) covering the frequency range 1.2×10^{-3} Hz. TO 0.05 Hz. with additional data in the frequency range 0.125 Hz. TO 780 Hz. It was further intended to test the validity of two-dimensional wedge shaped models for the thrust including the model proposed by Soper and Barber (1982) Figure (1.2). It was considered that the Lewisian Foreland should be more resistive than the Moine hinterland owing to the low porosities of the non granular Lewisian Gneiss of the Foreland compared with the higher porosities of the Moinian siliceous granulites of the Hinterland (section 1.4). Hence it was considered that it should be possible to detect a thrust structure in the region of relatively high site density of approximately $0.2 \text{ sites Km}^{-1}$.

The original data set of Mbipom was collected along a profile part of which was adjacent to high tension transmission lines. Since the frequency range of this study included 50 Hz. and switching frequencies, an approximately parallel profile line 15 Kms. to the south of the profile of Mbipom was adopted in this study.

Since the S.P.A.M. equipment was vehicle bound it was necessary to position the sites near roads or tracks. This resulted in the bisection of three-dimensional structures in the region of grid references 265895 and 246901. The latter structure appears on both Bouguer gravity and aeromagnetic anomaly maps (Map (3) and Map (4)).

The positions of the principal sites are given in table (4.1) with the sounding frequencies used at each.

SITE	NATIONAL GRID REFERENCE	FREQUENCY RANGE OF SOUNDING
A	21279243	7.80×10^{-2} TO 1.25×10^{-1}
BAD*	21959475	5.00×10^{-2} TO 1.20×10^{-3}
ACH*	22789409	5.00×10^{-2} TO 1.20×10^{-3}
KIN*	23319364	5.00×10^{-2} TO 1.20×10^{-3}
B	23179103	7.80×10^{-2} TO 1.25×10^{-1}
C	23299052	7.80×10^{-2} TO 4.00
D	23939160	7.80×10^{-2} TO 1.25×10^{-1}
E	24599013	7.80×10^{-2} TO 1.25×10^{-1}
SHN*	25279176	5.00×10^{-2} TO 1.20×10^{-3}
F	25279021	2.00×10^{-1} TO 1.25×10^{-1}
TER*	25639142	5.00×10^{-2} TO 1.20×10^{-3}
LAI*	26059076	5.00×10^{-2} TO 1.20×10^{-3}
BNB*	26348955	5.00×10^{-2} TO 1.20×10^{-3}
G	27188943	7.80×10^{-2} TO 1.25×10^{-1}

* : DATA OF MBIPOM (1980).

TABLE 4.1. THE SITES.

4.2 THE DATA ACQUISITION.

The rate of data collection was limited by the occurrence of natural signal. Frequently there was a polarized signal usually in the east-west direction, with little or no coherent signal in the north-south direction. This was particularly the case in the frequency range 0.125 Hz. TO 4.0 Hz. However at a rate of approximately one in every four days there were satisfactory unpolarized signals over the entire frequency range in which the S.P.A.M. system operated (0.125 Hz. TO 780 Hz.). Hence there were five sites at which measurements were made throughout the complete frequency range with one additional site where measurements were limited to the frequency range 4.0 Hz. TO 780 Hz.

The region between F and G was strongly affected by 50 Hz. noise making measurements with the S.P.A.M. system impossible. Observations at site F were restricted to the range

0.125 Hz. TO 40 Hz. owing to the equipment saturation by 50 Hz. noise before the notch filters.

Owing to the in-field acquisition and analysis facilities of the S.P.A.M. system, it was possible to compare responses obtained at different times at the same site (Figure 4.1). These comparisons showed that smooth responses could be obtained with small random errors where the observations were unrepeatable.

These responses were obtained throughout the entire length of the profile including the north-western regions (Map 2) where little cultural noise was expected. They were thus attributed to source and telluric self-potential field effects. Furthermore the responses of adjacent sites could also be compared. On the assumption that the responses change only slowly with distance this enabled abnormal responses for a given locality to be identified.

The selection of acceptable data was thus to some extent qualitative.

4.3 THE DATA ANALYSIS

Each event window selected by the S.P.A.M. system consisted of 512 samples of magnetic and telluric data in the time-domain for each of the five Magnetotelluric components. The Fourier Transform produced 256 Fourier Coefficients which were divided into ranges on a frequency basis and averaged to produce 52 sets of impedance tensor elements Z_{ij} per window. A broader frequency range was then selected and the impedance values averaged both over the frequencies within the range and over all

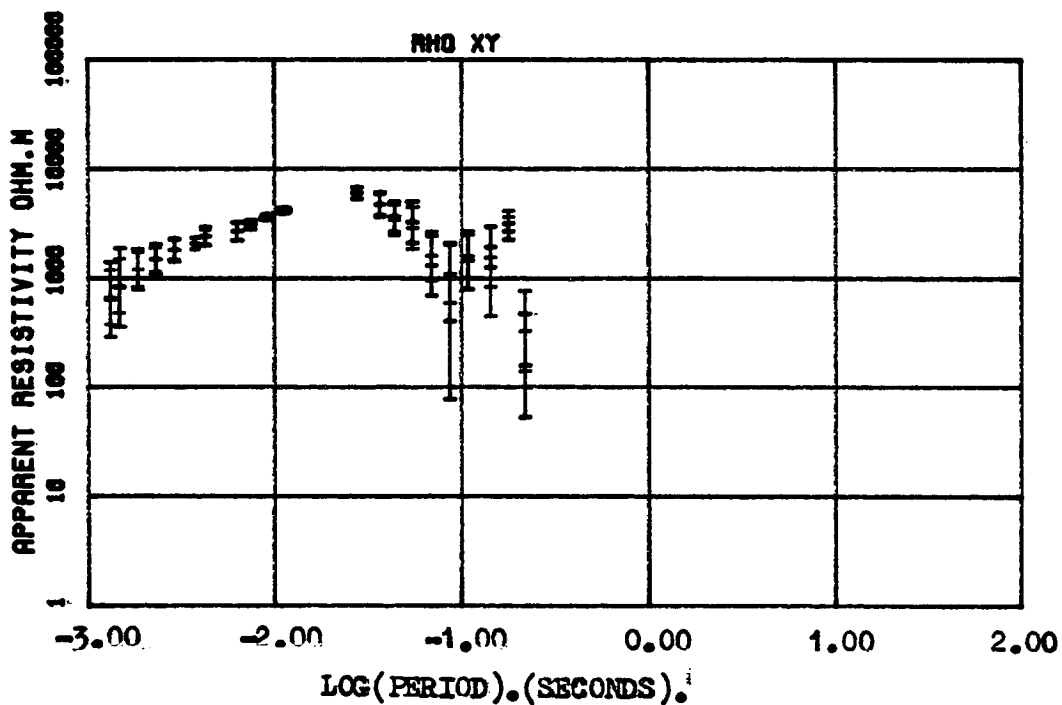
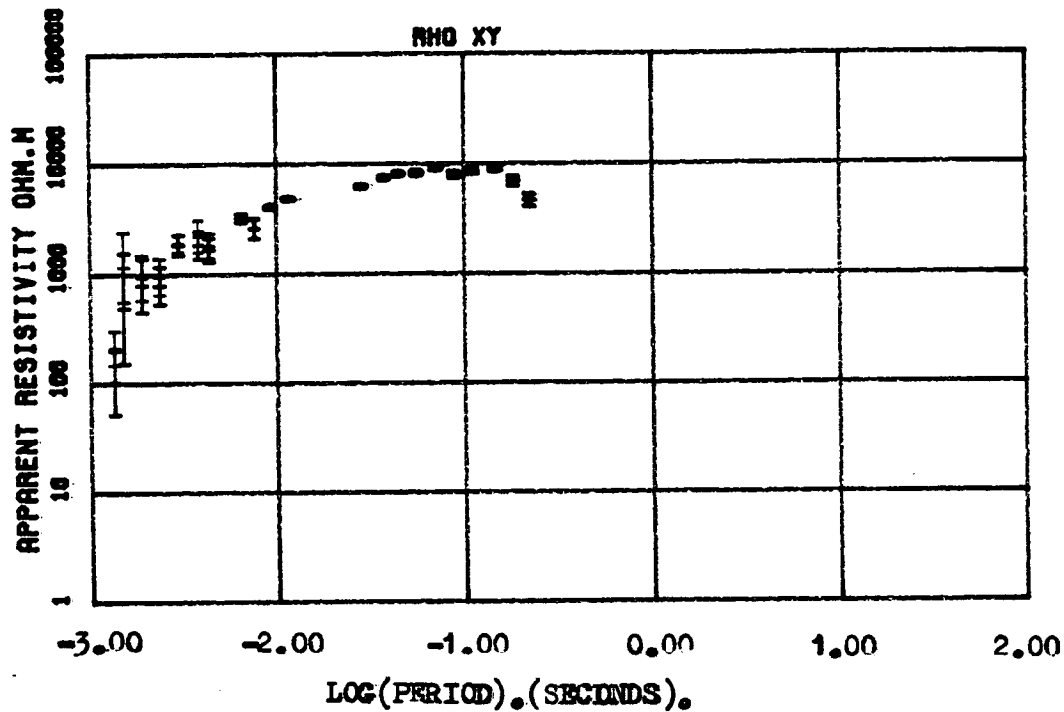


FIGURE 4.1. UNREPEATABLE DATA. THE DATA WAS COLLECTED AT NATIONAL GRID REFERENCE 22629218 ON DIFFERENT DAYS. THE ERRORS PRESENTED ARE DUE TO RANDOM NOISE. THE APPARENT RESISTIVITY ESTIMATES FROM THE SIX IMPEDANCE TENSOR ELEMENT ESTIMATORS ARE SUPERPOSED INDICATING THAT THESE CANNOT BE USED TO IDENTIFY THE DATA AS BEING UNREPEATABLE.

the acceptable windows. The values of Z_{ij} which were associated with a coherency less than some assigned minimum coherency were not included in the average. The impedance tensor was then rotated into its principal axes by maximising the off-diagonal terms. Alternatively the axes of the impedance tensor may be rotated through some fixed azimuth. The elements Z_{xy} and Z_{yx} of the rotated impedance tensor were then used to estimate the appropriate apparent resistivity and phase estimate.

4.4 THE BIAS ANALYSIS.

The bias associated with the apparent resistivity measurements was assessed by estimating the apparent resistivities associated with the four stable equations (56,57,60 and 61) of section (1.7). It was shown in section (1.8) that noise present in the data may bias the apparent resistivity estimates obtained from these equations in different directions. The term bias range as used below is defined as the maximum range in log(ohm-metres) or degrees between the mean estimates obtained from equations 56,57,60 and 61 (section 1.7) at a given frequency. Although use of a minimum acceptable coherency (section 1.9) of almost unity may be a satisfactory criterion for the rejection of data with incoherent noise, coherency does not directly indicate the level of bias present in the apparent resistivity estimates.

The effects of bias appeared to be present at all frequencies and sites in this study. However the bias range appeared to be least between 3.0 Hz. and 40 Hz. while at frequencies below 3.0 Hz. the bias range appeared to increase with decreasing frequency, and at frequencies above 400 Hz. a large bias range was also found.

In this study the presence of bias was taken to indicate that there was some inconsistency between the behaviour of the electric and magnetic fields measured in the field and the assumed theoretical behaviour of those fields upon which the forward modelling was based. For this reason the estimates of apparent resistivity and phase with a large range of bias were not used for modelling purposes. It should however be noted that a large bias range did not necessarily imply that all the associated apparent resistivity and phase measurements were incorrect.

The noise on the data was assumed to be predominantly on the telluric components and the impedance estimator which biased the impedance moduli upwards was used.

The anisotropy in apparent resistivity estimates did not exceed approximately 0.5 decades. In order to identify anisotropic responses

data with a bias range exceeding 0.2 decades was considered inconsistent and was not used for modelling.

It was found that the bias ranges frequently exceeded the standard errors obtained for both the apparent resistivity and phase estimates. For modelling purposes the bias ranges were considered random errors and of the values given in table (4.2).

4.5 THE MAGNETOTELLURIC RESPONSE FUNCTIONS.

The magnetotelluric responses are shown in Figure (4.2). The following earth response functions are shown:

- (1) Orthogonal apparent resistivity and phase responses after rotation through 15° .
- (2) The azimuths of the unrotated data.
- (3) The skew.
- (4) The number of estimates at each frequency.

The following observations were made concerning sites A,B,C,D,F and G.

The anisotropy at sites B,C,D,F and G were larger than at site A but did not exceed 0.5 Log (Ohm-Metres). Excluding frequencies above 100 Hz. and below 1 Hz. the skew is less than 0.2 at sites A,B,C and D but greater than 0.2 at sites F and G.

Site E shows anisotropy of at least 1 Log (Ohm-Metre) and skew scattered values.

The azimuths at each site vary widely.

All the data appear to exhibit bias at frequencies below 1 Hz. However the absence of a large bias range appears to be insufficient to guarantee the reliability of the data since sites A,F and G have data which are scattered yet have a low bias range.

4.6. THE QUALITATIVE INTERPRETATION OF THE MAGNETOTELLURIC RESPONSES.

The complete set of Magnetotelluric responses is now compared with the expected deep geology, the surface geology and the geophysical properties of the region.

BIAS RANGE	ASSUMED ERROR
0.0 TO 0.1 LOG(M.)	+0.1 LOG(M.)
0.1 TO 0.2 LOG(M.)	+0.2 LOG(M.)
GREATER THAN 0.2 LOG(M.)	DATA REJECTED.
0.0° TO 2.5°	+2.5°
2.5° TO 7.5°	+7.5°
GREATER THAN 7.5°	DATA REJECTED.

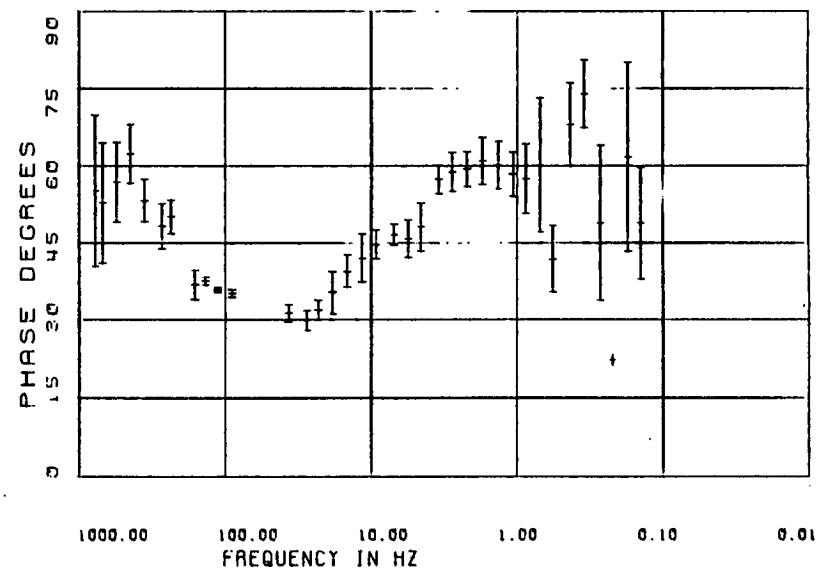
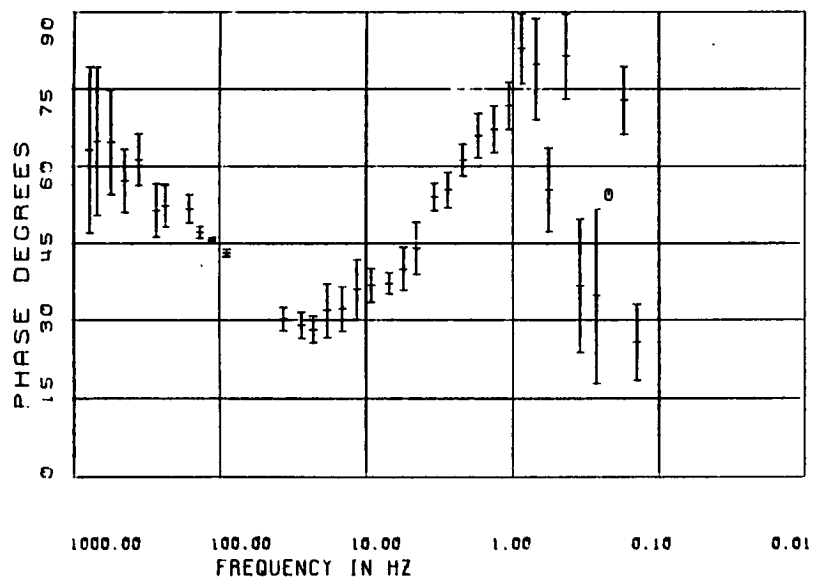
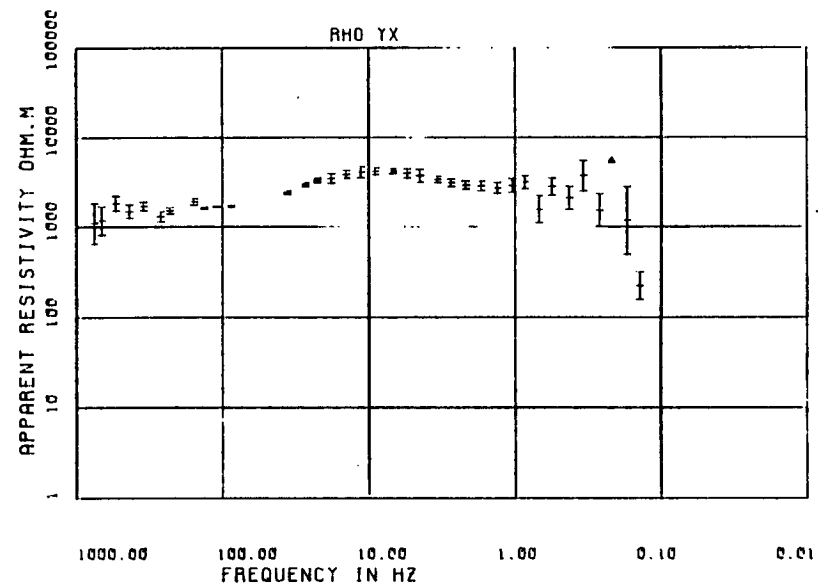
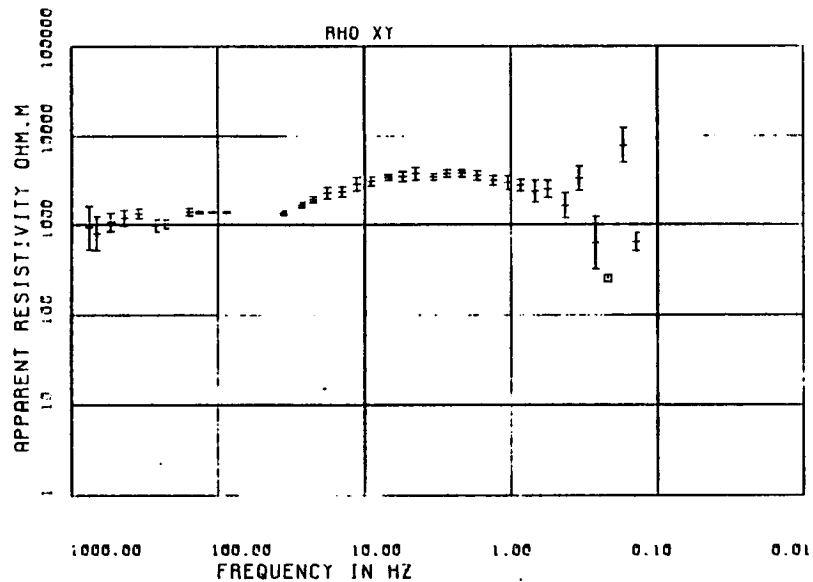
NOTE:

THE ASSUMED ERROR WAS GREATER THAN THE RANDOM ERRORS ON THE ACCEPTED DATA.

TABLE 4.2. THE BIAS RANGES.

FIGURE 4.2

THE MEASURED MAGNETOTELLURIC RESPONSE FUNCTIONS.



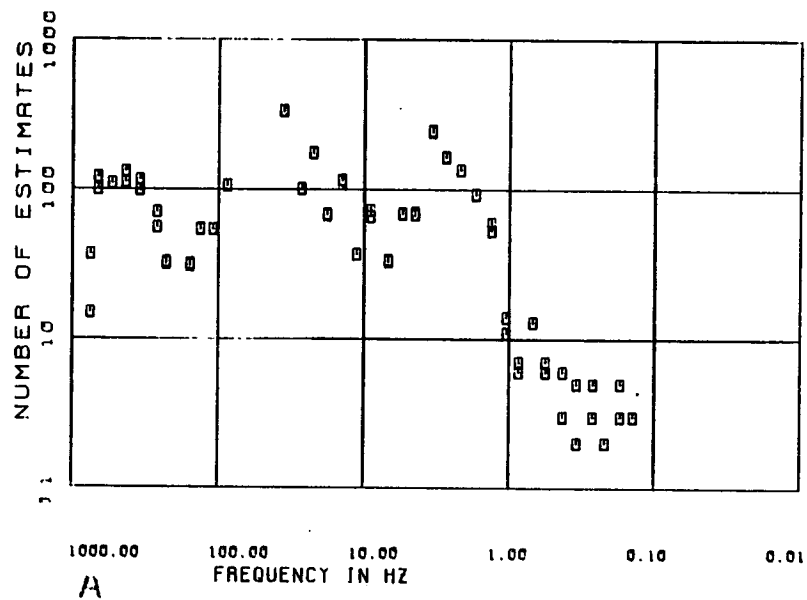
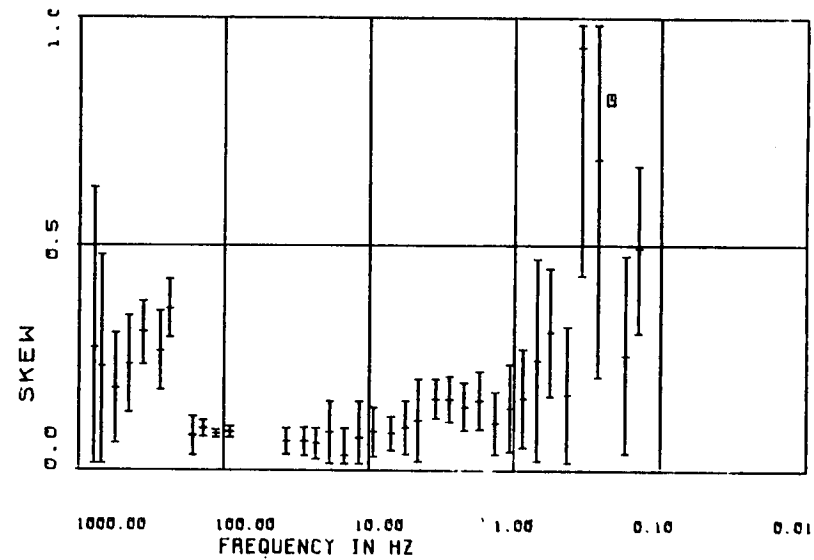
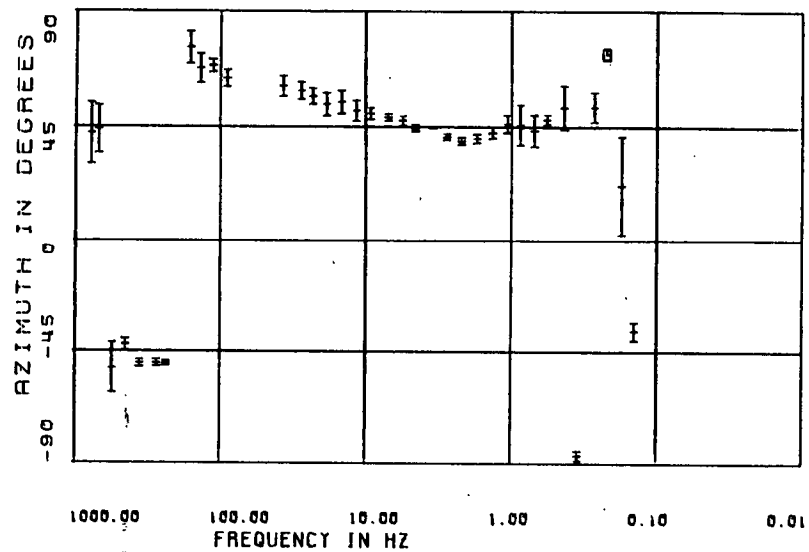
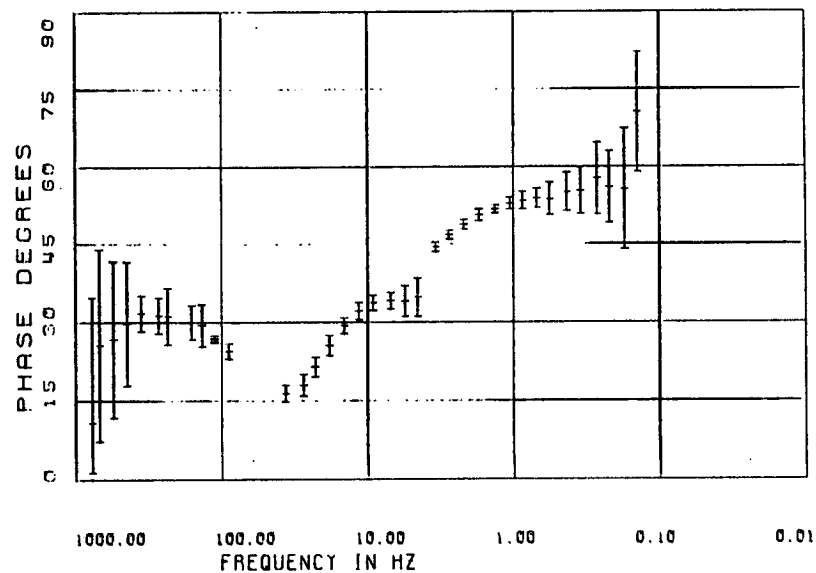
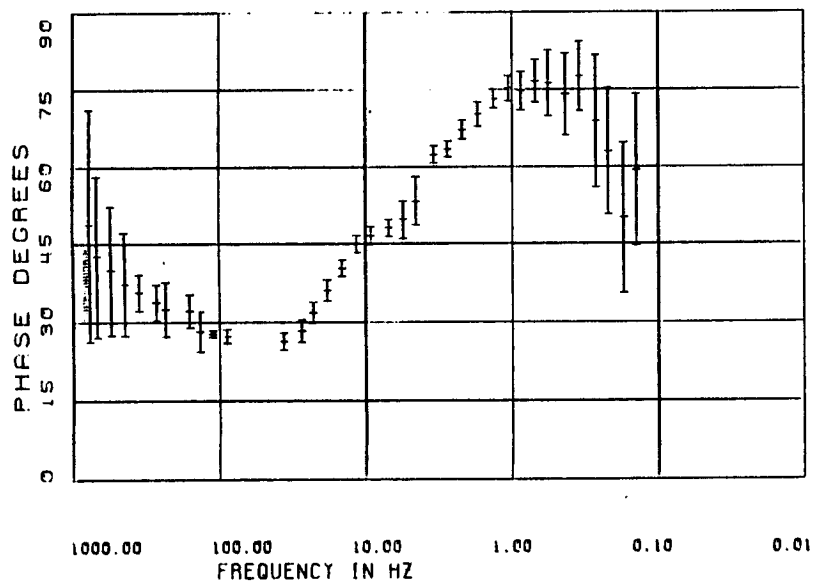
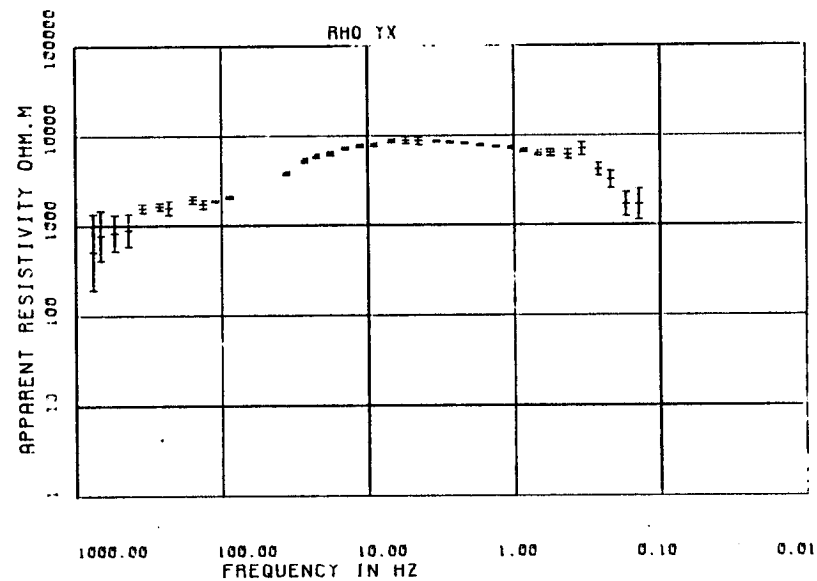
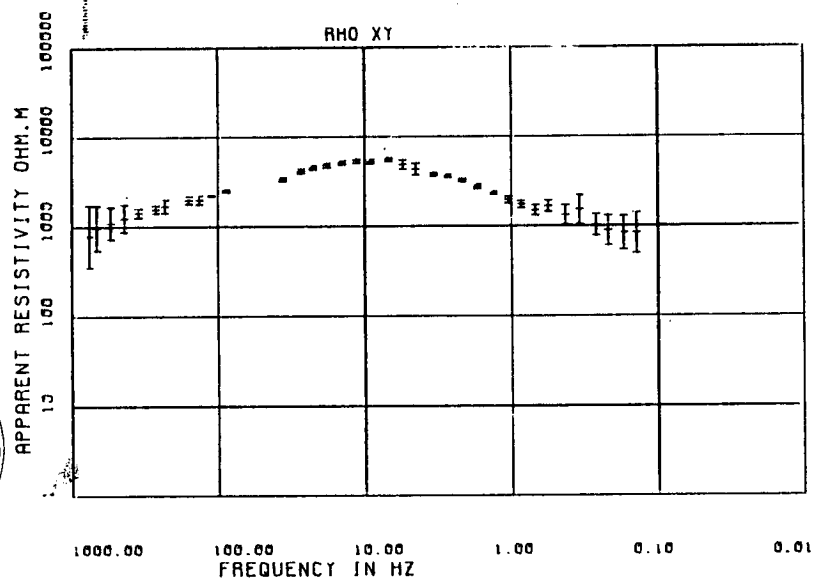


FIGURE 4.2 (2) SITE A.



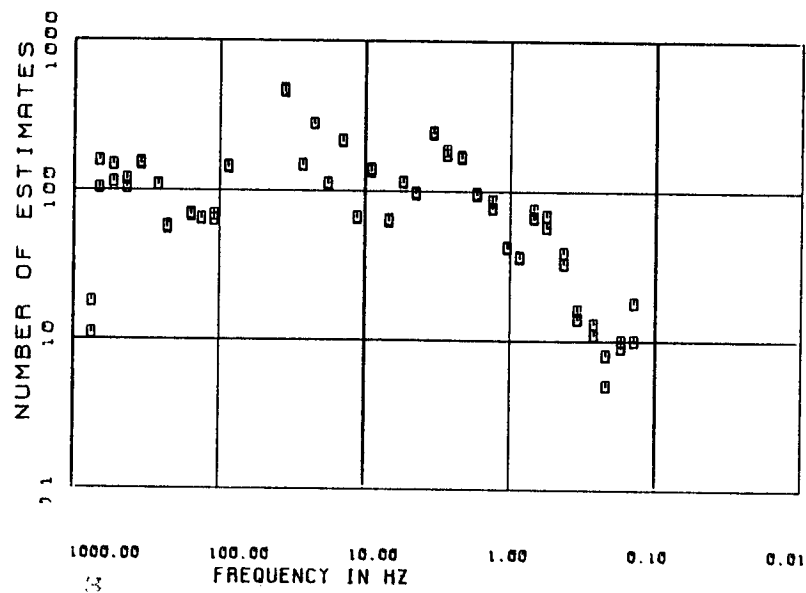
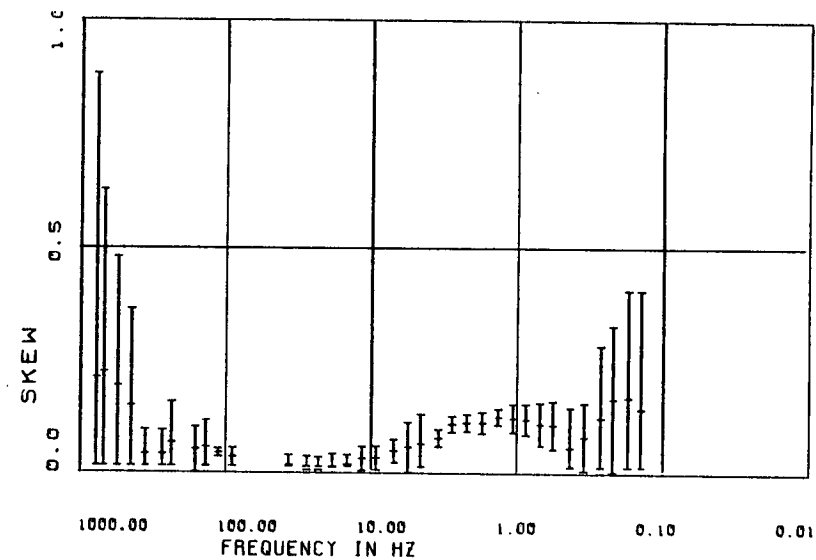
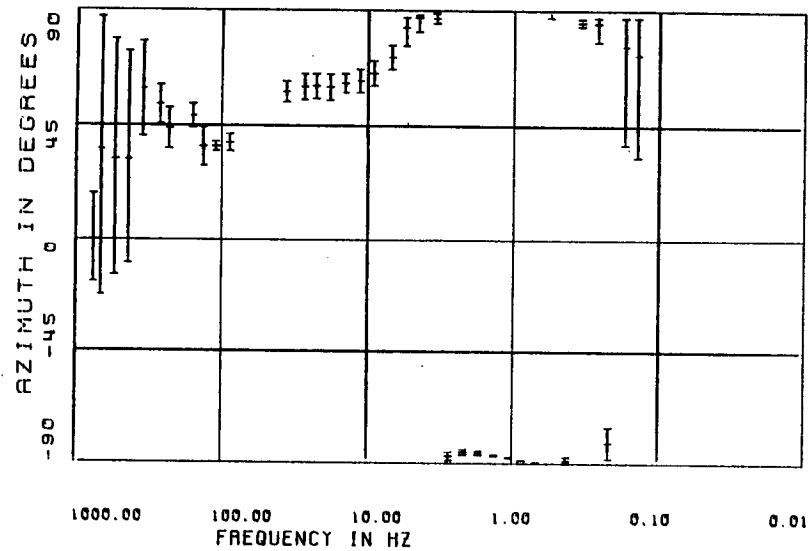
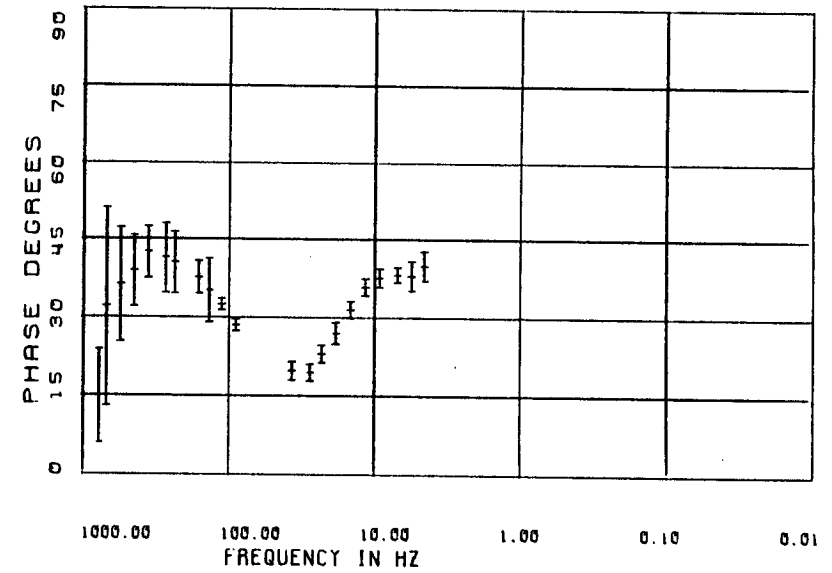
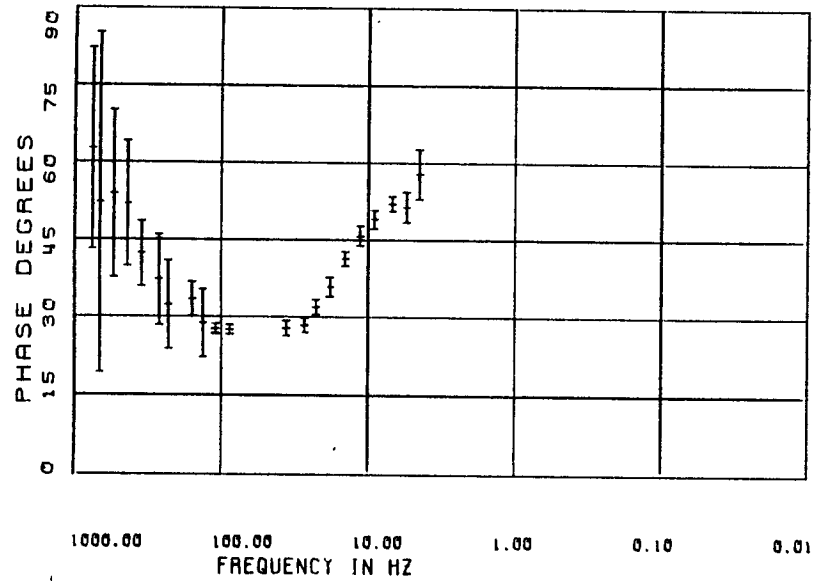
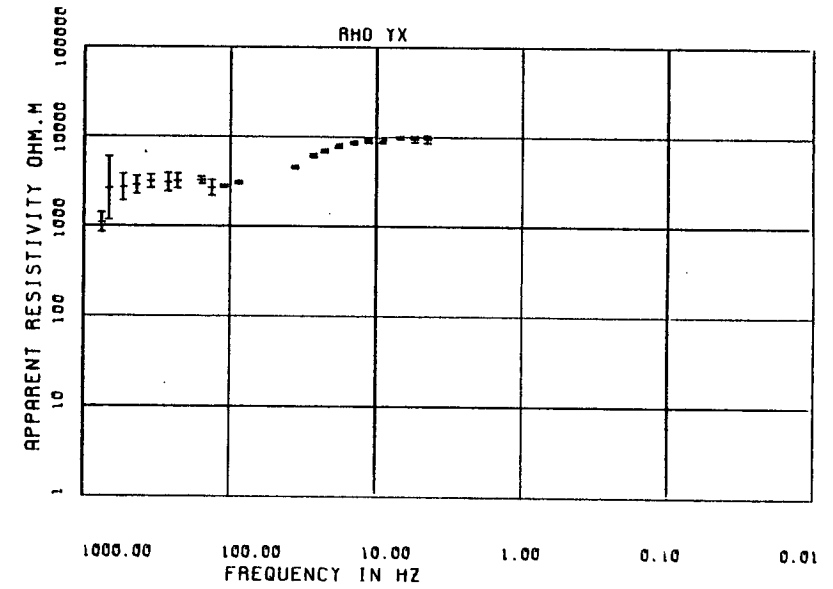
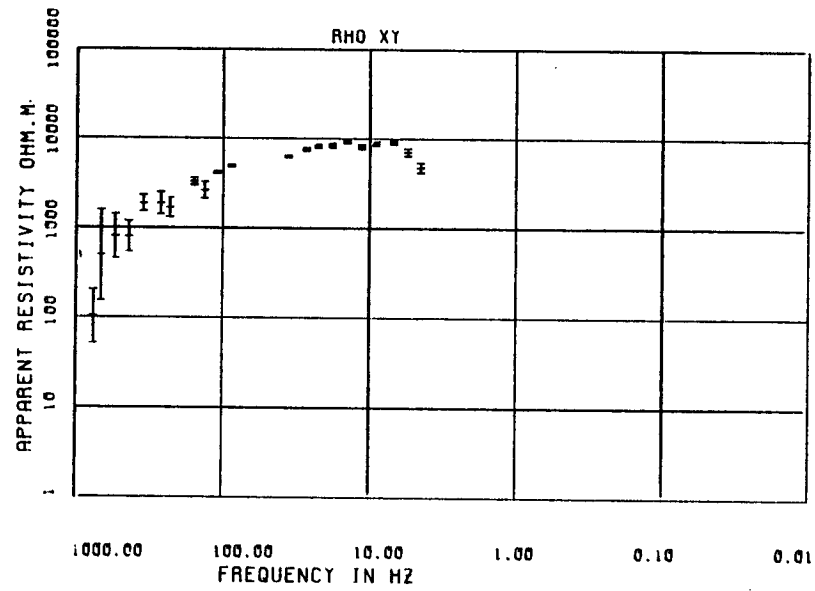
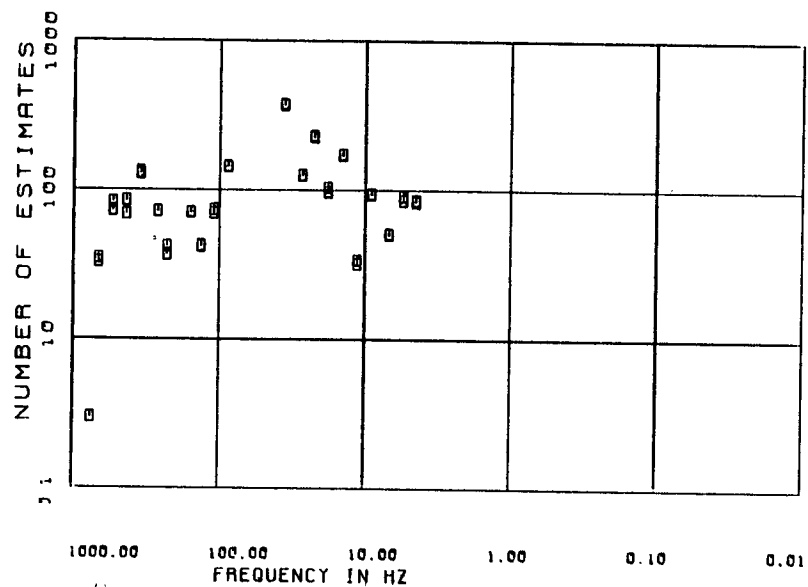
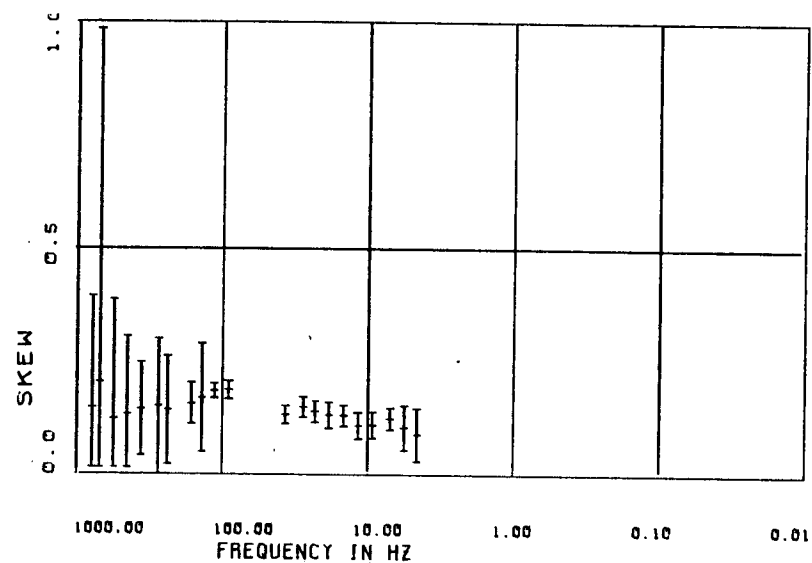
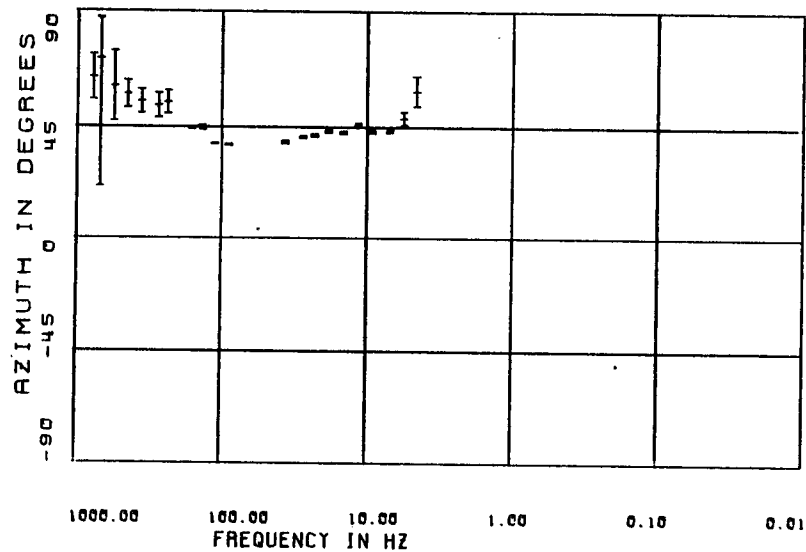
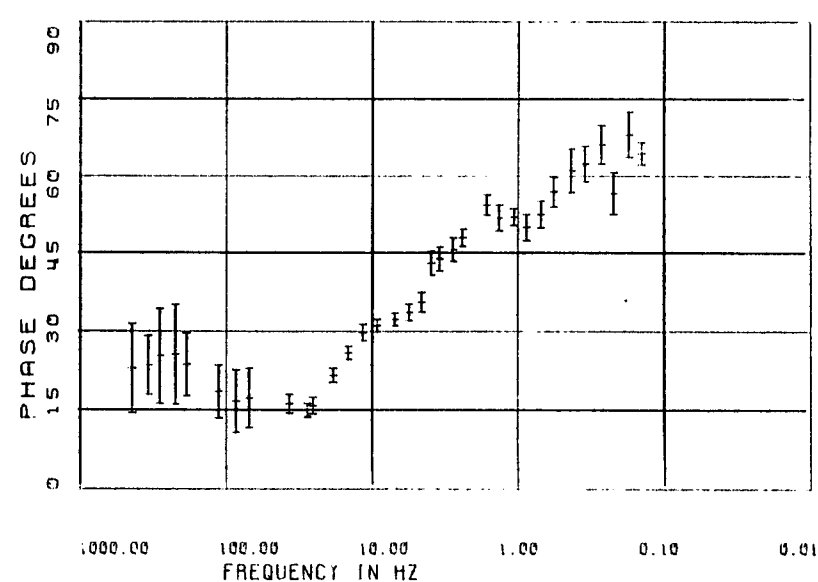
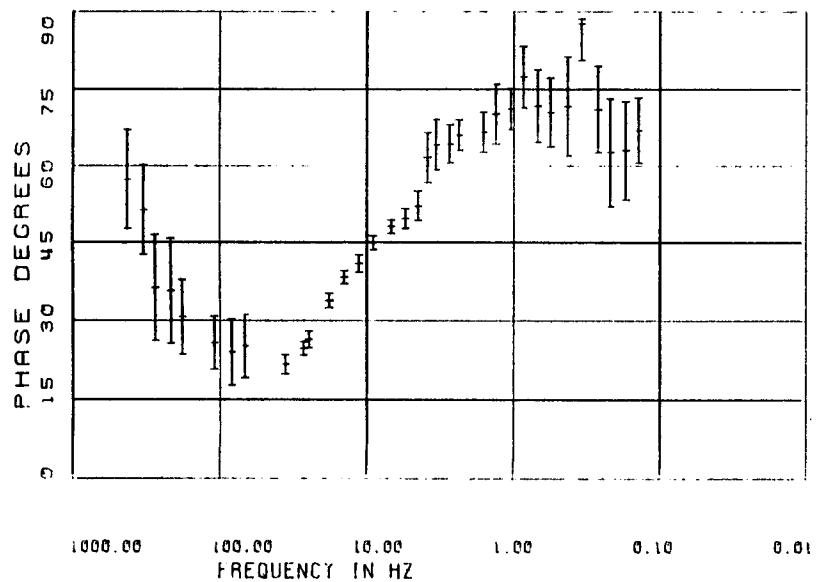
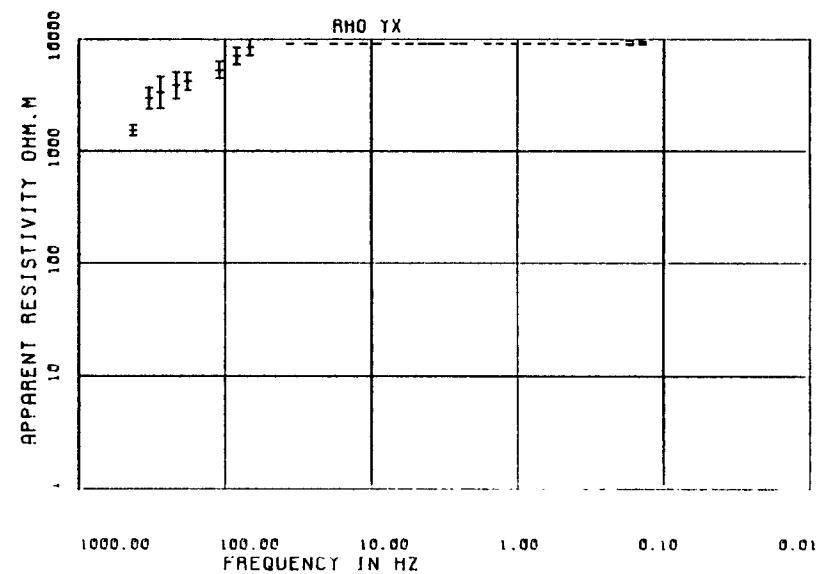
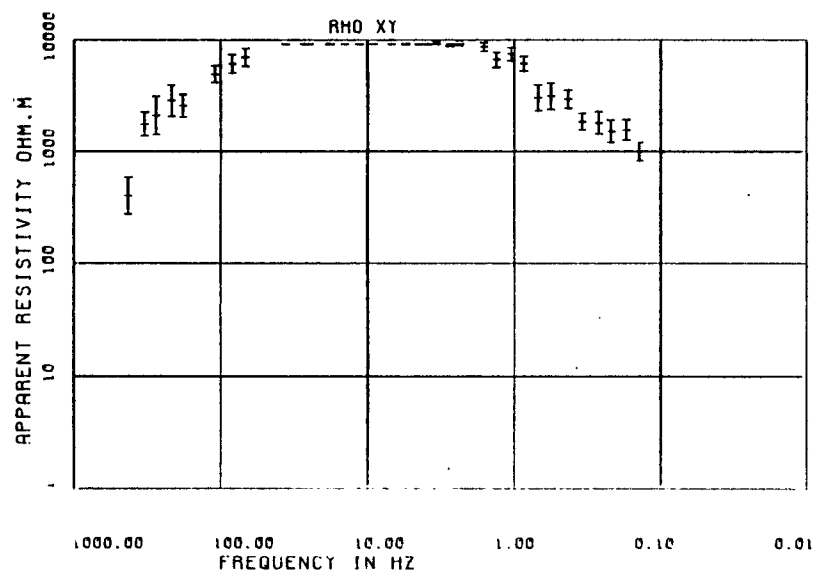


FIGURE 4.2 (4) SITE B.







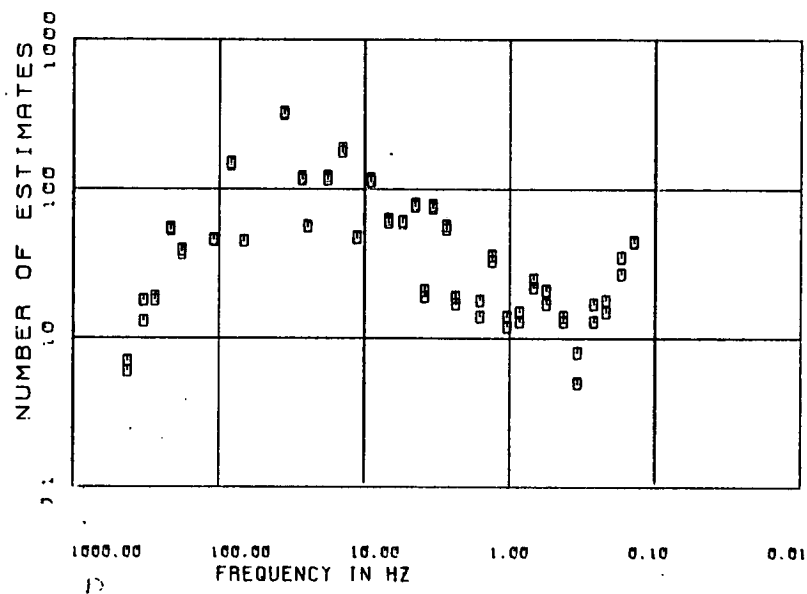
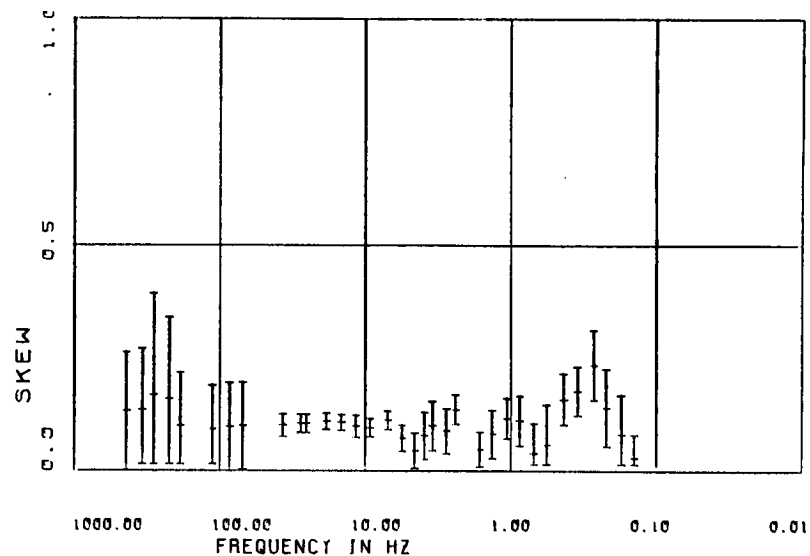
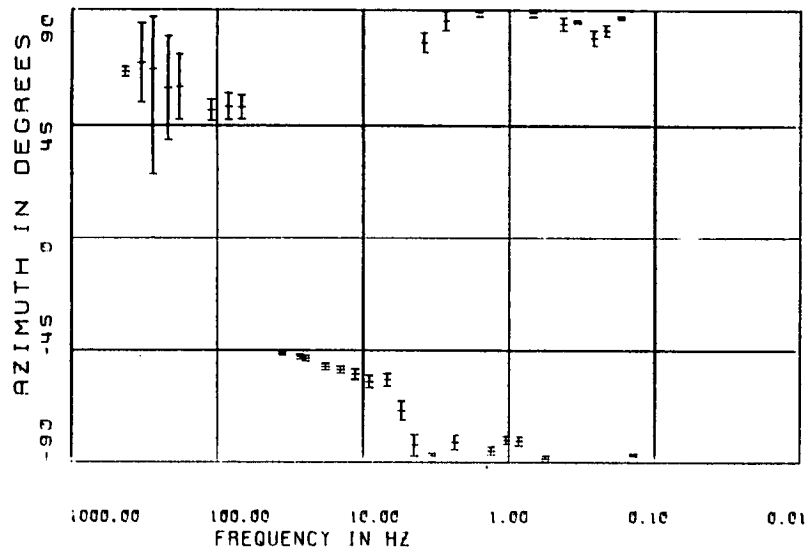
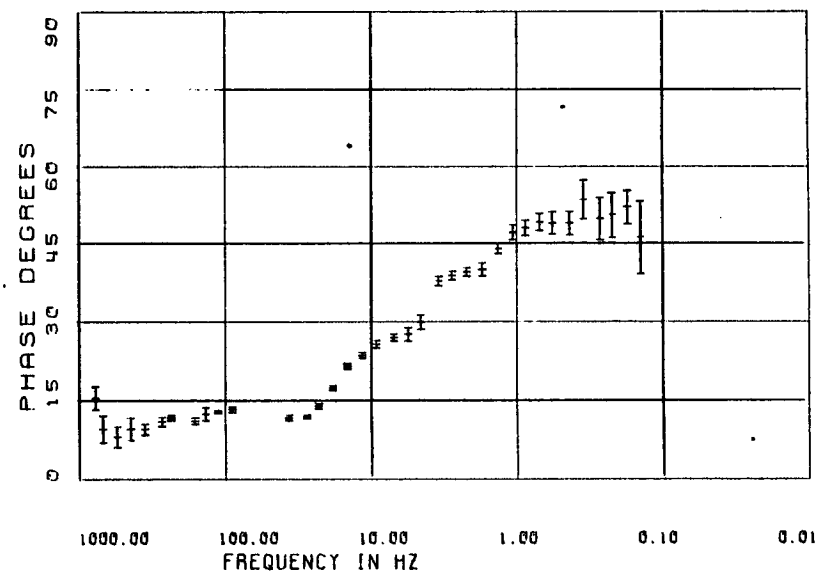
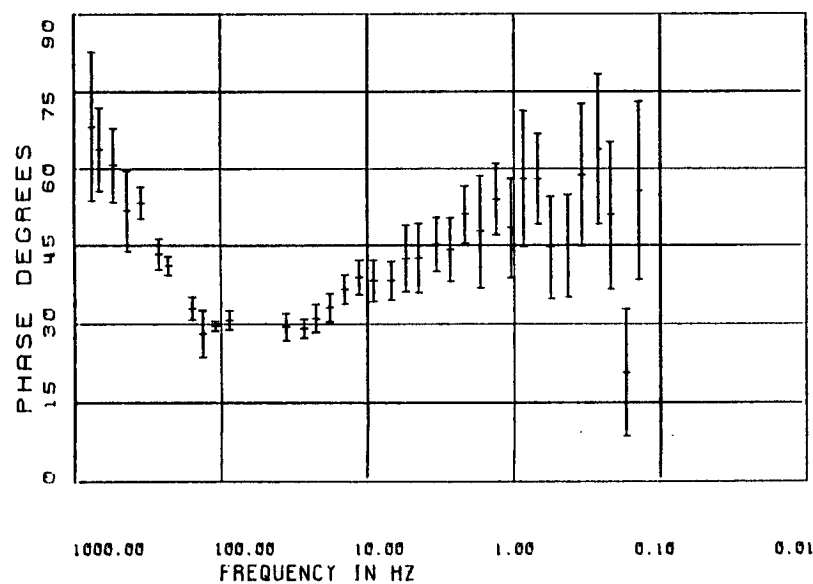
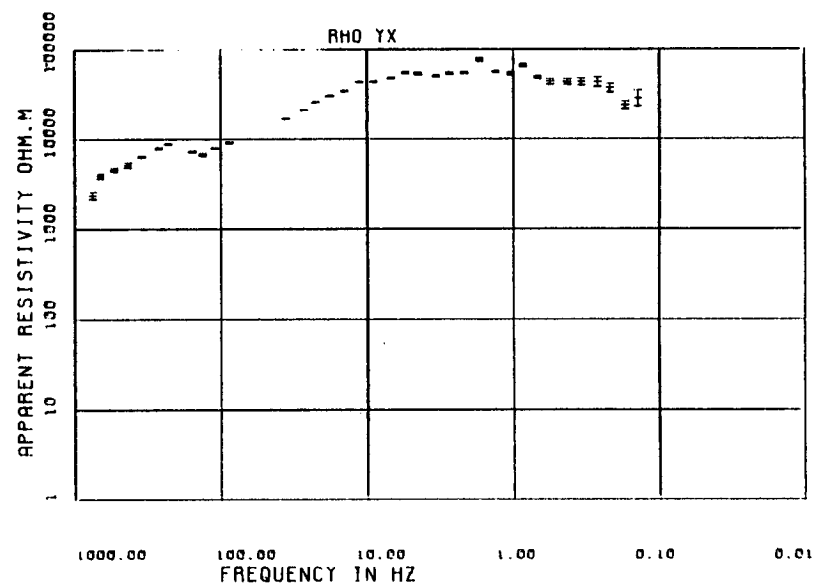
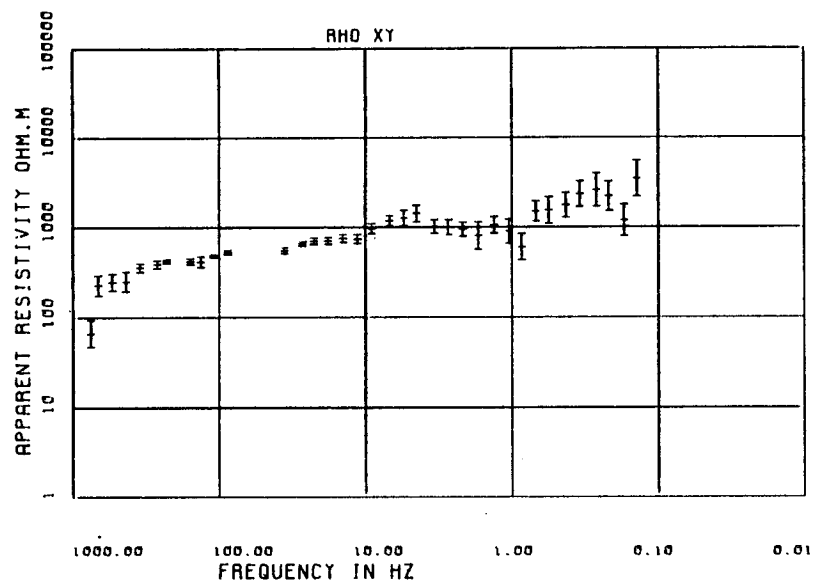


FIGURE 4.2 (8) SITE D.



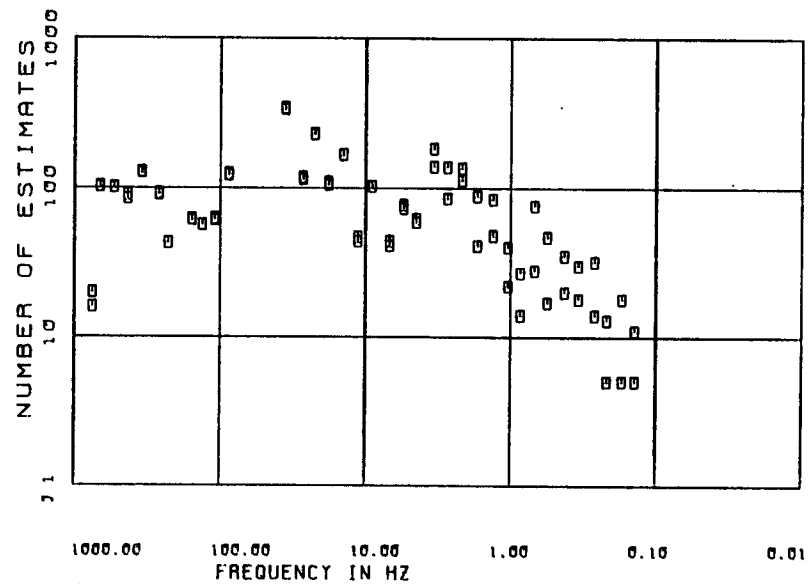
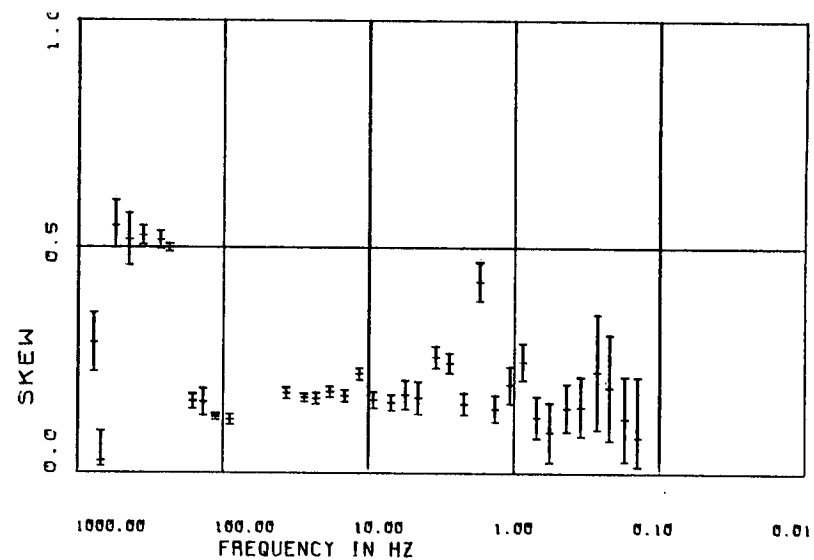
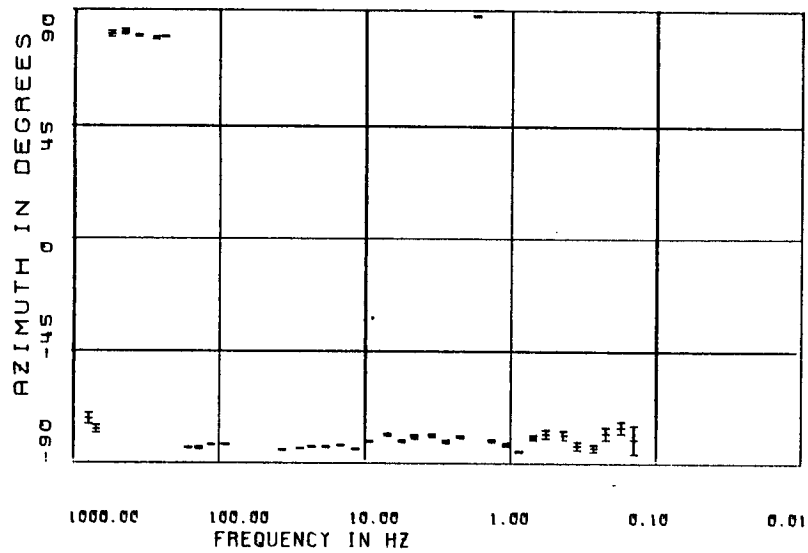
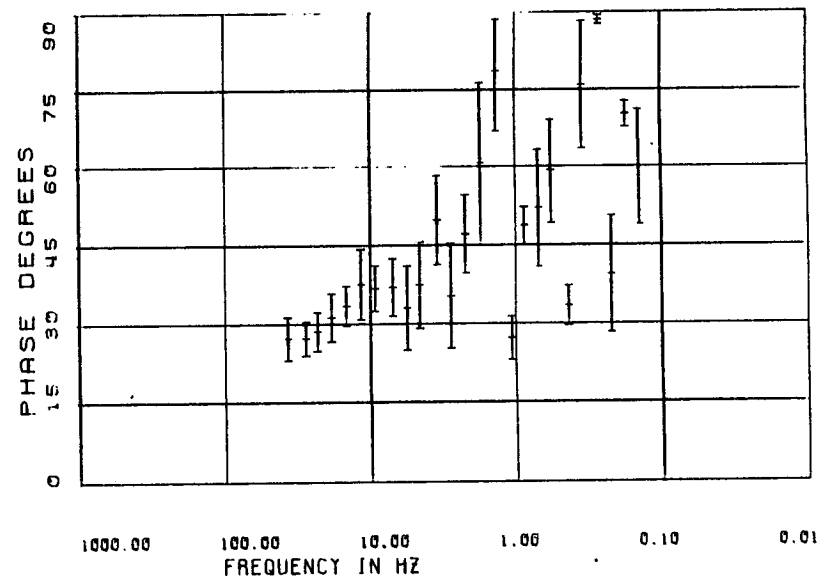
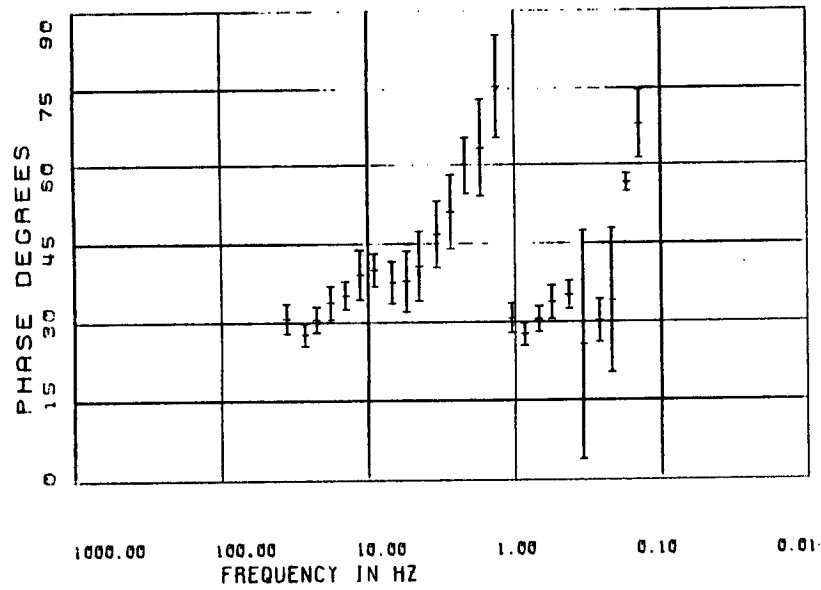
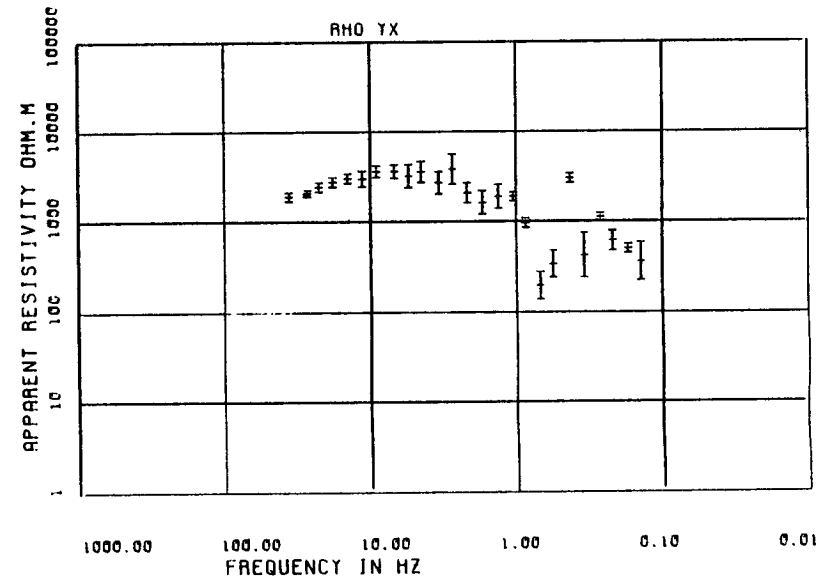
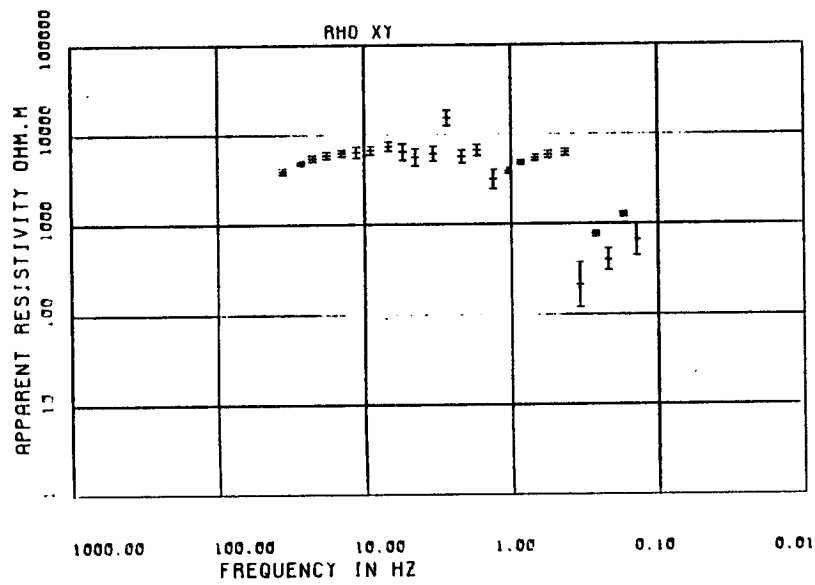


FIGURE 4.2 (10) SITE B.



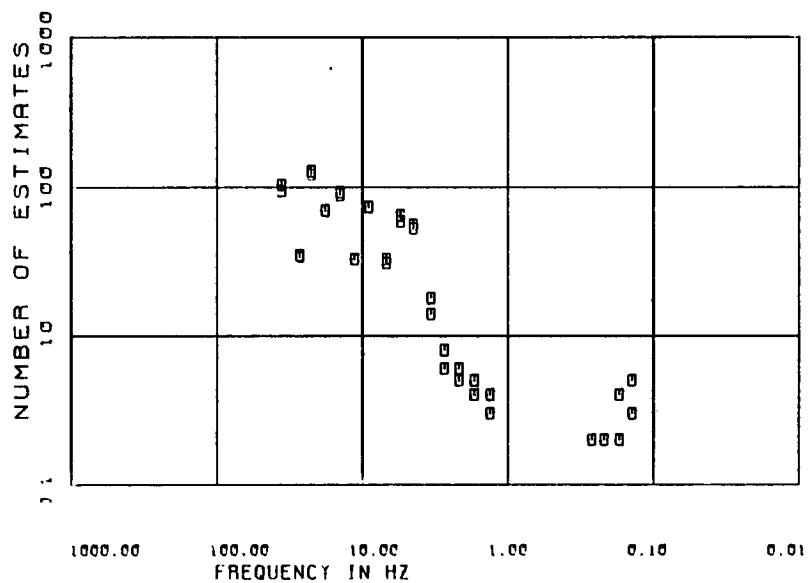
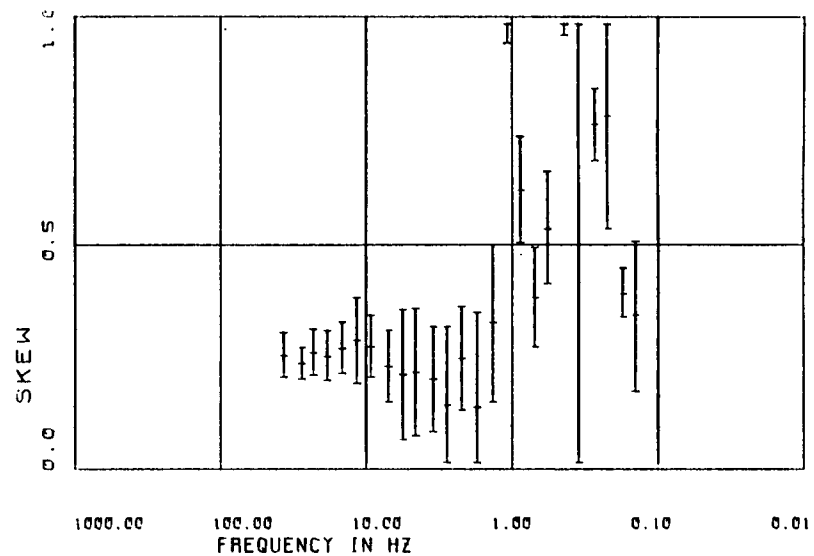
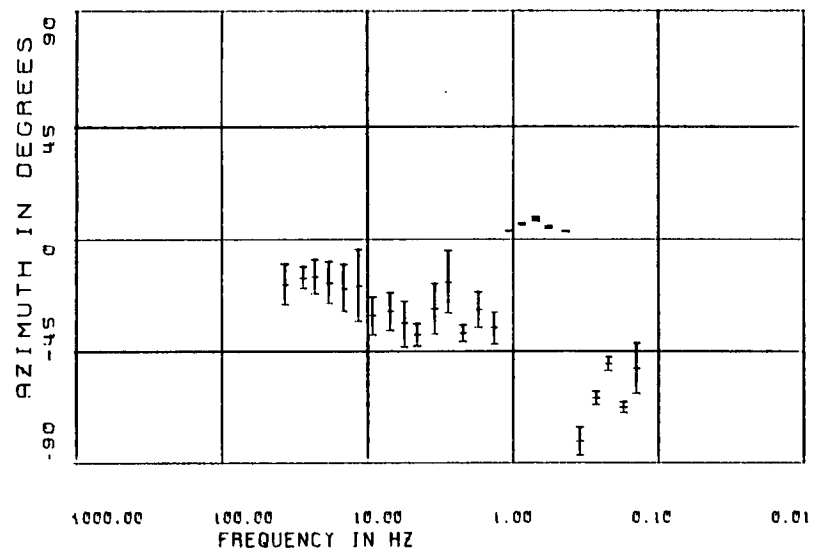
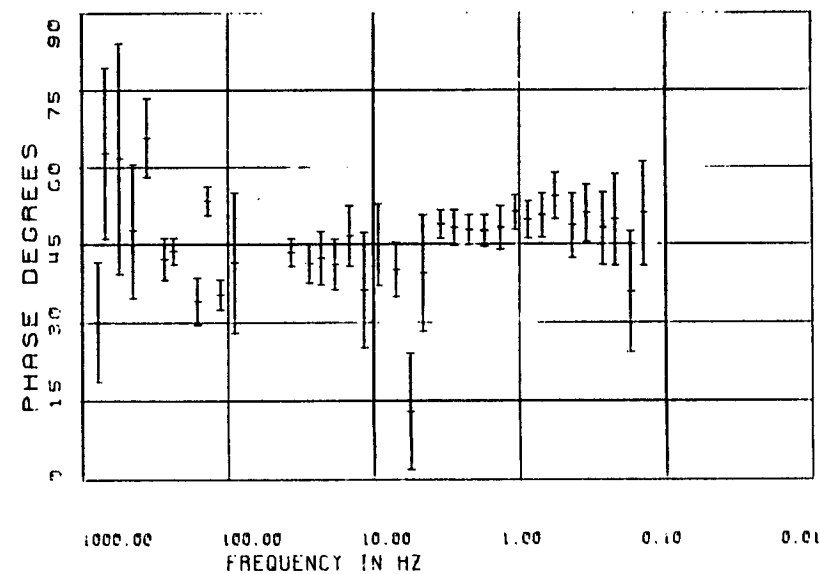
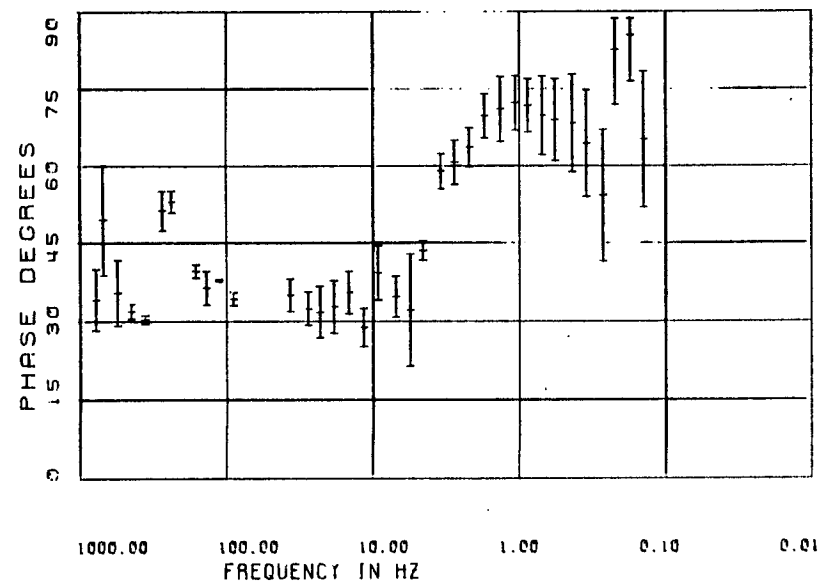
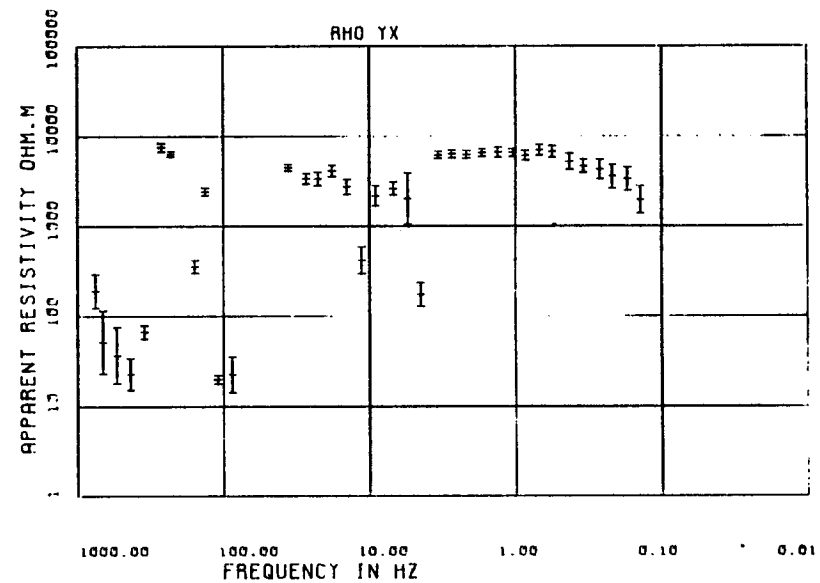
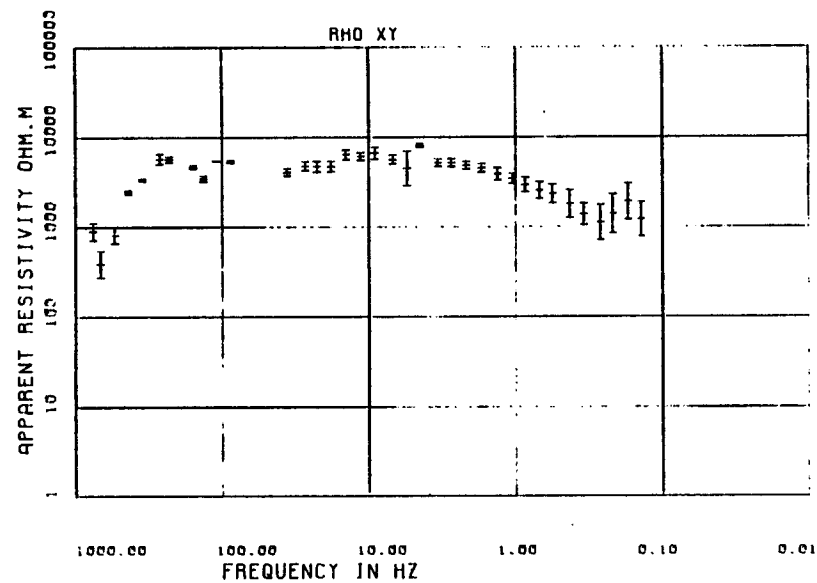


FIGURE 4.2 (12) SITE F.



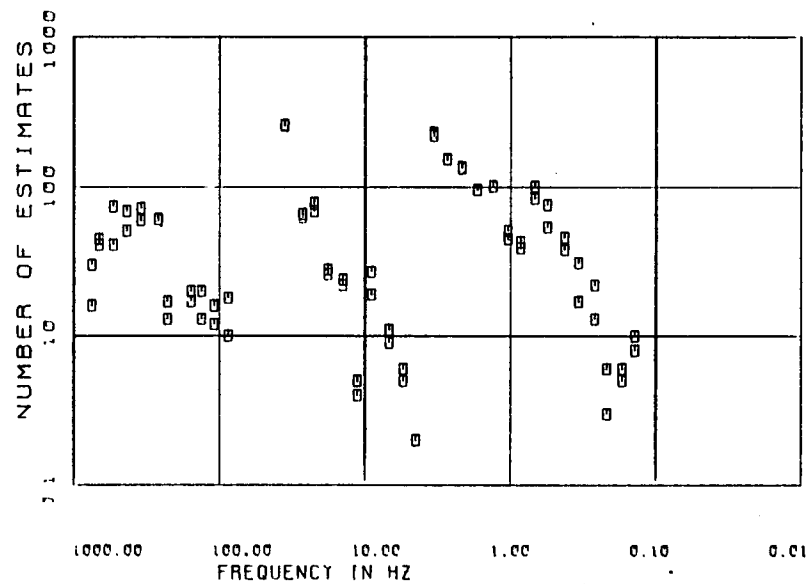
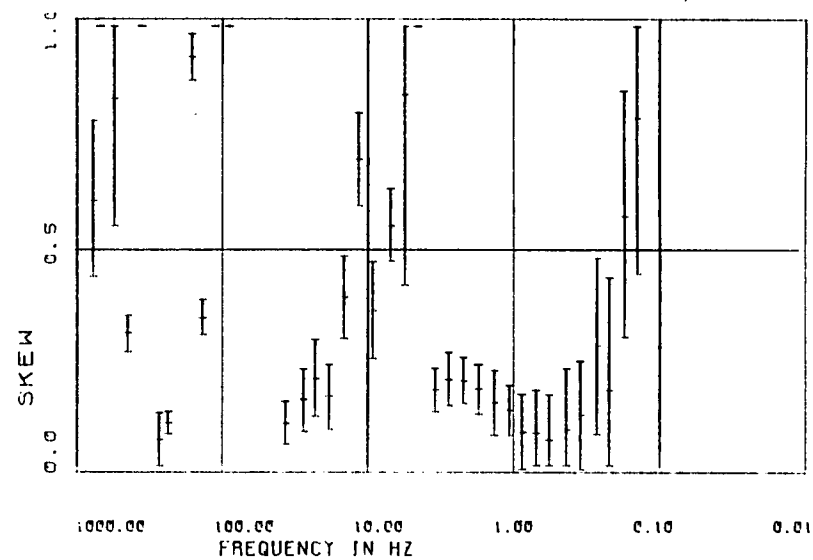
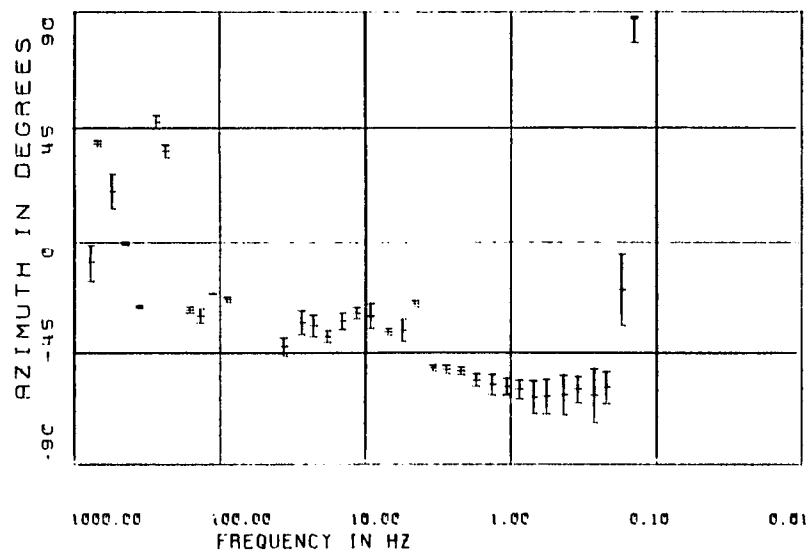


FIGURE 4.2 (14). SITE G.

4.6.1 THE MAGNETOTELLURIC RESPONSES AND THE EXPECTED DEEP GEOLOGY.

It had been expected as discussed in Section (4.1) that the Magnetotelluric responses should constitute two sets of data representative of the high resistivities expected on the Lewisian Foreland and the lower resistivities expected on the Moinian Hinterland. This however is not evident either from the apparent resistivity curves (Figure 4.2) or the one-dimensional models (Figure 5.1 and Figure 5.2).

A different subdivision of sites was then utilized. It is apparent that the Magnetotelluric sites may be divided into two sets according to the maximum apparent resistivity at each site (Table 4.3). Sites A,B,C,F and G do not have apparent resistivities greater than 1×10^4 ohm-metres and are henceforth described as normal sites for the study region. Sites D and E have apparent resistivities as large as 8×10^4 ohm-metres and are henceforth described as anomalous sites for the study region.

4.6.1.1 THE CLASSIFICATION OF THE MAGNETOTELLURIC RESPONSES AND THE INTRUSIVES.

In the following we shall assume that the granitic intrusives have resistivities in the region of 4.4×10^3 ohm-metres TO 1.3×10^8 ohm-metres (Telford ET.AL. 1976) are embedded in country rocks which according to the normal Magnetotelluric sites have a resistivity in the range 1×10^3 ohm-metres TO 1.2×10^4 ohm-metres (Figure 5.1), (Figure 5.2). Hence the granite intrusives were expected to constitute positive resistivity anomalies or to be of approximately the same resistivity as the country rock. Inspection of Table (4.4) indicates that the anomalous sites are relatively remote from the surface evidence of granite intrusives. Furthermore the sites relatively near the known granite intrusives are normal.

Hence we may conclude that either the granite intrusives have the same resistivity as the country rock or that the Magnetotelluric method was unable to detect them in this area.

4.6.1.2. THE CLASSIFICATION OF THE MAGNETOTELLURIC RESPONSES AND THE GEOPHYSICAL ANOMALIES.

Inspection of Table (4.5) indicates that the anomalous sites are relatively remote from the gravity anomalies. Furthermore the sites relatively near the gravity and aeromagnetic anomalies are normal. Sites near the aeromagnetic anomalies are both normal and anomalous. Hence we conclude that the Magnetotelluric Method is unable to detect

SITE	DESIGNATION	MAXIMUM LOG(APPARENT RESISTIVITY)
A	NORMAL	3.5
B	NORMAL	4.0
C	NORMAL	4.0
D	ANOMALOUS	4.5
E	ANOMALOUS	4.75
F	NORMAL	3.8
G	NORMAL	3.75

TABLE 4.3. THE MAXIMUM APPARENT RESISTIVITIES AT THE SITES.

SITE	MAXIMUM APPARENT RESISTIVITY		NEAREST GRANITE INTRUSIVES		REMARKS
	LOG(OHM-METRES)		NAME	DISTANCE AREA KMS. KMS ²	
A	3.6			0.5	NUMEROUS DYKES.
B	4.0		LOCH BORROLAN	1	
			LOCH AILSH	3	
C	4.0		LOCH BORROLAN	8	
			LOCH AILSH	8	
D	4.5		LOCH BORROLAN	10	
			LOCH AILSH	6	1. UNRELIABLE DATA. 2. LATERAL EXTENT OF GRUDIE GRANITE IS UNKNOWN BUT IS AT THE CENTRE OF AN EXTENSIVE 1.4×10^{-4} MS ⁻² GRAVITY ANOMALY.
E	4.8		GRUDIE	2	
F	3.9		GRUDIE	2	1. UNRELIABLE DATA. 2. LATERAL EXTENT OF GRUDIE GRANITE IS UNKNOWN BUT IS AT THE CENTRE OF AN EXTENSIVE 1.4×10^{-4} MS ⁻² GRAVITY ANOMALY.
G	3.8		MIGDALE	5	
			ROGART	9	

TABLE 4.4.

SITE	MAXIMUM APPARENT RESISTIVITY LOG(OHM-METRES)	NEAREST AEROMAGNETIC DISTANCE KMS.	ANOMALY nT.	NEAREST GRAVITY DISTANCE KMS.	ANOMALY MS ⁻²
A	3.6	3.6	-100	44	-1.4X10 ⁻⁴
B	4.0	2.0	300	15	-1.4X10 ⁻⁴
C	4.0	1.0	-80	21	-1.4X10 ⁻⁴
D	4.5	1.0	-180	17	-1.4X10 ⁻⁴
E	4.8	1.0	-150	9.0	-1.4X10 ⁻⁴
F	3.9	3.0	100	2.4	-1.4X10 ⁻⁴
G	3.8	3.6	100	20	-1.4X10 ⁻⁴

TABLE 4.5

the structures to which the gravity and aeromagnetic anomalies in this are due.

CHAPTER V

THE ONE-DIMENSIONAL INVERSION

5.1 ONE-DIMENSIONAL MODELLING.

At this point, as the data have been analysed we now require to obtain a conductivity structure from the data prior to any interpretation. The first step involved the determination of one-dimensional models for each site and then their compilation to construct an approximate two-dimensional conductivity section. As we are only interested in plausible conductivity structures at this stage the entire data sets were used in the construction of these models.

5.2 THE INVERSION PROCEEDURE.

The one-dimensional modelling programme used was a Hedgehog routine modified from a Monte-Carlo routine by Dawes. This routine was suitable for a non-linear search for models provided the range of models admitted at each iteration was sufficiently large.

The algorithm used a Monte-Carlo search in an iterative manner so as to reduce the range of possible models at each iteration. Let P_i be the i^{TH} parameter; a logarithm of resistivity or depth. Initially $(P_i)_{\text{MAX}}$, $(P_i)_{\text{MIN}}$ and $(P_i)_{\text{AV}}$ are specified for the first iteration. Let R be one of a set of random numbers having a mean of zero and a variance of unity. Sets of random parameters are calculated as below:

$$P_i = P_i + R [(P_i)_{\text{MAX}} - (P_i)_{\text{AV}}] : R > 0. \quad 1$$

$$P_i = P_i + R [(P_i)_{\text{AV}} - (P_i)_{\text{MIN}}] : R < 0 \quad 2$$

The corresponding model responses are calculated (Section 2.3) from each set of random parameters, and the 20 models the responses of which best fit the data are used as the set of models from which the maximum parameter values $(Q_i)_{\text{MAX}}$ and minimum parameter values $(Q_i)_{\text{MIN}}$ are calculated together with a new parameter value $(P_i)_{\text{AV}}$.

The new search range for the parameters is now defined in the following arbitrary manner. Let α and β be constants and let $K \approx 1$ be a constant adjustable for each series of iterations. If $(P_i)_{\text{MAX}} / (Q_i)_{\text{MAX}} > \alpha$, the search range is expanded, and the new values of

$(P_i)_{MAX}$ and $(P_i)_{MIN}$ are given by:

$$(P_i)_{MAX} = (P_i)_{MAX} + K [(P_i)_{MAX} - (P_i)_{AV}] \quad 3$$

$$(P_i)_{MIN} = (P_i)_{MIN} - K [(P_i)_{AV} - (P_i)_{MIN}] \quad 4$$

If $(Q_i)_{MIN}/(P_i)_{MIN} < \beta$, the search range is contracted, and the values of $(P_i)_{MAX}$ and $(P_i)_{MIN}$ are given by:

$$(P_i)_{MAX} = (P_i)_{MAX} - K [(P_i)_{MAX} - (P_i)_{AV}] \quad 5$$

$$(P_i)_{MIN} = (P_i)_{MIN} + K [(P_i)_{AV} - (P_i)_{MIN}] \quad 6$$

These values of $(P_i)_{MAX}$, $(P_i)_{MIN}$ and $(P_i)_{AV}$ are used as starting values for the second iteration.

After a given number of iterations (usually approximately 40), the 20 models whose responses best fit the data are plotted together with their responses. Although this does not give a formal statement of the error on the model parameters, it does allow the spread of models to be displayed with their associated spread of responses.

One of three possible measures of fit may be selected for use in the Hedgehog programme. A least squares criterion and weighted (by the data error) least squares criterion are available, as is an error bars criterion where the fit index is proportional to the number of error bars which the model response intersects.

5.3 THE MODIFIED BOSTICK TRANSFORM.

The modified form of the Bostick Transform (Bostick 1977) utilizing the phase data given below:

$$S = S_A [[\pi/2\phi] - 1] \quad 7$$

$$D = [S_A / \omega \mu_0]^{1/2} \quad 8$$

Where ρ is the resistivity, D is the depth, ρ_A is the apparent resistivity and ϕ is the phase.

5.4 THE ONE-DIMENSIONAL INVERSION RESULTS.

As already stated all one-dimensional models were obtained for all the response estimates of Figure (4.2) where the north and east measurement axes have been rotated by 15° . These are presented site by site in Figure (5.1). In each case the best fitting models derived using the algorithm described in Section (5.2) are superimposed on the results obtained using the modified Bostick Transform (Section 5.3).

FIGURE 5.1.

THE ONE-DIMENSIONAL MODELS.

1D MODEL FOR SITE A ROTATED NORTH

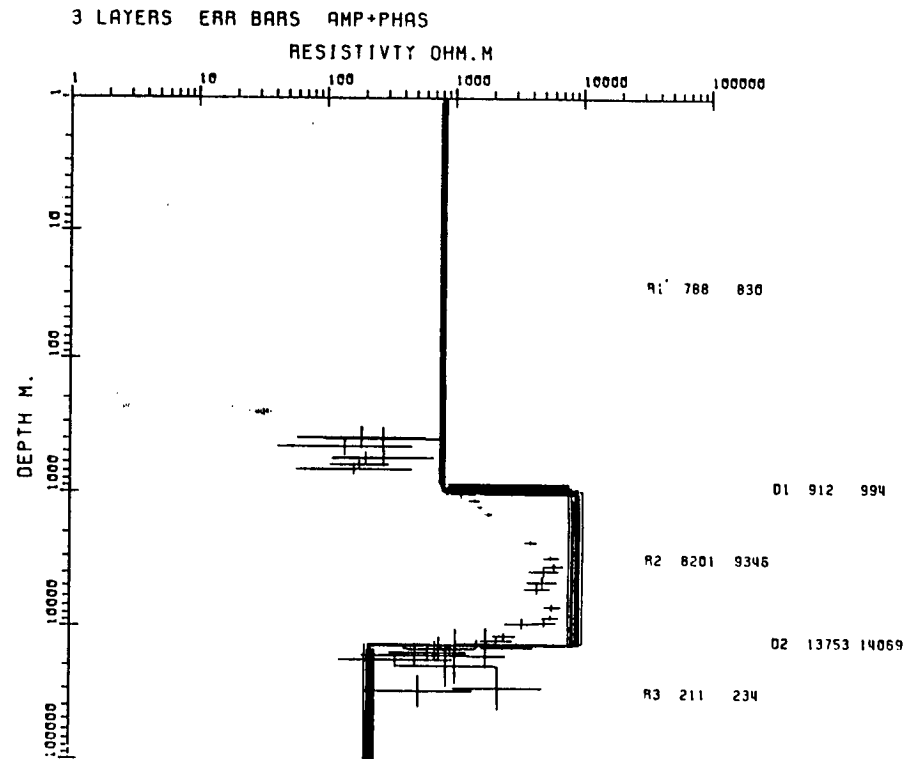
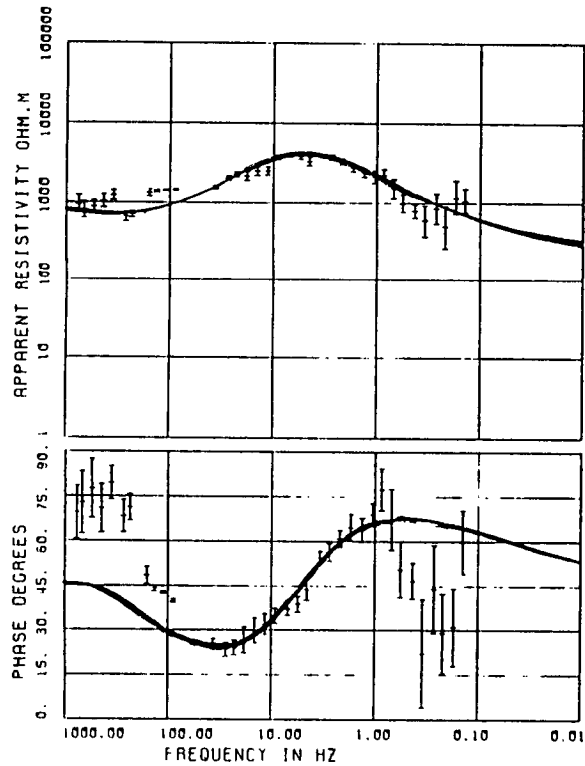


FIGURE 5.1 (1)

1D MODEL FOR SITE A ROTATED EAST

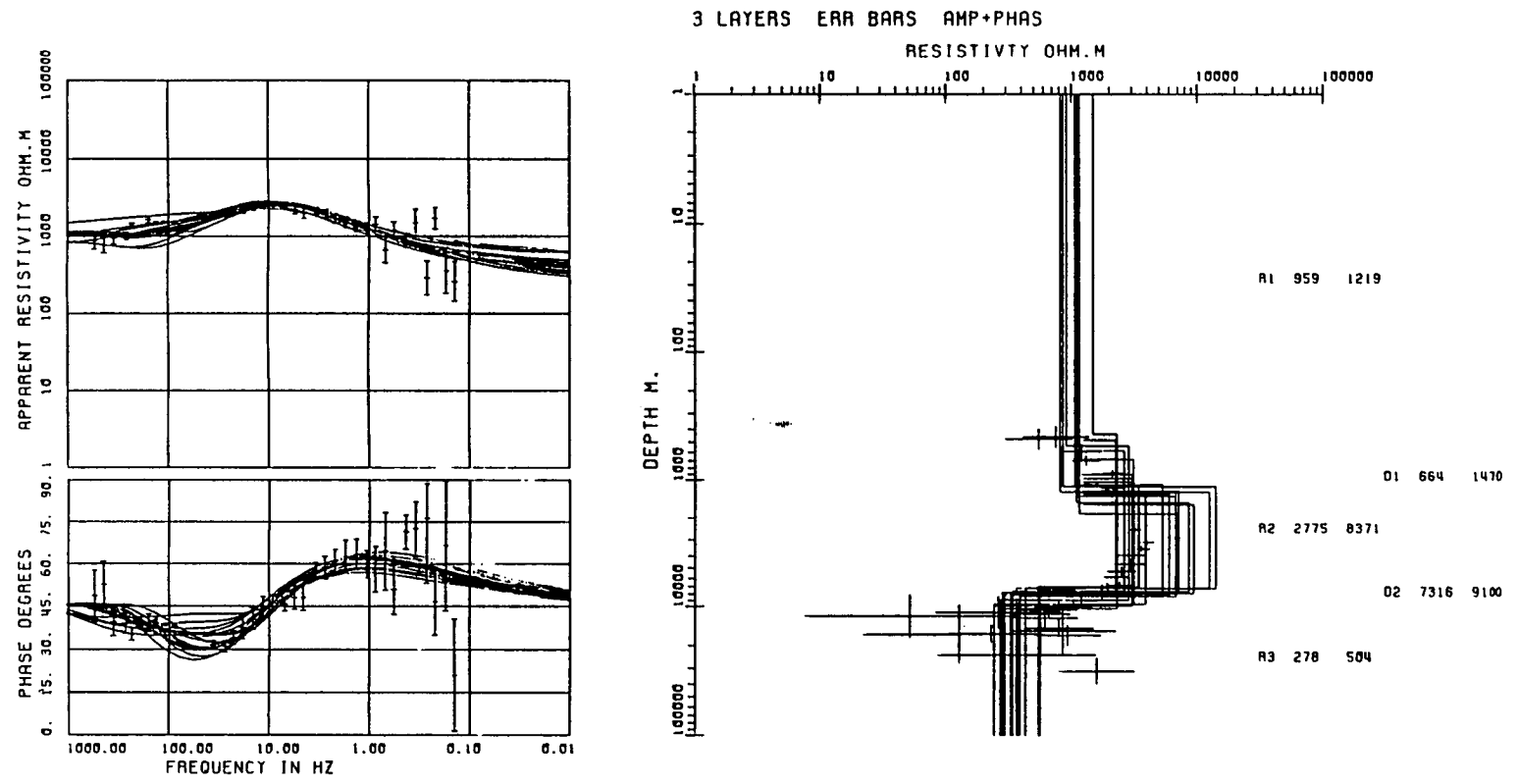


FIGURE 5.1 (2)

1D MODEL FOR SITE B ROTATED NORTH

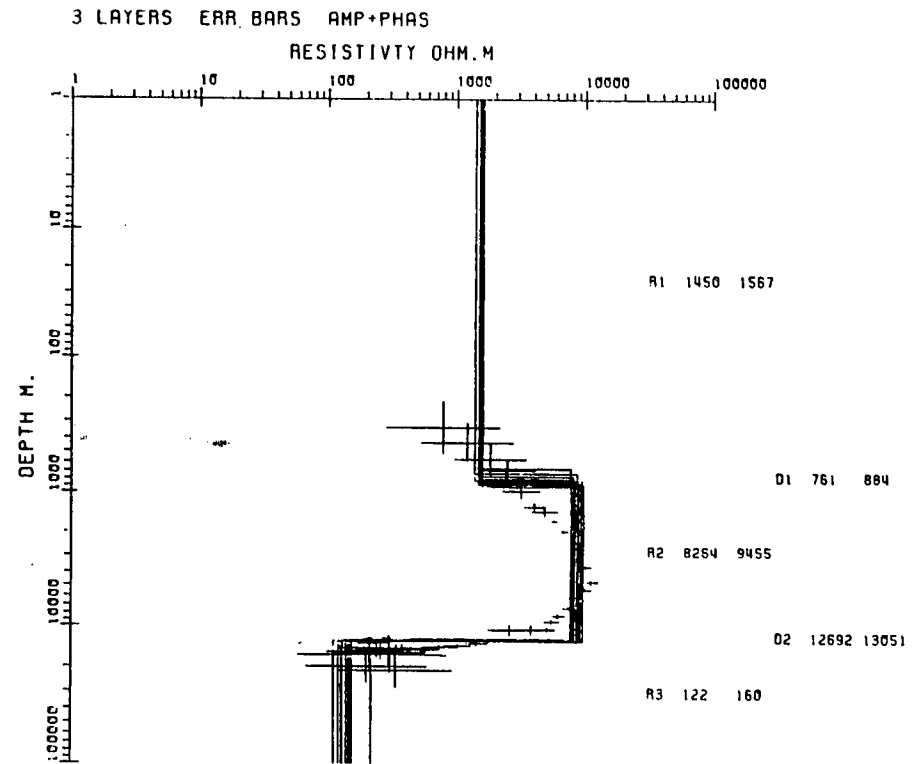
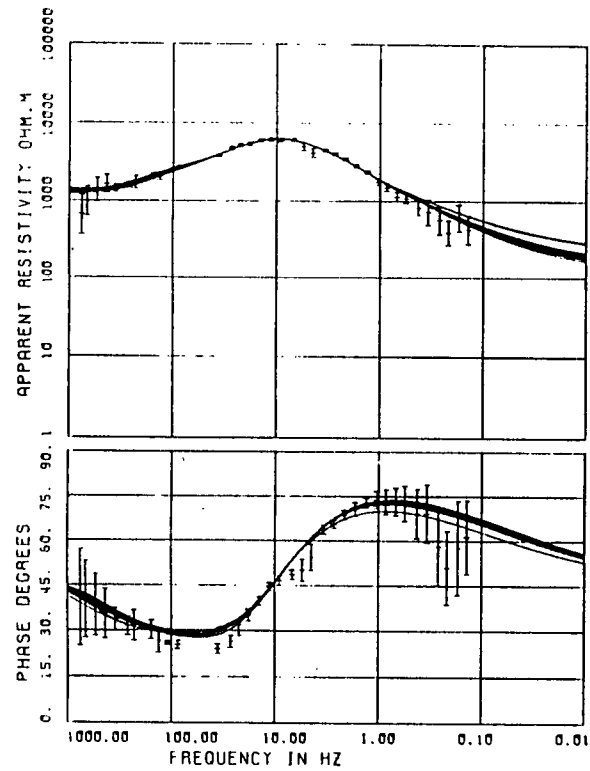


FIGURE 5.1 (3)

1D MODEL FOR SITE B ROTATED EAST

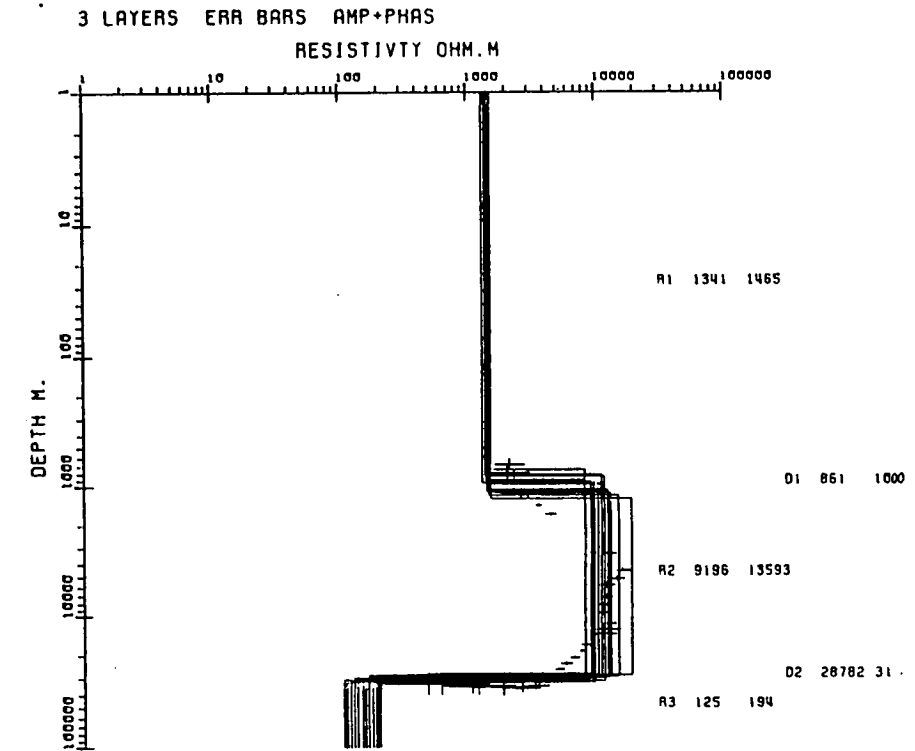
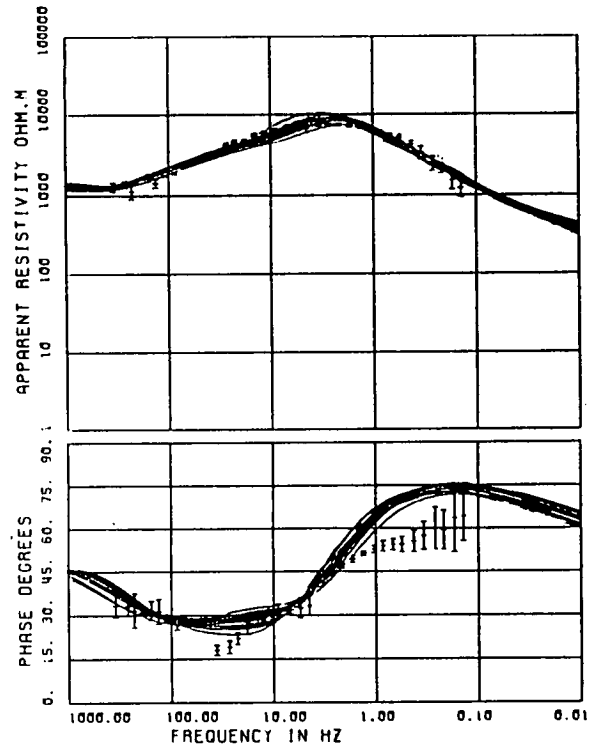


FIGURE 5.1 (4)

1D MODEL FOR SITE C ROTATED NORTH

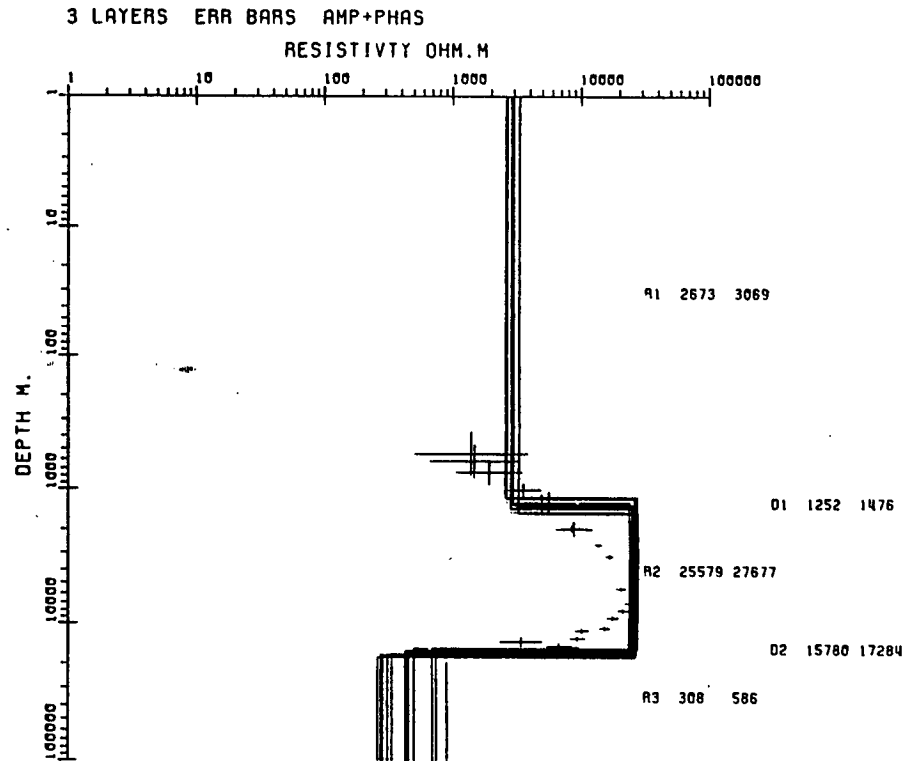
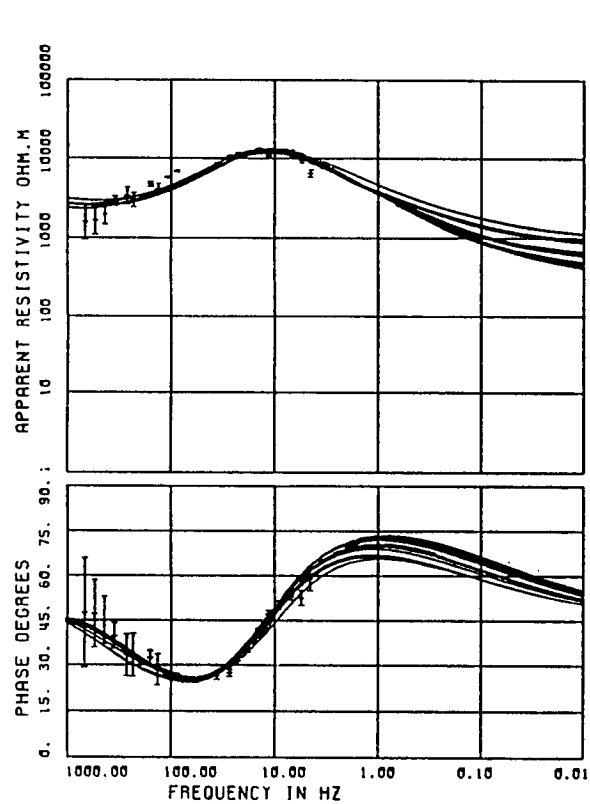


FIGURE 5.1 (5)

92

1D MODEL FOR SITE C ROTATED EAST

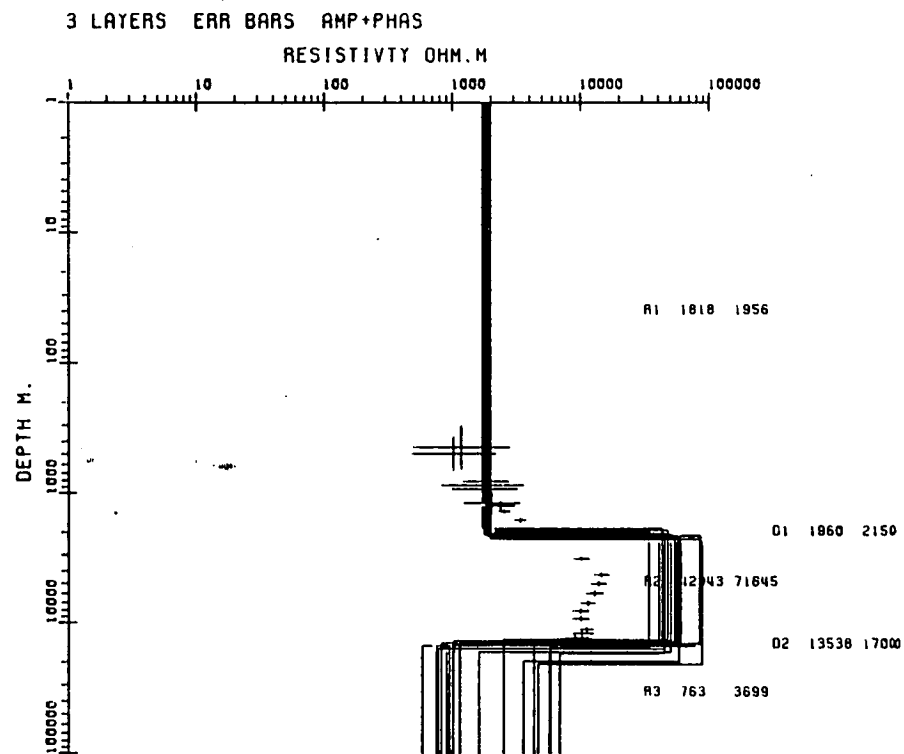
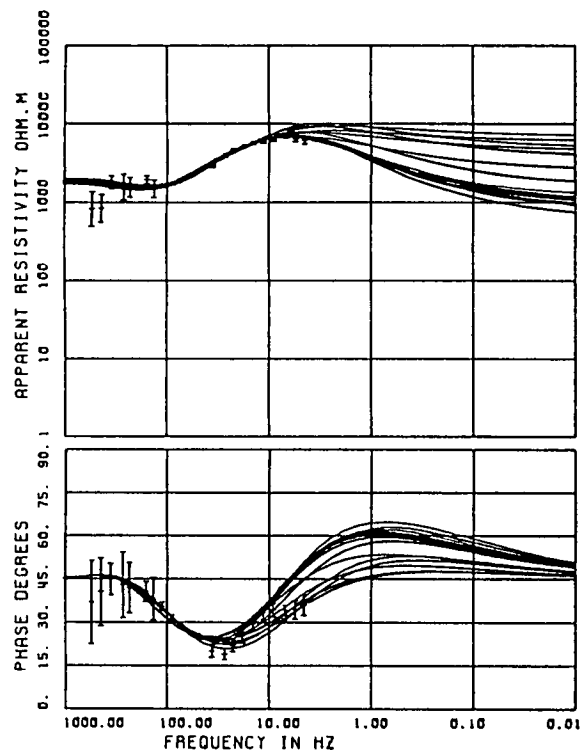


FIGURE 5.1 (6)

1D MODEL FOR SITE 'D' ROTATED NORTH

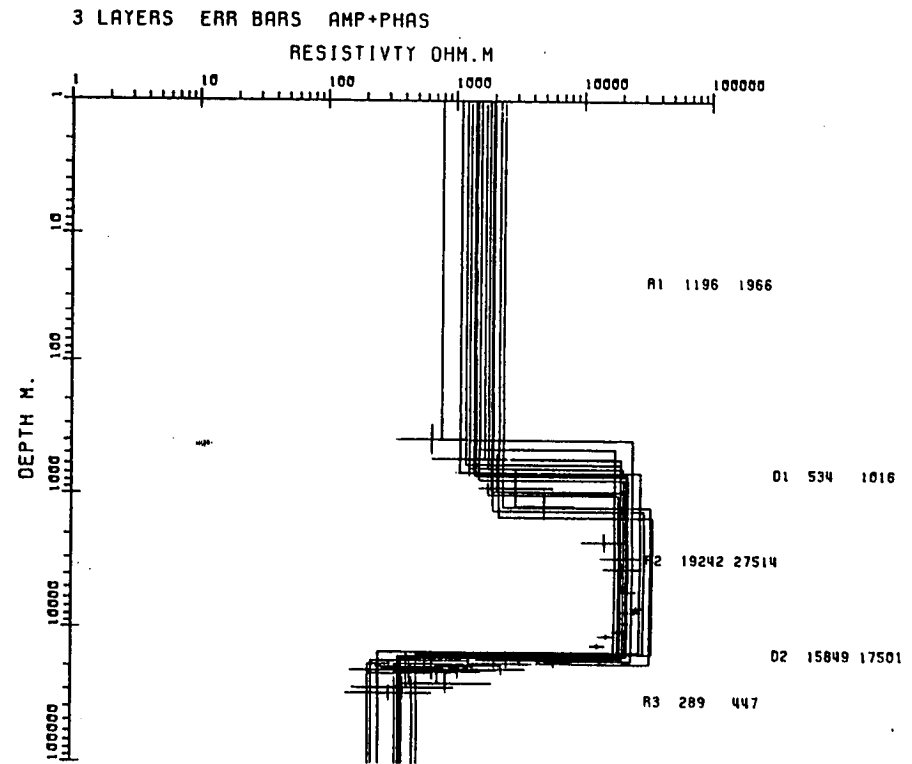
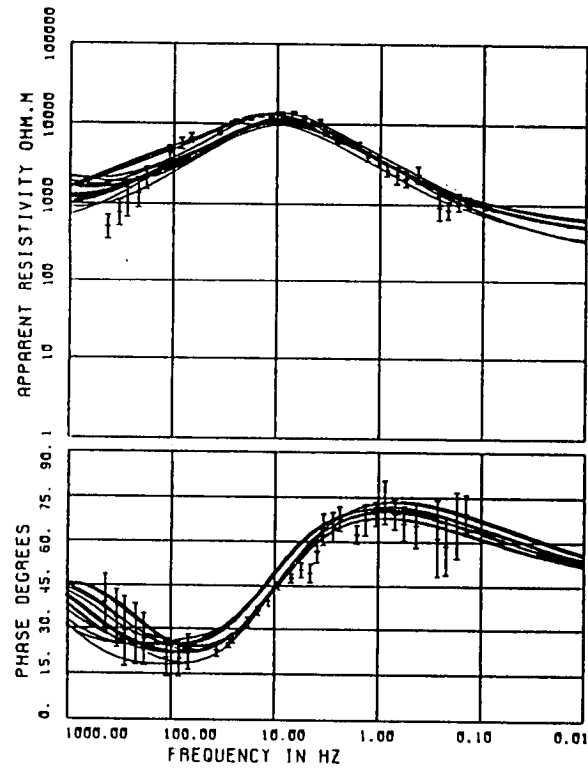


FIGURE 5.1 (7) .

1D MODEL FOR SITE D ROTATED EAST

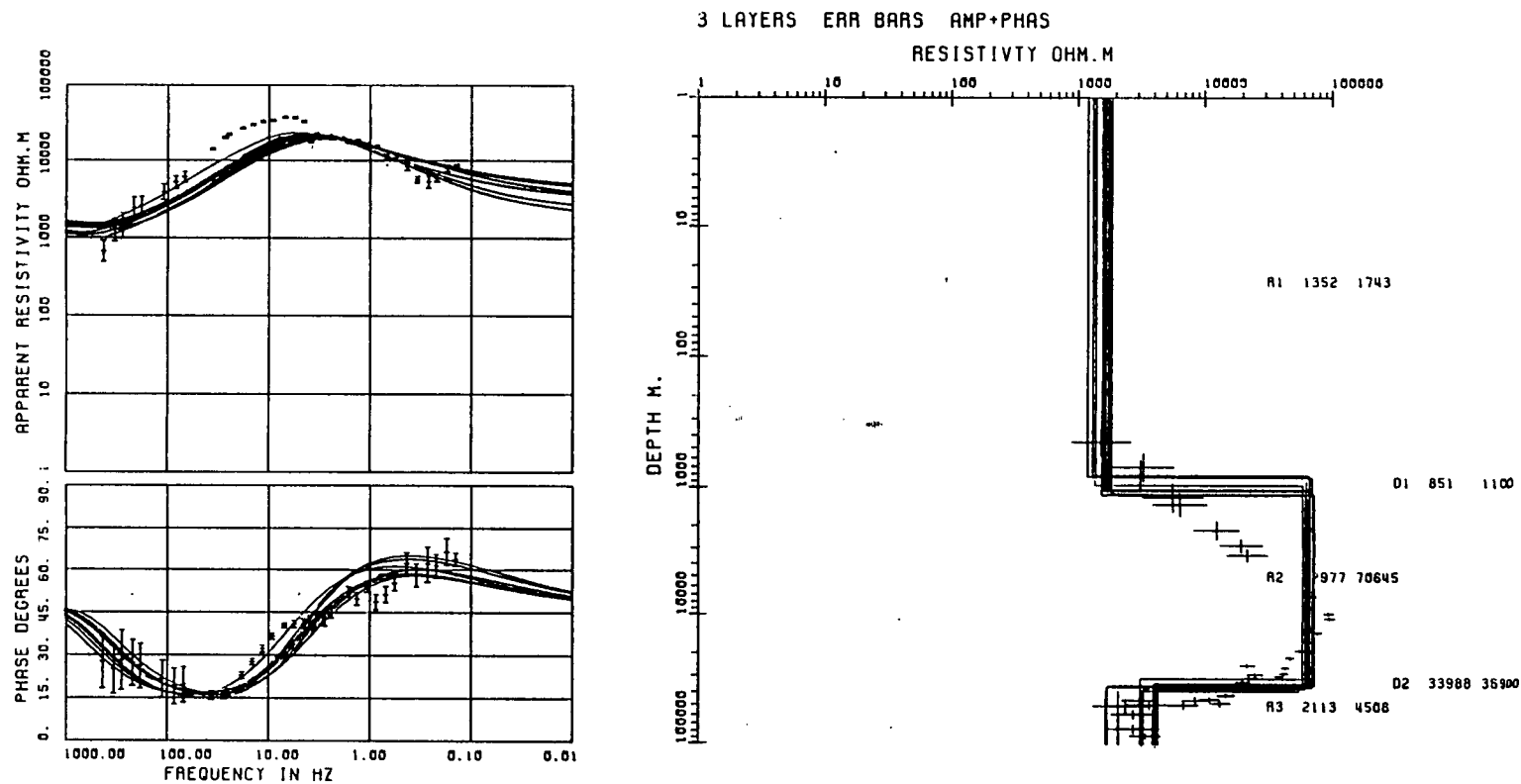


FIGURE 5.1 (8).

1D MODEL FOR SITE E ROTATED NORTH

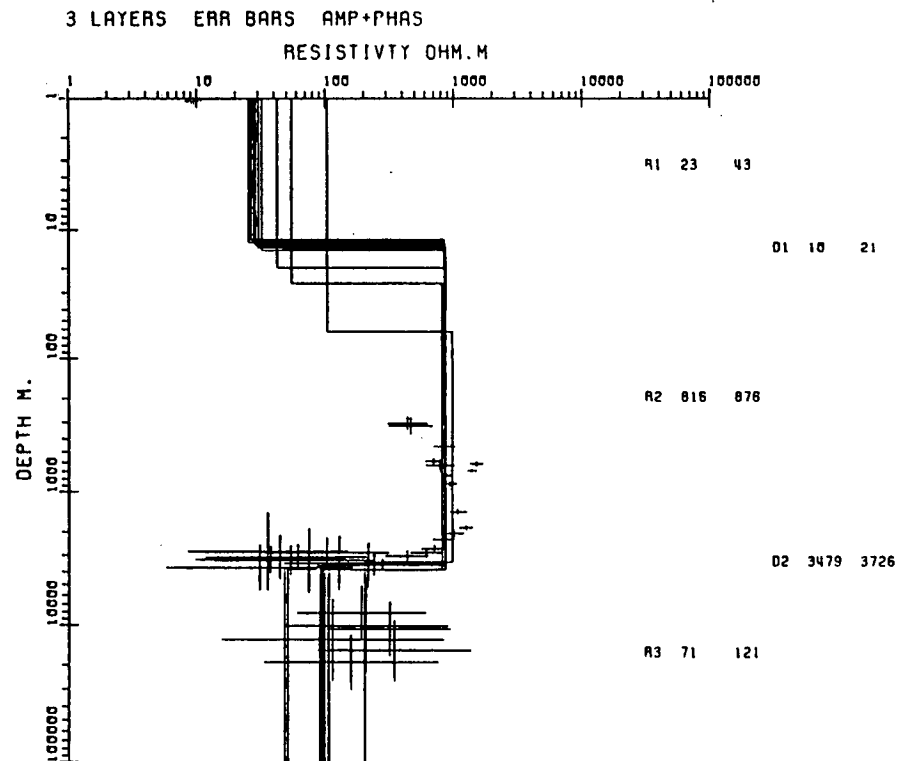
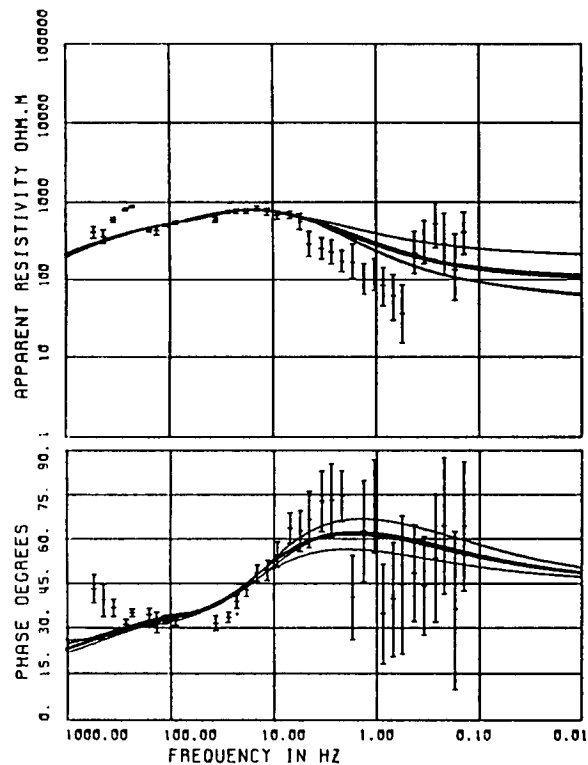


FIGURE 5.1 (9)

1D MODEL FOR SITE E ROTATED EAST

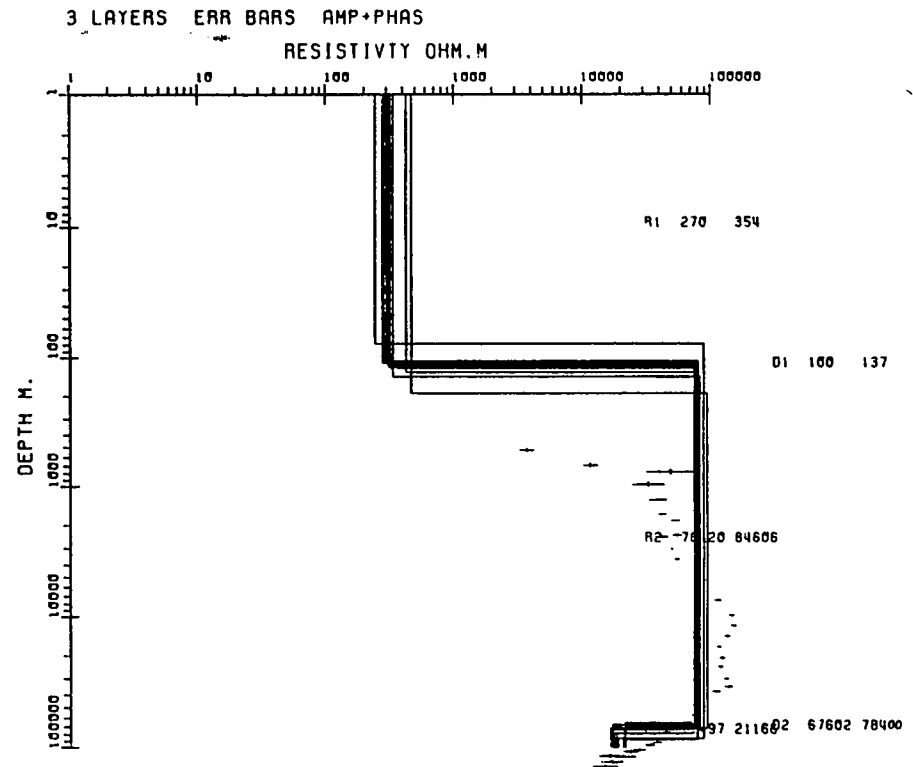
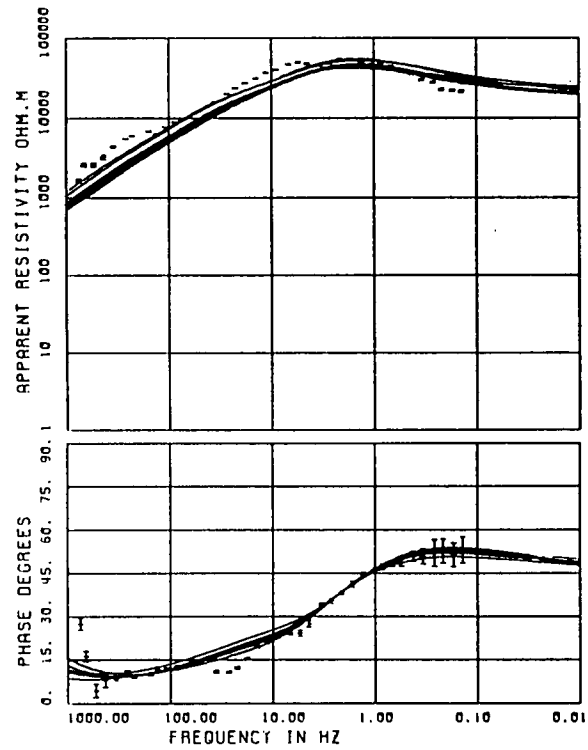


FIGURE 5.1 (10).

1D MODEL FOR SITE F ROTATED EAST

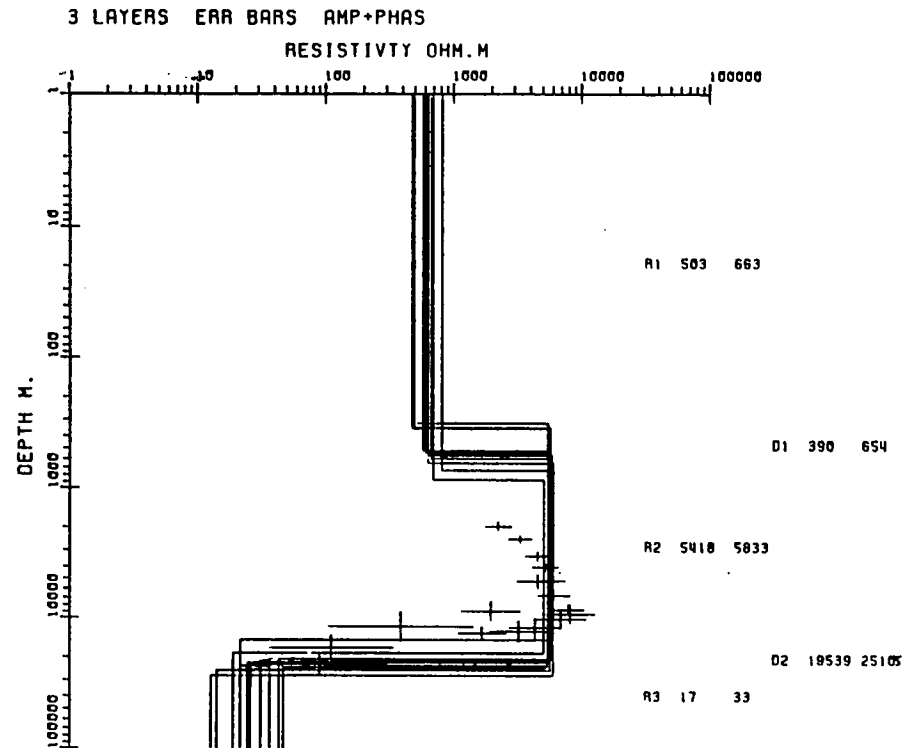
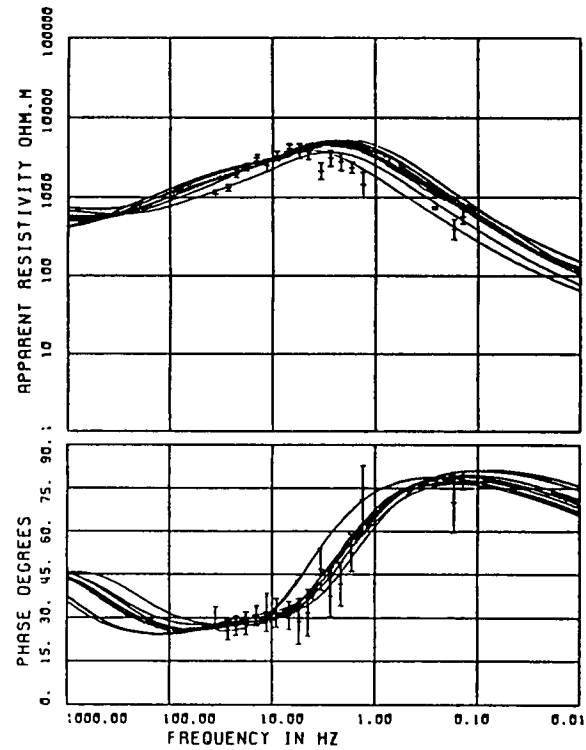


FIGURE 5.1 (12).

1D MODEL FOR SITE G ROTATED NORTH

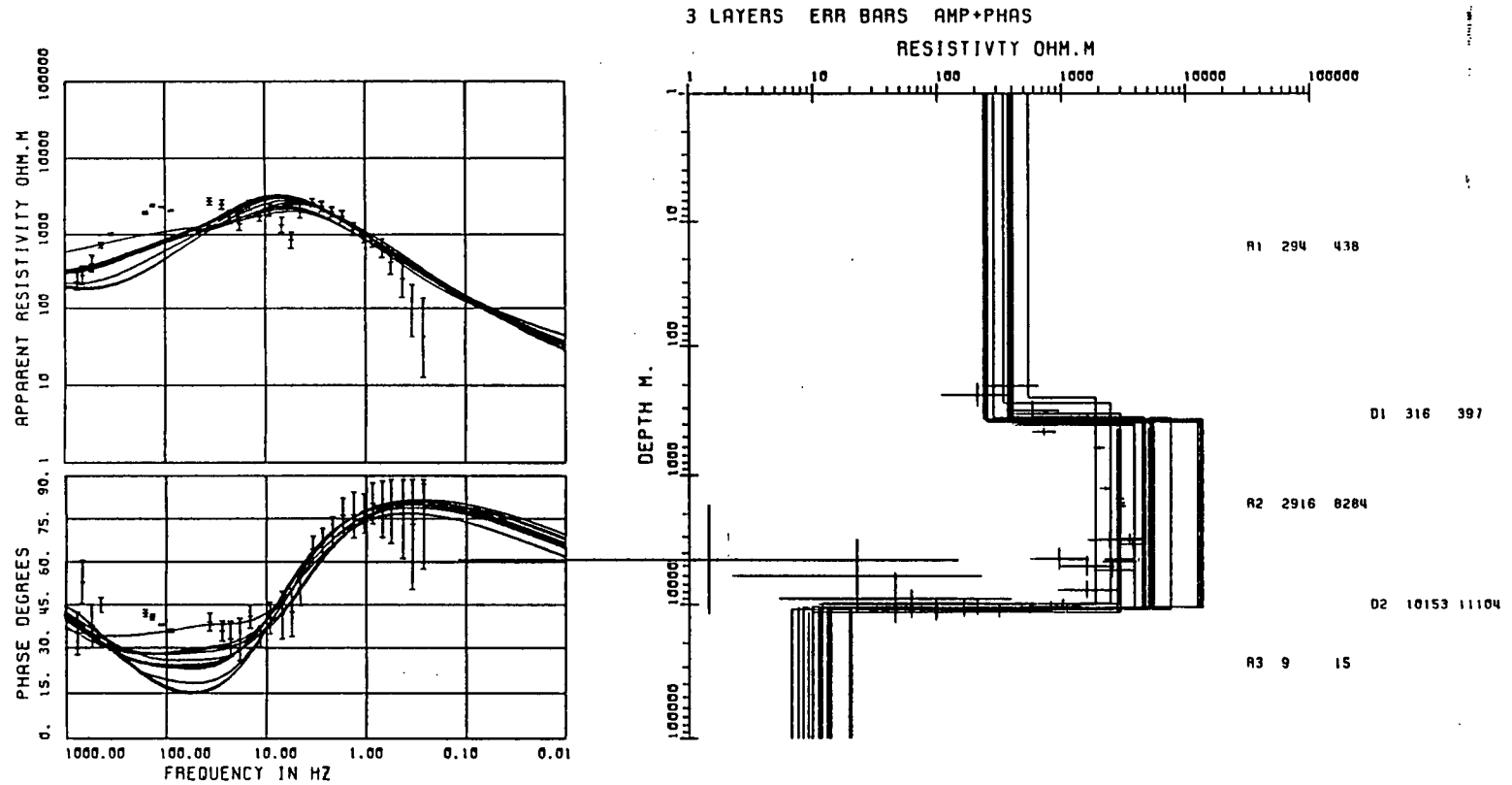


FIGURE 5.1 (13).

1D MODEL FOR SITE G ROTATED EAST

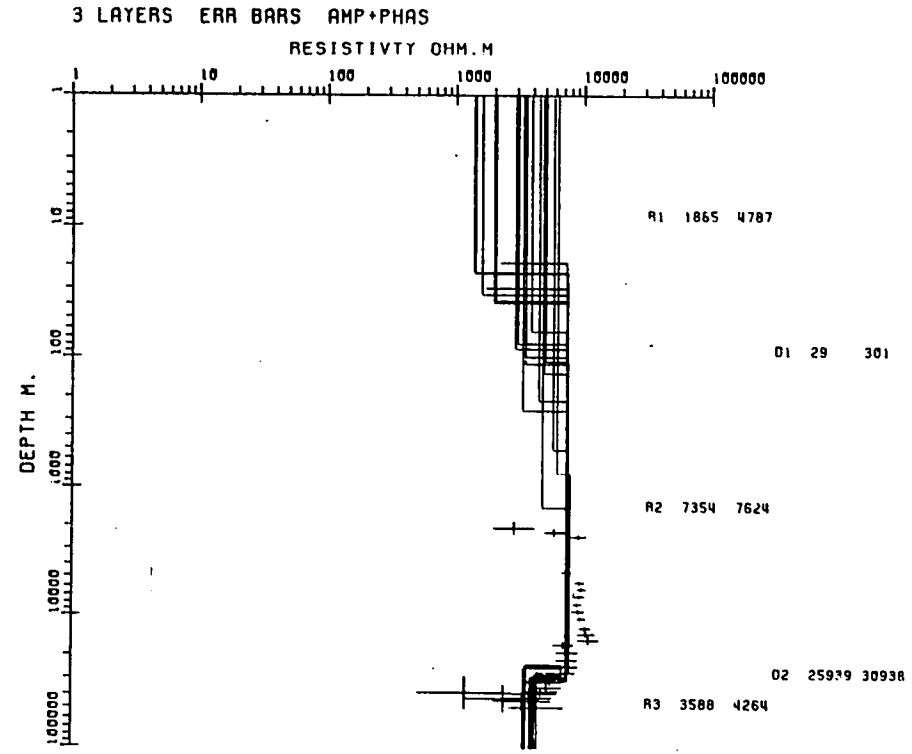
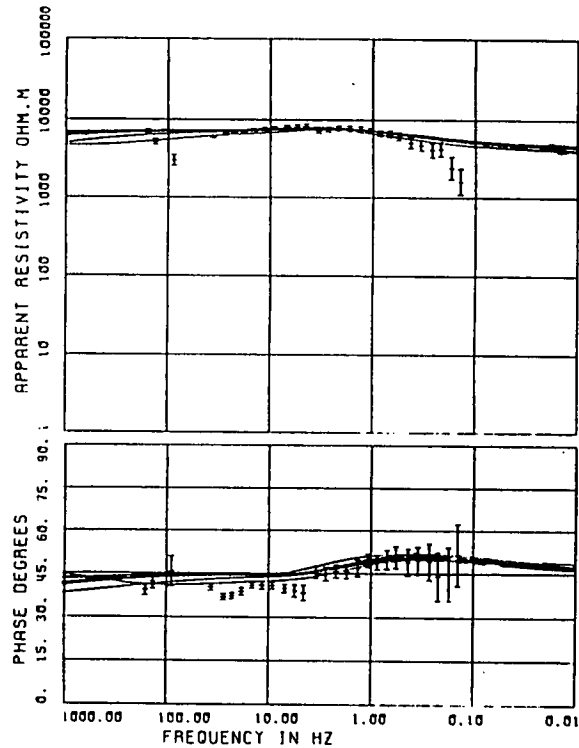


FIGURE 5.1 (14).

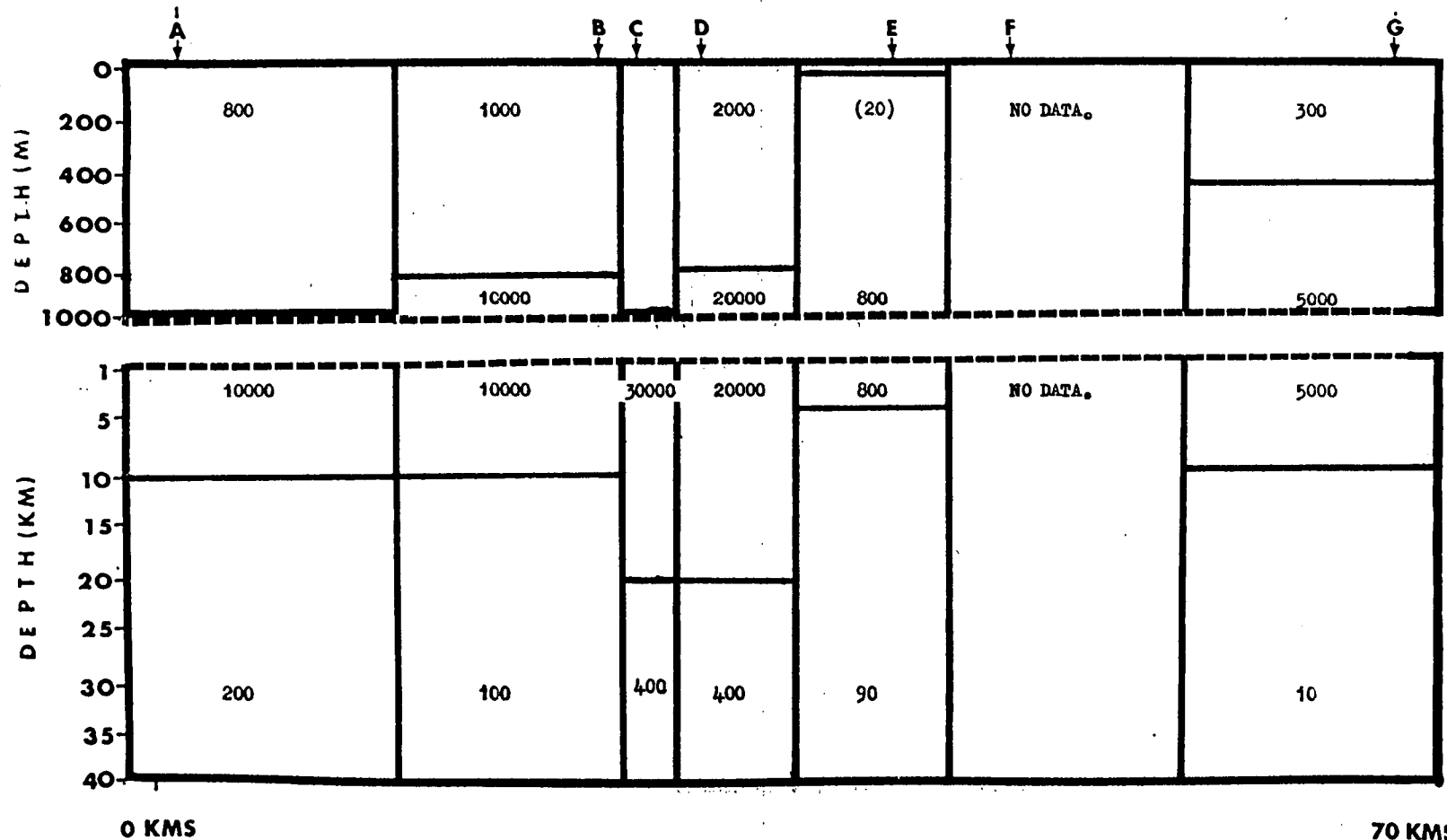
The computed responses for the one-dimensional models are superimposed on the observed responses as shown in Figure (5.1). They are also collected to form conductivity sections for each of the rotated measurement axes along the profile between sites A and G.

These models (Figure 5.1 and Figure 5.2) show little difference in conductivity structure between the Lewisian Foreland and the Moinian Hinterland. However many of the models incorporate layers having resistivities in the range 1×10^4 ohm-metres TO 1×10^5 ohm-metres and these layers extend to considerable depth near the centre of the profile.

At the frequencies used, the skin-depths in such highly resistive layers may extend to 50 Kms. Since the one-dimensional model sections of Figure (5.1) and Figure (5.2) indicate a lateral variation in conductivity structure over horizontal distances of the order of tens of kilometers, we cannot draw any useful any conclusions from these one-dimensional models. For this reason two-dimensional modelling was subsequently conducted as discussed in Chapter VIII.

NATIONAL GRID REFERENCE
21279243

NATIONAL GRID REFERENCE
27188943

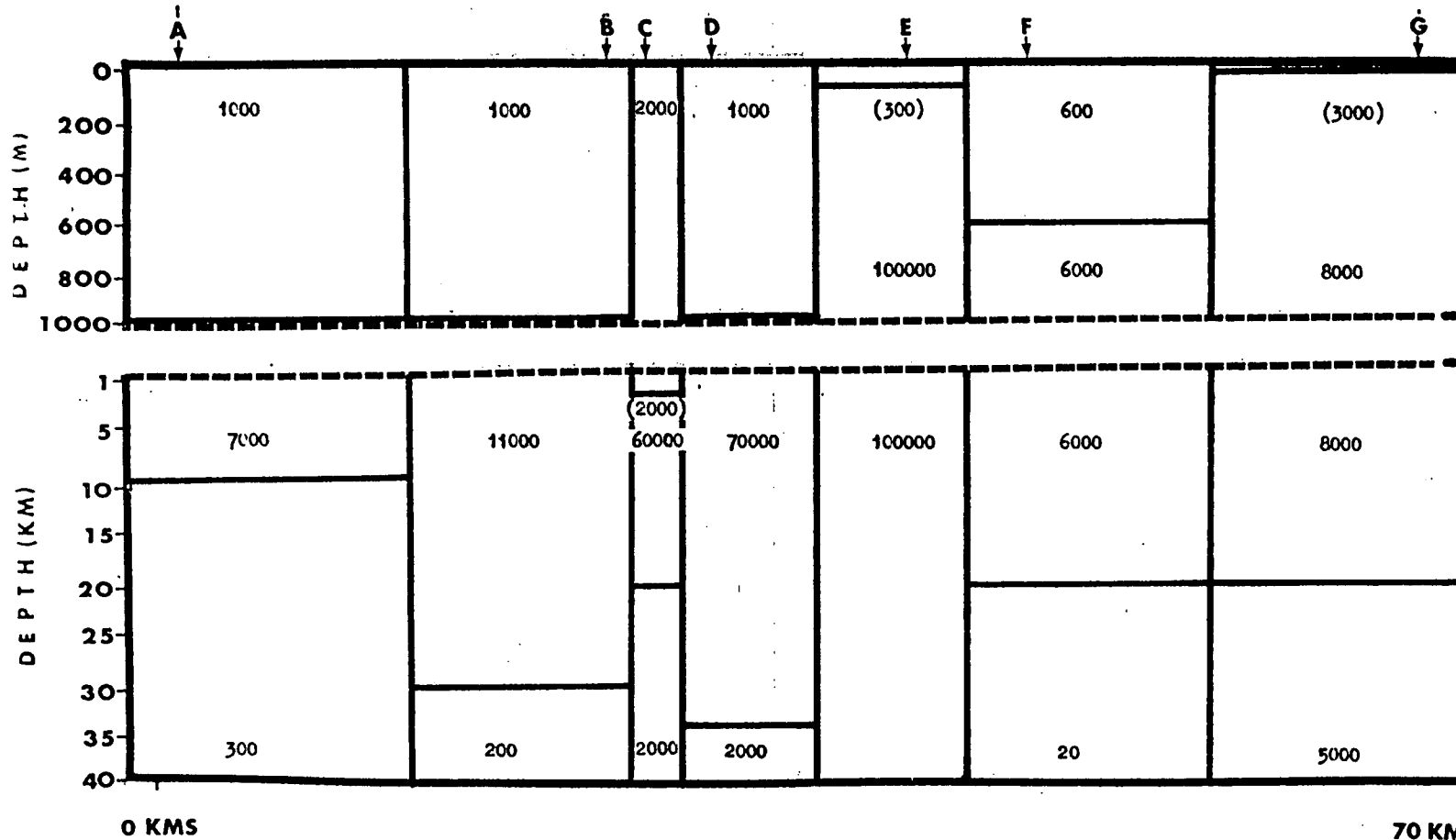


OHM-METRES

FIGURE 5.2. (1). THE COMPILATION OF ONE-DIMENSIONAL MODELS FOR THE ROTATED NORTH AXIS.

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NATIONAL GRID REFERENCE
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OHM-METRES

FIGURE 5.2. (2). THE COMPILATION OF ONE-DIMENSIONAL MODELS FOR THE ROTATED EAST AXIS.

CHAPTER VI

THE OPTIMIZATION THEORY FOR INVERSION

6.1 OPTIMIZATION AND STATISTICAL INVERSION THEORY.

This section considers the use of the truncation and ridge regression methods applied to inversion in terms of optimization and statistical interpretation.

6.1.1 A PRACTICAL MODELLING PROBLEM.

Consider an approximate two-dimensional model derived by collating one-dimensional models produced at each of the measuring sites by say Hedgehog inversion technique applied in this study. Let this model consist of block resistivities and orthogonal boundaries. Designate the value of a block resistivity or the position of a boundary as a parameter.

It should be possible given sufficient parameters, to change them to improve the fit of the model responses to the anisotropic response estimates. One approach changes the parameters one at a time by trial and error. Unfortunately however there is often little indication as to how much a parameter should be perturbed. Several trial changes may be necessary to optimize the model fit at this stage. However it may then be found that a parameter has been overadjusted to compensate for errors in the other parameters of the model. Thus when the other parameters are adjusted it may be necessary to return to the first parameter to correct the over-adjustment or bias.

These two problems may be overcome to some extent by linearizing the model over some restricted range. The Jacobian of the model response derivatives with respect to a number of parameters is obtained. Using a minimization of variance technique the parameters are adjusted simultaneously to a set of optimum values which lie within the restricted range of linearity. The process is then repeated. This method has the further advantage that the entire data set is considered simultaneously so that the interaction of the model parameters is recognized.

It may be found however that the initial set of parameters is ultimately insufficient to describe a model with a response which fits

the data. Further parameters may then have to be made available. However by the time a deficiency in the number of parameters has been identified a number of iterations may have been made and hence the adjustments of the initial set of parameters may be biased.

The initial choice of parameters is clearly important. However the linearization method is unable to allocate the parameters. Although a fine grid of blocks would be ideal, this would have required a finite difference forward modelling program (section 7.1) would have to be used in order that the computing time would not become prohibitive.

In this study only models with a few block resistivities were considered.

6.1.2 THE GENERAL THEORY

Let $x_1, \dots, x_n$ be the parameters and $\phi_1, \dots, \phi_m$ be the discrete model responses. Let $\psi_1, \dots, \psi_m$ be the set of discrete measured responses. In general the ϕ_i and x_i are related by some non-linear function.

$$\phi_j = \phi_j(x_i) \quad i=1, n, \quad j=1, m \quad 1$$

It is required to minimize the misfit of the calculated model to the data (Jupp and Vozoff (1974), Jupp and Vozoff (1977), Lawson and Hanson (1974), Luenburger (1968), Plackett (1961), Price (1964), Rodgers (1976), Smith (1969), Twomey (1977)). The measured responses ψ however are associated with unequal errors ϵ_i and are heterogeneous in units. Thus assuming the errors on the data to be independent the sum $\sum (\psi_i - \phi_i / \epsilon_i)^2$ is minimized. To effect this we solve an equation similar to (2).

$$A^T A \underline{x} = A^T \underline{y} \quad 2$$

The minimization is effected by local linearization of the model response function ϕ_j . Let A_0 be the Jacobian of $\partial \phi_j / \partial x_i$ for $i=1, n$ and $j=1, m$. Let the errors ϵ_i on the data be independent so that $\text{COV}(\underline{y})$ is a diagonal matrix with entries $1/\epsilon_{ii}^2$. Then we may define the scaled data $\underline{y}$ as below:

$$A = [\text{COV}(\underline{y})]^{1/2} A_0 \quad 3$$

$$\underline{\tilde{y}} = [\text{COV}(\underline{y})]^{1/2} \underline{\psi} \quad 4$$

The scaled equations may now be solved for $\underline{x}$. It may be shown that (2) minimizes the sum of squared residuals by differentiation of the

expression:

$$\phi = \left| \underline{y} - A \underline{x} \right|^2 = \sum_{j=1}^m \left[y_j - \sum_{i=1}^n a_{ij} x_i \right]^2 \quad 5$$

We may decompose the square matrix $A^T A$ using the decomposition :

$$A^T A = S^T D S \quad 6$$

In this representation the columns of S constitute the eigenvectors and the diagonal of D constitutes the eigenvalues of the equation :

$$A^T A \underline{x} = d \cdot \underline{x} \quad 7$$

It should be noted that the singular value decomposition of Lanczos may be written :

$$A = U \Lambda V^T \quad 8$$

where $S=V^T$ and $D=\Lambda^T \Lambda$. This second decomposition was used in this study in preference to that of equation (6). It may be shown that the least squares solution for x_i as given by (2) may be obtained using the expression :

$$\underline{x} = V \Lambda^{-1} U^T \underline{y} \quad 9$$

The Lanczos inverse A^+ is evaluated by determining Λ^{-1} in accordance with the conditions :

$$A^+ = V \Lambda^{-1} U^T \quad 10$$

$$\lambda \Rightarrow 1/\lambda \quad \text{IF } \lambda \neq 0 \quad 11$$

$$\lambda \Rightarrow 0 \quad \text{IF } \lambda = 0 \quad 12$$

6.1.3. THE NATURAL INVERSE OF LANCZOS.

The Natural Inverse of Lanczos (Lanczos (1961), Penrose (1954), Roxis (1984)) appears frequently in the following discussion. For completeness a description of the inverse and the associated notation is given below.

The $m \times n$ matrix A may be studied by enlarging it to an $(m+n) \times (m+n)$ square matrix and considering its eigenvalue equation:

$$\begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} \underline{u}_i \\ \underline{v}_i \end{bmatrix} = \lambda_i \begin{bmatrix} \underline{u}_i \\ \underline{v}_i \end{bmatrix} \quad 13$$

We may express (13) in matrix form :

$$A V = \Lambda U \quad 14$$

$$A^T U = \Lambda V \quad 15$$

After multiplication we may obtain:

$$A^T A \underline{V}_i = \lambda_i^2 \underline{V}_i \quad 16$$

$$A^T A \underline{U}_i = \lambda_i^2 \underline{U}_i \quad 17$$

Hence $\underline{v}_i^T \underline{v}_j = 0$, or the vectors $\underline{v}_i$ and $\underline{v}_j$ are orthogonal and $\underline{u}_i^T \underline{u}_j = 0$, or the vectors $\underline{u}_i$ and $\underline{u}_j$ are orthogonal for all λ_i .

The vectors $\underline{v}_i$ and $\underline{u}_i$ may be found independently of each other but for non-zero eigenvalues ($\lambda_i \neq 0$) the U and V spaces are coupled. Let there be p non-zero eigenvalues. It is convenient to divide the U space into U_p and U_0 and the V space into V_p and V_0 as below:

$$A^T A V_p = \lambda_p^2 V_p \quad 18$$

$$A^T A V_0 = 0 \quad 19$$

$$A^T A U_p = \lambda_p^2 U_p \quad 20$$

$$A^T A U_0 = 0 \quad 21$$

Any solution to:

$$A^T A V_p = \lambda_p^2 V_p \quad 22$$

may be added to any solution to:

$$A^T A V_0 = 0 \quad 23$$

to give the general solution for V.

Hence solutions for V where one or more of the λ_i are zero are non-unique and contain projections into the V_0 space.

A similar argument applies to the solutions for U.

6.1.3.1 THE ANALOGY WITH SQUARE SYMMETRIC MATRICES.

Let the matrix A be square and symmetric so that $m=n=p$. Then A may be decomposed as below where d is a diagonal matrix and $S^T S = S S^T = I$:

$$A = S^T D S \quad 24$$

For the square symmetric matrix by analogy of (13) with (24) we have:

$$U = V \quad 25$$

$$V^T V = V V^T = I \quad 26$$

$$U^T U = U U^T = I \quad 27$$

Whence

$$A^{-1} = B = V A^{-1} U^T \quad 28$$

6.1.3.2 THE GENERAL MXN MATRIX.

The inverse B may be extended to account for the general mxn matrix A of rank p as below:

$$B = V_P A^{-1}_P U_P^T \quad 29$$

Where

$$\lambda_i \Rightarrow 1/\lambda_i \quad \text{IF } \lambda_i \neq 0 \quad 30$$

$$\lambda_i \Rightarrow 0 \quad \text{IF } \lambda_i = 0 \quad 31$$

Then we have:

$$AB = U_P U_P^T = I_P \quad 32$$

Also

$$BA = V_P V_P^T = I_P \quad 33$$

Let $U_P \eta$ be an arbitrary vector in U_P space. Then the product AB leaves $U_P \eta$ unchanged as below:

$$AB U_P \eta = U_P U_P^T U_P \eta = U_P \eta \quad 34$$

Similarly let $V_P \eta$ be an arbitrary vector in V_P space. Then the product BA leaves $V_P \eta$ unchanged as below:

$$BA V_P \eta = V_P V_P^T V_P \eta = V_P \eta \quad 35$$

The matrix B is known as the Natural Inverse of A which operates only in p space.

6.1.3.3 THE GENERAL LINEAR SYSTEM.

Consider the equation:

$$A \underset{\sim}{x} = \underset{\sim}{y} \quad 36$$

We may use B to obtain the solution as below:

$$\underset{\sim}{x} = B \underset{\sim}{y} \quad 37$$

$$\underset{\sim}{x} = V_P A^{-1}_P U_P^T \underset{\sim}{y} \quad 38$$

If the equations are compatible then we have:

$$AB \underset{\sim}{y} = \underset{\sim}{y} \quad 39$$

Whence:

$$U_P A_P V_P^T V_P A_P^{-1} U_P^T \underset{\sim}{y} = \underset{\sim}{y} \quad 40$$

Hence the equations are only compatible if y is in U_p space and has the form $y = U_p \eta$ where η is some vector. The least-squares equations are not usually compatible.

If the equations are complete then we have:

$$\tilde{x} = B A \tilde{x} \quad 41$$

Whence:

$$\tilde{x} = V_p \Lambda_p^{-1} U_p^T U_p \Lambda_p V_p^T \tilde{x} \quad 42$$

Hence the equations are only complete if x is in V_p space and has the form $x = V_p \eta$ where η is some vector. The solution then has no projection into the V_0 space since $V_p^T V_0 = 0$.

6.1.3.4 THE LEAST SQUARES INVERSE.

Let A be an $m \times n$ matrix and let:

$$A \tilde{x} = \tilde{y} \quad 43$$

It was shown in section (6.1.2) that the least-squares solution for x may be obtained using:

$$\tilde{x} = [A^T A]^{-1} A^T \tilde{y} \quad 44$$

$$\tilde{x} = [V_p \Lambda_p U_p^T U_p \Lambda_p V_p^T]^{-1} V_p \Lambda_p U_p^T \tilde{y} \quad 45$$

$$\tilde{x} = V_p \Lambda_p^{-1} U_p^T \tilde{y} \quad 46$$

The least-squares solution x has no projection into the V_0 space since $V_0^T V_p = 0$.

6.1.4 THE STEP LENGTH LIMITATION.

The truncation technique (Marquardt (1970)) for step-length limitation uses the expression below :

$$\tilde{x}_T = V \Lambda_T^{-1} U^T \tilde{y} \quad 47$$

where the elements of Λ_T^{-1} are related to those of Λ by the transforms :

$$\lambda \Rightarrow 1/\lambda \quad \text{IF } \lambda \geq \lambda_0 \quad 48$$

$$\lambda \Rightarrow 0 \quad \text{IF } \lambda < \lambda_0 \quad 49$$

where λ_0 is some threshold eigenvalue.

The ridge regression technique for step-length limitation uses the expression :

$$[A^T A + \mu I] \underline{x}_R = A^T \underline{y} \quad 50$$

This is equivalent to the form :

$$\underline{x}_R = V \Lambda_R^{-1} U^T \underline{y} \quad 51$$

where the elements of Λ_R^{-1} are related to those of Λ by the transform:

$$\lambda \Rightarrow \frac{\lambda}{\lambda^2 + \mu^2} \quad 52$$

where μ is some damping factor.

It should be noted that $A^T \underline{y}$ is the component of the gradient vector resolved along the direction of the misfit $\underline{y}$ between the data and the model.

The gradient method uses the expression :

$$\underline{x}_G = K A^T \underline{y} \quad 53$$

where K is some arbitrary scalar chosen to restrict the step-length.

Alternatively the parameters which produce the small λ_i may be removed from the problem by for example inspecting the associated Ridge-Plots.

It may be shown that the Gauss Method (where $\lambda_0 = \mu = 0$) is not convergent when :

54

However the gradient method is always theoretically convergent. As μ is increased the ridge regression technique produces steps $\underline{x}_R$ which have decreasing length but which make a decreasing angle with $\underline{x}_G$.

The fact that $||\underline{x}_R||$ decreases with increasing μ is shown by utilizing the fact that $A^T A$ is a square matrix where $V^T V = V V^T = I$ and expressing $\underline{x}_R$ as below :

$$\underline{x}_R = V^T [A^2 + \mu I]^{-1} V A^T \underline{y} \quad 55$$

Let :

$$\underline{z} = V A^T \underline{y} \quad 56$$

Then we obtain :

$$|\underline{x}_R| = \sum_{i=1}^{i=K} \frac{\tau_i^2}{[A_i + \mu I]^2} \quad 57A$$

Since T_i and Λ_i are independent of μ $|x_R|$ decreases with increasing μ .

We may show that the angle between the gradient vector x_G and the ridge regression vector x_R decreases with increasing μ as below.

Let x_G be the correction vector of the gradient method and let x_R be the correction vector of the ridge regression method with a damping factor μ . Then as μ increases monotonically θ decreases monotonically. We have the angle θ given by :

$$\cos \theta = \frac{x_R^T x_G}{|x_R| |x_G|} \quad 57B$$

The gradient correction vector x_G is given by :

$$x_G = \alpha \left[\sum_{i=1}^{i=K} \left[y_i - f_i \right] \frac{\partial f_i}{\partial \theta_j} \right]^T \quad j=1, \dots, K. \quad 57C$$

The angle may be expressed as below :

$$\cos \theta = \frac{Y^T [\Lambda^2 + \mu I]^{-1} Y}{[Y^T [\Lambda^2 + \mu I]^{-2} Y]^{1/2} [x_G^T x_G]^{1/2}} \quad 57D$$

Whence :

$$\cos \theta = \frac{\sum_{j=1}^{j=K} \frac{V_j^2}{\lambda_j^2 + \mu}}{\left[\sum_{j=1}^{j=K} \frac{V_j^2}{\lambda_j^2 + \mu} \right] [x_G^T x_G]^{1/2}} \quad 57E$$

After differentiation we obtain :

$$\frac{d \cos \theta}{d\mu} = \frac{\left[\sum_{j=1}^{j=K} V_j^2 \prod_{i=1, i \neq j}^{i=K} [\lambda_i^2 + \mu] \right] \left[\sum_{j=1}^{j=K} V_j^2 \prod_{i=1, i \neq j}^{i=K} [\lambda_i^2 + \mu]^3 \right] - \left[\sum_{j=1}^{j=K} V_j^2 \prod_{i=1, i \neq j}^{i=K} [\lambda_i^2 + \mu] \right]^2}{\left[\sum_{j=1}^{j=K} \frac{V_j^2}{[\lambda_j^2 + \mu]^2} \right]^{3/2} \left[\prod_{j=1}^{j=K} [\lambda_j^2 + \mu]^2 \right] [x_G^T x_G]} \quad 57F$$

The denominator of (57F) is positive and the numerator may be expressed as :

$$\left[\sum_{j=1}^{j=K} \left[V_j \prod_{i=1, i \neq j}^{i=K} [\lambda_i^2 + \mu] \right]^2 \right] \left[\sum_{j=1}^{j=K} \left[V_j \prod_{i=1, i \neq j}^{i=K} [\lambda_i^2 + \mu]^3 \right]^2 \right] - \left[\sum_{j=1}^{j=K} \left[V_j \prod_{i=1, i \neq j}^{i=K} [\lambda_i^2 + \mu] \right]^{1/2} \left[V_j \prod_{i=1, i \neq j}^{i=K} [\lambda_i^2 + \mu]^3 \right]^{1/2} \right]^2 \quad 57G$$

Then by the Schwartz inequality $d(\cos \theta)/d\mu$ is positive for $\mu > 0$.

The truncation method also possesses the property that the step correction length $|x_T|$ decreases with assumed rank R of the matrix A . This may be shown using a similar argument to that used with the ridge regression technique yielding :

$$|x_T| = \sum_{j=1}^{j=R} \lambda_j^{-2} \left[\sum_{j=1}^{j=R} [V_j g_j] \right]^2 \quad 58A$$

where we have $g = A^T y$. As R decreases $|x_T|$ decreases.

We may derive the conditions under which the angle between the gradient vector x_G and the truncation vector x_T decrease with decreasing assumed rank R as below.

Let x_G be the correction vector of the gradient method and let x_T be the correction vector of the truncation method. Let θ be the angle

between x_G and x_T .

Then we have :

$$\cos \phi = \frac{x_T^T x_G}{|x_T| |x_G|} \quad 58B$$

Then :

$$x_T^T x_G = x_G^T V A^{-2} V^T x_G \quad 58C$$

Whence :

$$\cos \phi = \frac{1}{|x_G|} \frac{\sum_{u=1}^{u=R} \lambda_u^{-2} \left[\sum_{j=1}^{j=P} [x_{Gj} V_{ju}] \right]}{\left[\sum_{u=1}^{u=R} \lambda_u^{-4} \left[\sum_{j=1}^{j=P} [x_{Gj} V_{ju}] \right]^2 \right]^{1/2}} \quad 58D$$

Then :

$$|x_G| [\cos \theta_R - \cos \theta_{R-1}] = \frac{\sum_{u=1}^{u=R} \lambda_u^{-2} \left[\sum_{j=1}^{j=P} [x_{Gj} V_{ju}] \right]^2}{\left[\sum_{u=1}^{u=R} \lambda_u^{-4} \left[\sum_{j=1}^{j=P} [x_{Gj} V_{ju}] \right]^2 \right]^{1/2}} - \frac{\sum_{u=1}^{u=R-1} \lambda_u^{-2} \left[\sum_{j=1}^{j=P} [x_{Gj} V_{ju}] \right]}{\left[\sum_{u=1}^{u=R-1} \lambda_u^{-4} \left[\sum_{j=1}^{j=P} [x_{Gj} V_{ju}] \right]^2 \right]^{1/2}} \quad 58E$$

The denominator of (58E) is positive. The numerator is positive and the angle decreases when :

$$\lambda_R^2 \leq \frac{1}{2} \left[\frac{\sum_{u=1}^{u=R-1} \lambda_u^{-2} \left[\sum_{j=1}^{j=P} [x_{Gj} V_{ju}] \right]^2}{\sum_{u=1}^{u=R-1} \lambda_u^{-4} \left[\sum_{j=1}^{j=P} [x_{Gj} V_{ju}] \right]^2} - \frac{\left[\sum_{j=1}^{j=P} [x_{Gj} V_{jR}] \right]^2}{\sum_{u=1}^{u=R-1} \lambda_u^{-2} \left[\sum_{j=1}^{j=P} [x_{Gj} V_{ju}] \right]^2} \right] \quad 58F$$

Under certain circumstances the condition above may be simplified to $(\lambda_{R-1}/\lambda_{R-2}) \ll 1$. Nevertheless in this study the condition was rarely satisfied and where truncation to low ranks would have been necessary to secure sufficient step-length limitation the ridge regression technique was used.

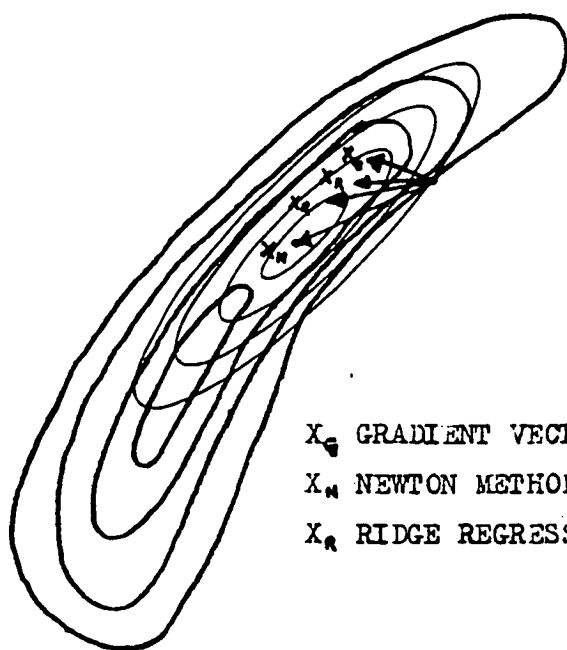
The effects of using the ridge regression or truncation techniques may be seen by reference to Figure (6.1). Where the gradient method is used the convergence to the minimum may be slow and hemstitching (Figure 4.2) may occur. When the Gauss-Newton method is used the vectors x_N lie along the ridges but the iterative series may diverge if (54) is not satisfied and $|x_N|$ may be sufficiently large to extend beyond the region of linearity. The ridge regression and truncation techniques produce x_R which lie between these extremes.

6.1.5 RIDGE REGRESSION AS CONSTRAINED OPTIMIZATION.

It is possible to envisage ridge regression as a constrained minimization problem : minimize $x_R^T x_R$ subject to the constraint :

$$[x_R - \langle x \rangle]^T A^T A [x_R - \langle x \rangle] = \phi_0 \quad 61$$

where ϕ_0 is the permissible sum squared bias in the estimate $\hat{x}_R$ and x is the unbiased least squares estimate. Using the method of Lagrange

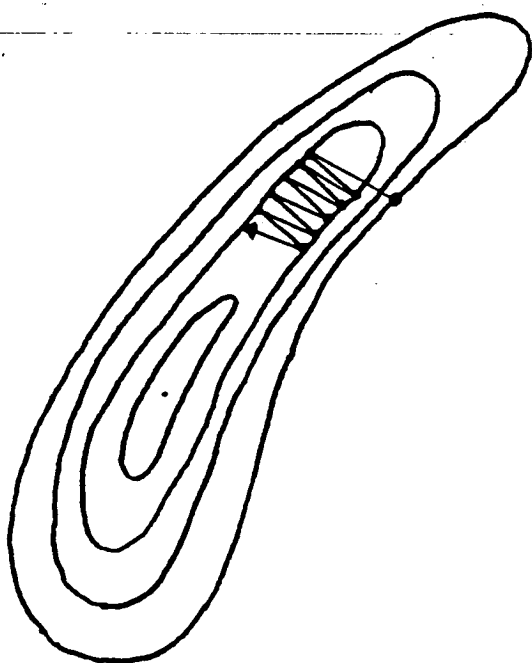


X_G GRADIENT VECTOR CORRECTION VECTOR.

X_N NEWTON METHOD CORRECTION VECTOR.

X_R RIDGE REGRESSION METHOD CORRECTION VECTORS.

THE GRADIENT AND RIDGE REGRESSION METHODS.



THE GRADIENT METHOD. HEMSTITCHING.

FIGURE 6.1. THE GRADIENT AND RIDGE REGRESSION METHODS. HEMSTITCHING.

multipliers (50) and (61) may be solved to obtain an estimate for x_R .

Alternatively an equivalent constrained problem is to minimize $(y - Ax_R)^T(y - Ax_R)$ subject to the constraint :

$$\underline{x}_R^T \underline{x}_R = R^2 \quad 62$$

where R is the step length. Using the method of Lagrange Multipliers (50) may be solved with (62) to obtain an estimate x_R .

Neither of these methods was used as they are unable to limit the magnitude of any given step correction vector element to a given range . The linearization of the variation in the model response with respect to the model parameters is only valid for limited ranges in the parameters. As the relationship between the largest step correction vector element and the possible bias ϕ_0 was not known the method of (61) was not used. The method of (62) was not used since the relationship between the largest step correction vector element and the step length R is only known as an inequality The consequent use of step correction vectors of unnecessarily short lengths would be inefficient. Hence in this study the magnitude of the step correction vector was limited by the adjustment of μ until the largest vector element equaled some maximum.

6.1.6 THE STATISTICAL PROPERTIES OF THE RIDGE REGRESSION AND TRUNCATION METHODS.

The ridge regression and truncation methods have been considered from the viewpoint of optimization and step-length limitation . In the following section we present a number of statistical advantages (Hoerl and Kennard (1970), Marquardt (1970)) of using these methods.

In the case of the truncation method the shorter principal component vectors were neglected. In the case of the ridge-regression method the shorter principal component vectors were relatively neglected. Hence the correction vectors moved in directions lying between those of the steepest gradients and the ridges or valleys of the $\epsilon^T \epsilon$ surface (section 6.1.4).

If in the region of the minimum, the objective function is sufficiently linear then the properties of the truncation and ridge regression methods should apply as they do to the linear problem. The stabilization methods may reduce the expected sum of squares error between the exact and estimated parameters by decreasing the random error and introducing a systematic bias error. This however increases the sum of squares misfit between the predicted model response and the data.

This is described below.

At the final iteration step, we may consider the model to be approximately linear. We may require an estimation of the error on a vector $\mathbf{x}$. Let the true value of $\mathbf{x}$ be that which satisfies:

$$A\mathbf{x} = \mathbf{y} + \boldsymbol{\xi} \quad 75$$

The estimate of $\mathbf{x}$ may in fact be quite remote from the true value of $\mathbf{x}$ as indicated by the variance expectation :

$$E [[\langle \mathbf{x} \rangle - \mathbf{x}]^T [\langle \mathbf{x} \rangle - \mathbf{x}]] = \sigma^2 \sum [\frac{1}{\lambda_i^2}] \quad 76$$

The variance on this expected value may be similarly large:

$$\text{VAR} [[\langle \mathbf{x} \rangle - \mathbf{x}]^T [\langle \mathbf{x} \rangle - \mathbf{x}]] = 2\sigma^4 \sum [\frac{1}{\lambda_i^4}] \quad 77$$

Let $\mathbf{x}_Z$ be some estimate of $\mathbf{x}$ where:

$$\mathbf{x}_Z = \mathbf{Z} \mathbf{x} \quad 78$$

Then the expectation $E[(\mathbf{x}_Z - \mathbf{x})^T (\mathbf{x}_Z - \mathbf{x})]$ is given by:

$$E [[\mathbf{x}_Z - \mathbf{x}]^T [\mathbf{x}_Z - \mathbf{x}]] = \sigma^2 \text{TRACE} [\mathbf{A}^T \mathbf{A}]^{-1} \mathbf{Z}^T \mathbf{Z} + \mathbf{x}^T [\mathbf{Z} - \mathbf{I}]^T [\mathbf{Z} - \mathbf{I}] \mathbf{x} \quad 79$$

The first term is the sum of the variances while the second term is the Euclidian distance between $\mathbf{x}_Z$ and $\mathbf{x}$ or the squared bias in the estimate $\mathbf{x}_Z$.

Both the estimates of the truncation and ridge regression methods satisfy linear relationships of the same form as (78). It may be shown for both truncation and ridge regression methods that it is possible to obtain a smaller expectation value $E[(\mathbf{x}_Z - \mathbf{x})^T (\mathbf{x}_Z - \mathbf{x})]$ than with the least squares method.

To demonstrate that this is the case for the ridge regression method we express (79) in the form :

$$E [[\langle \mathbf{x}_R \rangle - \mathbf{x}]^T [\langle \mathbf{x}_R \rangle - \mathbf{x}]] = \sigma^2 \sum_{i=1}^{i=P} \frac{\lambda_i^2}{[\lambda_i^2 + \mu]^2} + \mu^2 \sum_{i=1}^{i=P} \frac{[V^T \mathbf{x}]_i^2}{[\lambda_i^2 + \mu]^2} \quad 80$$

The differentiation of (80) yields :

$$\frac{dE [[\langle \mathbf{x}_R \rangle - \mathbf{x}]^T [\langle \mathbf{x}_R \rangle - \mathbf{x}]]}{d\mu} = -2\sigma^2 \sum_{i=1}^{i=P} \frac{\lambda_i^2}{[\lambda_i^2 + \mu]^3} + 2\mu \sum_{i=1}^{i=P} \frac{\lambda_i^2 [V^T \mathbf{x}]_i^2}{[\lambda_i^2 + \mu]^3} \quad 81$$

At $\mu=0$ the expectation $E[(\mathbf{x}_R - \mathbf{x})^T (\mathbf{x}_R - \mathbf{x})]$ is given by $\sigma^2 \sum 1/\lambda_i^2$ while as $\mu \rightarrow \infty$ the squared bias tends asymptotically to $\mathbf{x}^T \mathbf{x}$. From (81) at $\mu=0$ the variance term decreases at a greater rate than the squared bias term increases with μ and hence the expectation $E[(\mathbf{x}_R - \mathbf{x})^T (\mathbf{x}_R - \mathbf{x})]$ assumes values less than $E[(\mathbf{x} - \mathbf{x})^T (\mathbf{x} - \mathbf{x})]$.

Now consider the truncation method. For an assumed rank R of the matrix $A^T A$ equation (79) yields:

$$E[[X_T - \hat{X}]^T [X_T - \hat{X}]] = \sigma^2 \sum_{i=1}^{i=K} [1/\lambda_i^2] + \sum_{i=K+1}^{i=P} \hat{X}_T^T V_{P-R}^T V_{P-R} \hat{X} \quad 82$$

The condition:

$$E[[<X> - \hat{X}]^T [<X> - \hat{X}]] > E[[X_T - \hat{X}]^T [X_T - \hat{X}]] \quad 83$$

Is satisfied when:

$$\sum_{i=K+1}^{i=P} [\sigma^2 \lambda_i^2 - [V_{P-R} \hat{X}]_i] > 0 \quad 84$$

The condition for the truncation method is seen to be more complex than for the ridge regression technique.

It should be noted that the truncation method or ridge regression method may decrease $E[(x_Z - x)^T (x_Z - x)]$ but at the same time this increases the residual sum of squares misfit. If we assume that the response is smooth and that the data are randomly scattered about that response, then $E[(x_Z - x)^T (x_Z - x)]$ decreases with an increase in the residual sum of squares misfit as expected.

At the first iteration step vector we have further assumed that the model is linear. This may not necessarily be true and only a few of the model parameters may show a linear relationship with the responses. If the non-linear parameters are excluded the final step vector estimate is liable to be biased and if all the parameters are used the final step estimate may of necessity be small or in error due to the effects of non-linearity in conjunction with small eigenvalues.

Nevertheless where the region about the minimum is approximately linear the expectation $E[(x_Z - x)^T (x_Z - x)]$ may be minimized to produce a form of optimal solution. This solution however reduces the errors from the random spread of values about x by introducing an unknown bias. Although the expectation value is reduced the introduction of the bias term may itself introduce difficulties in interpretation.

6.1.7 THE ESTIMATION OF THE ERRORS ON THE PARAMETERS.

Let us assume that the minimum residual sum of squares has been reached in accordance with any distortions arising from the biasing. We now require an estimate of the range of values each parameter may assume (Hoerl and Kennard (1970), Jackson (1973), Marquardt (1970), Roxis (1984)).

6.1.7.1 THE PARAMETER COVARIANCE MATRIX.

One possibility is to examine the parameter covariance matrix $(A^T A)^{-1}$. Let the general estimate $\underline{x}_z$ be related to the true value of $\underline{x}$ by (78). Then we obtain :

$$\text{VAR}[\underline{x}_z] = \sigma^2 Z [A^T A]^{-1} Z^T \quad 85$$

In the case of the ridge regression this becomes :

$$\text{VAR}[\underline{x}_R] = \sigma^2 [A^T A + \mu I]^{-1} [A^T A] [A^T A + \mu I]^{-1} \quad 86$$

In the case of the truncation method where $A^T A$ has an assumed rank R we obtain :

$$\text{VAR}[\underline{x}_T] = \sigma^2 V \Lambda_R^{-1} V^T \quad 87$$

The estimates of the diagonal of the covariance matrix indicate the variance associated with the individual parameters. However the region of constant variance Q_v for parameter combinations $\underline{x}$ are hyper-ellipsoids satisfying :

$$\underline{x}^T [A^T A] \underline{x} = Q_v \sigma^2 \quad 88$$

6.1.7.2 THE PARAMETER ELLIPSOID.

It is further possible to identify the maximum parameter range associated with any linear combination $\underline{b}$ of parameters.

Let Q_v be the maximum variance. Then we may minimize $\underline{x}^T \underline{b}$ subject to the constraint :

$$\underline{x}^T [A^T A] \underline{x} = Q_v \sigma^2 \quad 89$$

The Lagrangian function L is given by :

$$\mathcal{L} = \underline{x}^T \underline{b} + \frac{1}{2\alpha} [\sigma^{-2} \underline{x}^T [A^T A] \underline{x} - Q_v] \quad 90$$

Let H be the generalised inverse of A . Then we obtain :

$$\underline{x} = H \left[\underline{y} \pm \left[\frac{\sigma^2 Q_v}{\underline{b}^T H H^T \underline{b}} \right]^{1/2} H^T \underline{b} \right] \quad 91$$

This method is capable of yielding the range of $\underline{x}$ required so that when $\underline{x}$ is projected onto some arbitrary vector $\underline{b}$ the variance limit Q_v is encountered.

The covariance matrix has identical principal components to that of the system under consideration. The eigenvalues of $A^T A$ thus represent the variances associated with the principal components of the system.

Let $Q_y = \sigma$. Let b be a vector with a single unit element $b_i = 1$ and all other elements zero. The range of the corresponding parameter x_i is equivalent to the standard deviation for that parameter evaluated from the parameter covariance matrix.

6.1.7.3 THE MOST SQUARES METHOD OF JACKSON (1976).

Another possible approach is to define some threshold which the residual sum of squares misfit may not exceed. The residuals ϵ may be defined as below :

$$\underline{\epsilon}_R = \underline{y} - A\underline{x} \quad 92$$

For a fixed sum of squares residual $\epsilon_R^T \epsilon_R$ the parameters form hyper-ellipsoids given by :

$$Q = \underline{x}^T A^T A \underline{x} - 2 \underline{x}^T A^T \underline{y} + \underline{y}^T \underline{y} \quad 93$$

We may define a threshold Q_0 and a projection of x onto a arbitrary unit vector b and ascertain the range of values x may assume by minimizing $x^T b$ subject to the constraint :

$$\underline{x}^T A^T A \underline{x} - 2 \underline{x}^T A^T \underline{y} + \underline{y}^T \underline{y} = Q_0 \quad 94$$

The Lagrangian function L is given by :

$$\mathcal{L} = \underline{x}^T b + \frac{1}{2\alpha} [\underline{x}^T A^T A \underline{x} - 2 \underline{x}^T A^T \underline{y} + \underline{y}^T \underline{y} - Q_0] \quad 95$$

Let H be the generalised inverse of A . Then we obtain :

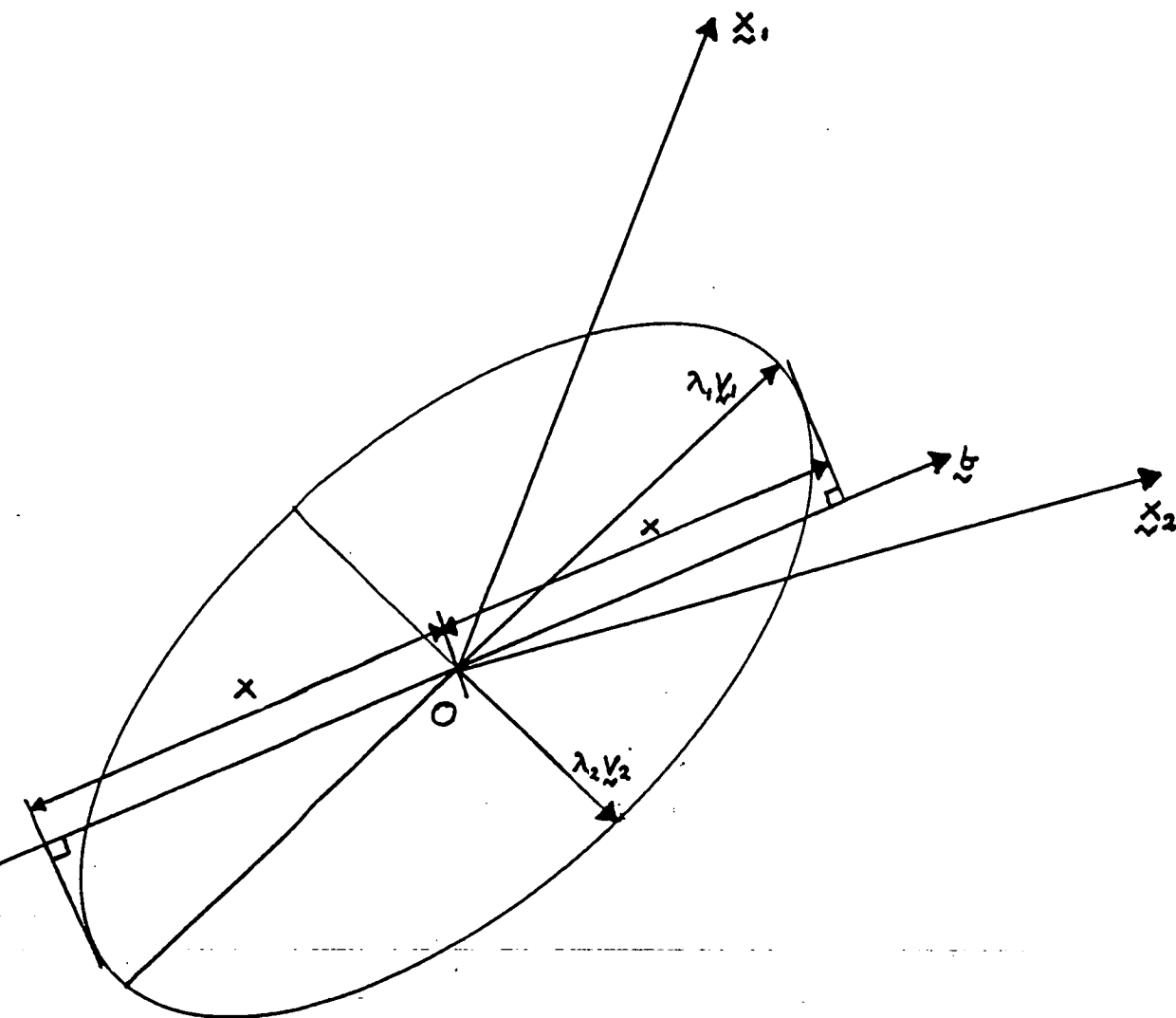
$$\underline{x} = H \left[\underline{y} \pm \left[\frac{Q_0 - Q_{LS}}{b^T H H^T b} \right]^{1/2} H^T b \right] \quad 96$$

Where Q_{LS} is the sum of squares misfit for the least squares solution to (92).

This method is capable of yielding the range of x required so that when x is projected onto some arbitrary vector b the residual sum of squares misfit threshold is encountered. The vector b may be chosen to have one element with all the other elements zero or it may be chosen as a principal axis of the problem or as some linear combination of variables which one may assume to be related to each other.

The procedure may be illustrated by reference to the two-dimensional case shown in Figure (6.2).

The ellipse shown here satisfies (93) for a given value of Q . Let b be a combination of parameters. We evaluate the extreme values of λ to find λb which lie on the boundary of the ellipse and hence satisfy (93).



$$\underline{\underline{x}} = \underline{\underline{H}} \left[\underline{\underline{y}} + \left[\frac{Q_v}{\underline{\underline{b}}^T \underline{\underline{H}} \underline{\underline{H}}^T \underline{\underline{b}}} \right]^{1/2} \underline{\underline{H}}^T \underline{\underline{b}} \right]$$

DIAGRAM FOR $Q = 1$

- $\underline{\underline{x}}_1, \underline{\underline{x}}_2$ THE ORIGINAL VECTOR PARAMETERS.
- $\lambda_1 \underline{\underline{v}}_1, \lambda_2 \underline{\underline{v}}_2$ THE PRINCIPAL COMPONENTS.
- $\underline{\underline{b}}$ THE PARAMETER COMBINATION VECTOR.
- $\underline{\underline{x}}$ THE PARAMETER COMBINATION RANGE.

FIGURE 6.2. THE PARAMETER ELLIPSE.

It is seen that (91) and (96) are identical when :

$$Q_0 - Q_{LS} = Q_V \sigma^2 \quad 97$$

Let $Q_V = \sigma$. When b is a vector with a single unit element $b_i = 1$ with all the other elements zero, the range of the corresponding element x_i is equivalent to the standard deviation for that element evaluated from the parameter covariance matrix.

6.1.7.4 THE PARAMETER BASIS.

The methods above give ranges for the individual parameters which are independent of the parameter basis on condition that matrix Z is diagonal in (85).

This may be illustrated by reference to Jacobian A . Let the parameter basis be changed so that the Jacobian may be represented by AL where L is a diagonal matrix. The expression $(A^T A)^{-1}$ in (85), (91) and (96) after the change of basis may be written as $L^{-1}(A^T A)^{-1}L^{-1}$. Expressions for the parameter ranges which use the diagonal term $(L^{-1}(A^T A)^{-1}L^{-1})_{ii}$ only for each parameter x_i yield parameter ranges for x_i independent of the parameter basis. Expressions which use linear combinations of the diagonal terms $(L^{-1}(A^T A)^{-1}L^{-1})_{ii}$ or the off-diagonal terms $(L^{-1}(A^T A)^{-1}L^{-1})_{ij}$ for $i \neq j$ yield parameter ranges dependent upon the parameter basis.

Thus for a vector b with a single unit element $b_i = 1$ and all other elements zero, the parameter range for x_i is parameter basis independent whereas that for x_j where $i \neq j$ is basis dependent. Where the vector has more than one non-zero element the parameter range is basis dependent.

6.1.7.5 THE APPENDED DATA.

It is questionable however whether the range of a parameter estimated using a technique known to append arbitrary data to the data set or introduce bias into the estimate is a valid range. The effect of the arbitrary data is to reduce the variance from $1/\lambda_i$ TO $1/(\lambda_i^2 + \mu)$ and to reduce the range of values which the parameters may satisfy.

If we require only use of the non-augmented model data then we may either use only the parameters which may be estimated without bias or use the entire parameter set with a non-augmented Jacobian. In both cases the parameter ranges are calculated from less data than the parameter estimates. Hence even though the model has been linearized the calculated parameter range may lie assymmetrically about the

parameter estimates.

6.1.7.6 THE NON-LINEARITY.

The methods described in Section 6.1.7.1 TO Section 6.1.7.5 are strictly only applicable to linear objective functions unless used as part of an iterative scheme. The Hessian of $\epsilon^T \epsilon$ is given by :

$$H = 2 \sum \frac{\partial \epsilon_k}{\partial x_i} \frac{\partial \epsilon_k}{\partial x_j} + 2 \sum \epsilon_k \frac{\partial^2 \epsilon_k}{\partial x_i \partial x_j} = 2A^T A + 2 \sum \epsilon_k \frac{\partial^2 \epsilon_k}{\partial x_i \partial x_j} \quad 98$$

An assumption of the method is that $H \approx 2A^T A$.

In the case of non-linear objective functions the $\epsilon^T \epsilon$ surface is no longer quadratic. In the case of approximately linear objective functions the linear estimation of the error may be sufficient but in more non-linear cases the iterative application of (91) or (96) may be necessary.

A further difficulty of non-linearity is that if the solution is displaced from the minimum then the elements of the Jacobian may be poorly estimated.

Since the solution is derived by an iterative process in which the Jacobian is evaluated several times, the comparison of successive Jacobians should reveal any non-linearity present.

THE ERRORS ON THE MODEL PARAMETERS.

The errors on the model parameters were in this study estimated using two methods. The error on the individual parameters was estimated by setting the maximum residual sum of squares error Q_0 such that :

$$Q_0 = Q_{LS} + \sigma^2 \quad 99$$

Since the Jacobian was that used for the final iteration step the errors may be incorrectly estimated. No iterations were conducted for the error estimations.

Unresolved adjacent parameters of similar values were averaged together by summing the appropriate columns of the Jacobian. The new parameters were estimated and the errors on the parameters calculated for the individual parameters. This differs from the procedure of maximizing the sum of the parameters $x^T b$ since the amalgamated parameters may take only one value. Since in this study the Jacobian was that used for the final iteration step the errors may be underestimated. No iterations were conducted for the error estimations.

6.2 THE DISADVANTAGES OF THE RIDGE REGRESSION AND TRUNCATION TECHNIQUES.

Section (6.1) considered the use of the ridge regression and truncation techniques from the viewpoint of optimization and statistical interpretation. In this section we show that the ridge regression technique relies upon the addition of fictitious data to the data set. Furthermore we show that the technique of adjusting the ridge regression damping factor with each iteration is not consistent with the use of a single set of a-priori information.

6.2.1 THE A-PRIORI INFORMATION APPROACH.

Now we show that a single iteration of the model using the ridge regression technique relies upon the addition of a-priori information to the Jacobian and the right hand side error vector (Marquardt (1970)).

It has been shown that for ridge regression the forms :

$$\underline{X}_R = [A^T A + \mu I]^{-1} A^T \underline{y} \quad 100$$

And :

$$\underline{X}_R = V \underline{\Delta} U^T \underline{y} \quad 101$$

Where :

$$\underline{\Delta} = \text{DIAG} \left[\frac{\lambda_i}{\lambda_i^2 + \mu} \right] \quad 102$$

Are equivalent.

6.2.2 THE ITERATION OF THE RIDGE REGRESSION TECHNIQUE.

In this section we show that ridge regression may be represented as a statistical problem where the diagonal damping factor matrix added to the Jacobian represents a covariance matrix, (Tarantola and Valette 1982, Tarantola and Valette 1982). An expression for the iteration is derived and it is shown that changing the damping factor for the ridge regression with each iteration changes the covariance of the statistical problem. This is usually assumed to be constant a-priori information in statistical problems.

It may be shown that (100) is equivalent to the addition of fictitious data to the experimental data. This is seen by considering the partition :

$$\begin{bmatrix} A^T & H_K^T \end{bmatrix} \begin{bmatrix} A \\ H_K \end{bmatrix} \underline{X}_R = \begin{bmatrix} A^T & H_K^T \end{bmatrix} \begin{bmatrix} \underline{y} \\ 0 \end{bmatrix} \quad 103$$

Then if :

$$H_K^T H_K = \mu I \quad 104$$

We obtain the expression (100).

The additional information implies that the elements of x_R have all been measured by some response which is directly proportional to the parameters and that these responses fit the data.

It may be shown however that (100) is a special case of a more general formulation.

Let x be the set of data and parameters and let C_0 be the covariance of x as below :

$$\underline{x} = \begin{bmatrix} \underline{d} \\ \underline{p} \end{bmatrix} \quad 105$$

$$C_0 = \begin{bmatrix} C_{d_0 d_0} & C_{d_0 p_0} \\ C_{p_0 d_0} & C_{p_0 p_0} \end{bmatrix} \quad 106$$

Let $f(x)$ be a non-linear function where :

$$f(x) = d - g(p) = 0 \quad 107$$

If $f(x)$ is linear and if the data have a Gaussian distribution the parameters will also have a Gaussian distribution. We require to minimize the weighted residual sum of squares :

$$[\underline{x} - \underline{x}_0]^T C_0^{-1} [\underline{x} - \underline{x}_0] \quad 108$$

Where x_0 is the set of data and a-priori parameters. Using the method of Lagrange Multipliers we obtain the expression :

$$\underline{x}_{K+1} = \underline{x}_0 + C_0 F_K^T [F_K C_0 F_K^T]^{-1} [F_K [\underline{x}_K - \underline{x}_0] - f(\langle \underline{x}_K \rangle)] \quad 109$$

Where :

$$F_{ik} = \left. \frac{\partial f_i}{\partial x_k} \right|_{x_k} \quad 110$$

For (107) F_{ik} is given by the partitioned matrix :

$$F = [I \quad -G] \quad 111$$

Where :

$$G = \frac{\partial g_i}{\partial p_k} \quad 112$$

Using (105), (106), (107) and (111) we obtain from (109) the expression :

$$\underline{p}_{K+1} = \underline{p}_0 + [C_{p_0 p_0} G_K^T - C_{p_0 d_0}] [C_{d_0 d_0} - C_{d_0 p_0} G_K^T - G_K C_{p_0 d_0} + G_K C_{p_0 p_0} G_K^T]^{-1} [\underline{d}_0 - g(\underline{p}_K) + G_K [\langle \underline{p}_K \rangle - \underline{p}_0]] \quad 113$$

If further we assume that the data and the parameters are independent we obtain :

$$C_{d_0 p_0} = C_{p_0 d_0}^T = 0 \quad 114$$

Whence :

$$\underline{p}_{K+1} = \langle \underline{p}_K \rangle + [G_K^T C_{d_0 d_0}^{-1} G_K + C_{p_0 p_0}^{-1}]^{-1} [G_K^T C_{d_0 d_0}^{-1} [\underline{d}_0 - g(\langle \underline{p}_K \rangle)] + C_{p_0 p_0}^{-1} [\underline{p}_0 - \langle \underline{p}_K \rangle]] \quad 115$$

This is the solution for the non-linear problem.

We may compare (100) with (115) whence we obtain :

$$\langle X \rangle = \underline{p}_{k+1} - \underline{p}_k \quad 116$$

$$A = C_{dodc}^{-1/2} \underline{g}_k \quad 117$$

$$\underline{y} = d_0 - \underline{g}(\langle p_k \rangle) \quad 118$$

$$\mu I = C_{p_0 p_0} \quad 119$$

However (115) has one additional term $C_{p_0 p_0}^{-1}[p_0 - p_k]$. If we assume during an iteration step that $p_0 = p_k$ then (100) is equivalent to (113) and the a-priori parameters are those at which the iteration starts. In a series of iterations, the a-priori parameters are changed with each step and this makes the solution dependent upon the starting point of the iteration series in some complex way.

However in the iterations in Section (8.7) and Section (8.8), ridge regression was used iteratively to limit the magnitude of the elements in the step correction vector. The a-priori data added to the data set in this way (Section 6.2.1) adds no further information to the problem and therefore cannot be considered as necessarily constituting conditions under which a solution is to be obtained. Hence the a-priori data is arbitrary and we may set $C^{-1}(p_0 - p_k)$ equal to zero by setting $p_0 = p_k$ at each iteration.

There are however a number of disadvantages associated with the use of (115).

The expression (115) is stabilized using $C_{p_0 p_0}$, the covariance of the a-priori data which remains constant throughout the iteration sequence. However it was found in this study that the damping factor μ in (100) could be decreased as the iteration proceeded. This resulted in a step correction vector of maximum length, consistent with the linearity approximation. Hence the use of (115) may require a larger number of iterations than (100) to obtain a solution.

For this reason (100) was used in this study in preference to (115).

CHAPTER VII

FURTHER INVERSION STUDIES

7. FURTHER INVERSION STUDIES.

This chapter contains the derivation of a number of expressions which should be of considerable utility in future studies. They were not applied to the inversion of the present field data as they were developed at a later stage. .

7.1 THE PERTURBATION OF THE MODEL PARAMETERS.

Swift (1965) and Jupp and Vozoff (1975) presented a method for the computation of the Jacobian as required by the two-dimensional inversion. The extension of this technique by the author is now described. The modified method allows the calculation of the response of a perturbed two-dimensional model to greater than first order accuracy and hence allows the calculation of the mean value of a derivative of a non-linearly varying response over a finite parameter interval. When used to first order accuracy the computation time for a Jacobian using the algorithm is approximately 0.065 of that required for the computation using single runs of the Brewitt-Taylor and Weaver programme.

7.1.1. THE METHOD DESCRIBED BY SWIFT (1965), JUPP AND VOZOFF (1976).

Consider the electrical network analogue of the two-dimensional model for E or H polarizations. For the E-polarization the electric field is assumed constant at the top of an air layer above the surface of the conductivity structure while for the H-polarization the magnetic field is assumed constant at the surface of the conductivity structure. These electric and magnetic fields are as represented by voltage generators.

The boundary conditions applied to the sides of the network are those of a one-dimensional structure, that is no horizontal electric field. The lower boundary of the network is also assumed to have no horizontal electric field and to extend to infinite depth, without changes in the electrical properties of the medium. This is effected using a matched termination.

It is thus seen that the current sources and sinks in the network remain unchanged by the specific structure under consideration provided the perturbation of the model parameters is not too extensive.

Let A be the admittance matrix, x be the nodal voltage vector and y be the constant source current vector for the network. Then we have :

$$X = A^{-1}y \quad 1$$

Differentiating (1) with respect to the model parameters α represented by the network we obtain :

$$\frac{\partial A}{\partial \alpha} X + A \frac{\partial X}{\partial \alpha} = 0 \quad 2$$

Then :

$$\frac{\partial X}{\partial \alpha} = A^{-1} \left[\frac{\partial A}{\partial \alpha} X \right] \quad 3$$

Hence by replacing y by $(\partial A / \partial \alpha) x$ we may obtain the voltage change at the network nodes due to the perturbation α in the model.

7.1.2. THE ITERATIVE METHOD.

The method described above can be extended to an iterative method. The perturbation of x can be expressed as a series.

The advantage in using the iterative method is that a first order approximation to x can be unsatisfactory when the series for x converges slowly. This occurs with inaccurate initial solutions or with the larger perturbations to the model when the spectral radius of the terms is near unity. The iterative method below also allows for changes in y in the case of H-Polarization.

Let the initial equation be :

$$[A + \Delta] X = y \quad 4$$

Let the perturbed equation be :

$$[A + \Delta + \delta A] X' = y + \delta y \quad 5$$

Let the Zollenkopf inverse of $(A + \Delta)$ be estimated as A^{-1} . In order to obtain a solution to (5) we apply the residual iterative algorithm for x'_{i+1} as below :

$$X'_{i+1} = A^{-1} [y + \delta y - [\Delta + \delta A] X'_i] \quad 6$$

Repeated application of (6) yields a series for x_I :

$$X'_I = A^{-1} \left[[I - [\Delta + \delta A] A^{-1}] + [[\Delta + \delta A] A^{-1}]^2 + \dots + [-[\Delta + \delta A] A^{-1}]^{I-1} [y + \delta y] + [-I]^{I-1} [[\Delta + \delta A] A^{-1}]^{I-1} [\Delta + \delta A] X_0 \right] \quad 7$$

The solution to (4) is obtained from (7) with :

$$\underline{X}_N = A^{-1} [I - \Delta A^{-1} + [\Delta A^{-1}]^2 + \dots + [-\Delta A^{-1}]^N] \underline{y} \quad 8$$

The solution to (5) is obtained from (7) with $x_0 = A^{-1}y$ as below :

$$\underline{X}'_M = A^{-1} \{ [I - [\Delta + \delta A]A^{-1}] + [[\Delta + \delta A]A^{-1}]^2 + \dots + [-[\Delta + \delta A]A^{-1}]^{M-1} \} [\underline{y} + \delta \underline{y}] + [-[\Delta + \delta A]A^{-1}]^M \underline{y} \quad 9$$

The perturbation $\delta x_1 = (x' - x)$ is then obtained as below :

$$[\underline{X}' - \underline{X}]_N = \underline{X}'_M - \underline{X}_N \quad \text{FOR } M=N \quad 10$$

For the series (10) to converge as $n \rightarrow \infty$ and $m \rightarrow \infty$, the series (8) and (9) must be convergent. In practice convergence can only be ascertained for a finite expansion from the terms in the series and by the application of (11) to determine the error ϵ given by :

$$\epsilon = | \underline{y} + \delta \underline{y} - [A + \Delta + \delta A] \underline{X}' | \quad 11$$

An alternative method for obtaining an estimate for $(x' - x)$ is given below. An expression for x_N is obtained to order N from (8). In (7) we set $x_0 = x_N$ and expand to order I. Then the series produced using the latter method is given by δx_2 where :

$$\delta x_2 = \delta x_1 + A^{-1} \{ [I - [\Delta + \delta A]A^{-1}] + [[\Delta + \delta A]A^{-1}]^2 + \dots + [-[\Delta + \delta A]A^{-1}]^I [-I]^N [\Delta A^{-1}]^{N+1} \} \underline{y} \quad 12$$

The expressions (8) and (7) should be expanded in order that (10) and (12) are identical to accuracy.

In many cases owing to the relative magnitudes of the elements in A and $(\Delta + \delta A)$ the resistivities of the model are increased for E-Polarization and decreased for H-Polarization in order to produce the most rapid convergence. The method may also be used for changes in frequency where the frequency is decreased. However in this application the convergence is not rapid.

7.1.1.3. THE JACOBIAN ESTIMATE.

The expression (10) for δx_1 is equivalent to that of Vozoff (1975) when N-1 and M-1. The expression (12) for δx_2 is equivalent to that of Vozoff (1975) when N-0 and M-1. These forms are first order approximations for δx , and are suitable for forming a Jacobian matrix.

Consider a Taylor series for $f(X+h)$. Comparison of the series to first order with (10) or (12) shows that the first order coefficient of (10) or (12) is the derivative of f at $f(X)$, that is the derivative determined at one side of the interval h.

Suppose now that f is non-linear but that we know the range h over which we require the first derivative. We can obtain a mean derivative over that range by using the series solutions of (7) or (9), and hence take account of some of the non-linearity in f . In practice the range h can be obtained approximately from a previous value for h determined using a Jacobian as described in the Vozoff (1975) method.

Such an approach is particularly useful where the errors on the models obtained from the two-dimensional inversion are required (section 6.1.7), as these are frequently large.

The alternative iterative method of section (7.1.2) is compared in Figure (7.1) with the method of Vozoff for the example of a quarter space.

7.2 THE BREWITT-TAYLOR AND WEAVER APPROXIMATE SOLUTION FOR A HALF-SPACE.

The Brewitt-Taylor and Weaver equations are used to derive the dependence of the approximate apparent resistivity and phase upon the horizontal mesh spacing and skin depth.

7.2.1 THE FINITE DIFFERENCE MESH

The finite difference formulation of the two dimensional requires the construction of a rectangular mesh of continuous lines of nodes parallel to the cartesian x and y axes. The nodes of the mesh must be sufficiently closely spaced to represent the electromagnetic field accurately but be sufficiently far apart to keep to a minimum the number of nodes and network equations to be solved.

To obtain an estimate of the necessary spacing we may consider a one-dimensional half space and apply the two dimensional equations.

Let the vertical mesh spacing be linear so that $k=k_2=k_4$ (Figure 2.2). Let the conductivity of the half space be σ . Since there is no variation in σ with y there are no horizontal currents and a capacitor-resistor ladder network analogue for E-polarization and H-polarization (Figure 7.2) yields a characteristic impedance in terms of the skin-depth δ given by :

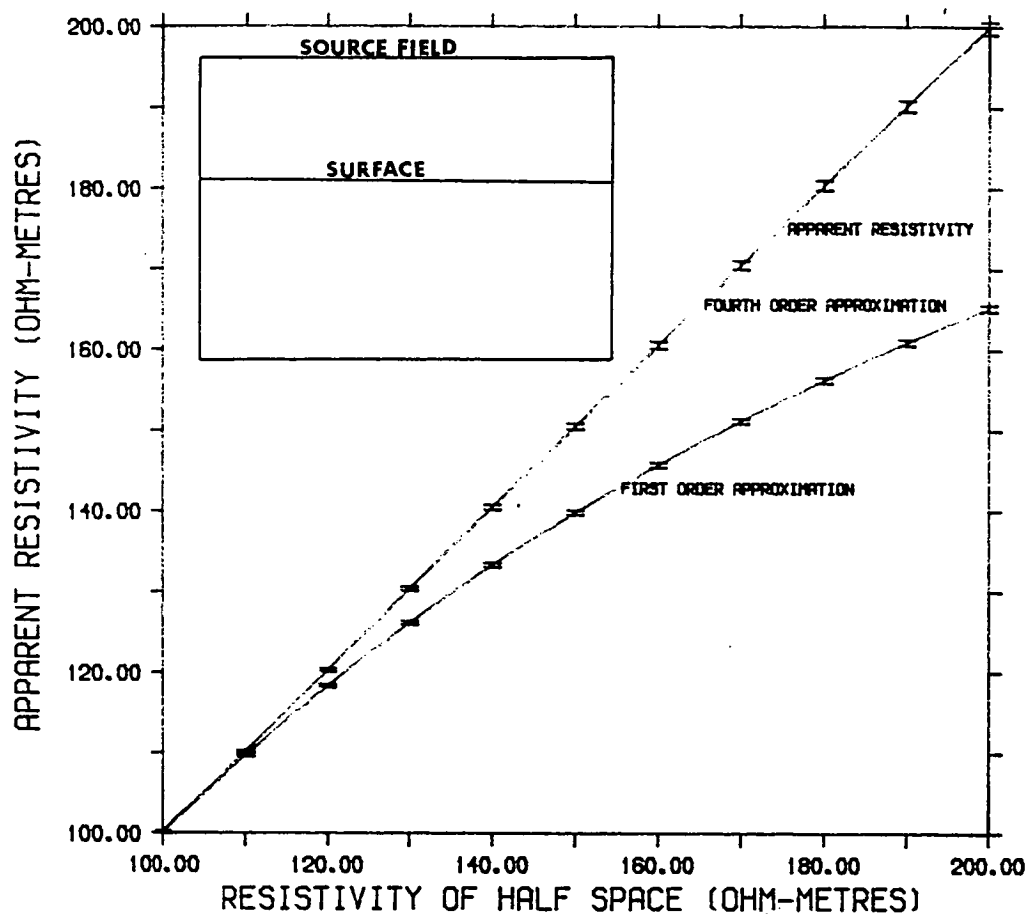
$$Z_0 = \frac{\kappa^2}{2} + \sqrt{\frac{\kappa^4}{4} - j \frac{\kappa^2 \delta^2}{2}} \quad 13$$

For E-polarization with a continuous variation of resistivity at the conductivity-structure air interface (Brewitt-Taylor and Weaver (1976)) as used for the modelling in this study we have from equation (6.35) :

$$S_A = \frac{\omega \mu}{\kappa^2} \left| \frac{Z_0 \delta^2}{Z_0 + \delta^2} \right|^2 \quad 14$$

$$S_A \approx S \left[1 - \frac{\kappa^4}{8\delta^4} \right] \quad \text{WHERE } \delta > h \quad 15$$

$$\phi \approx \pi/4 - \left[\frac{\kappa^2}{4\delta^2 + \kappa^2} \right] \quad \text{WHERE } \delta > h \quad 16$$



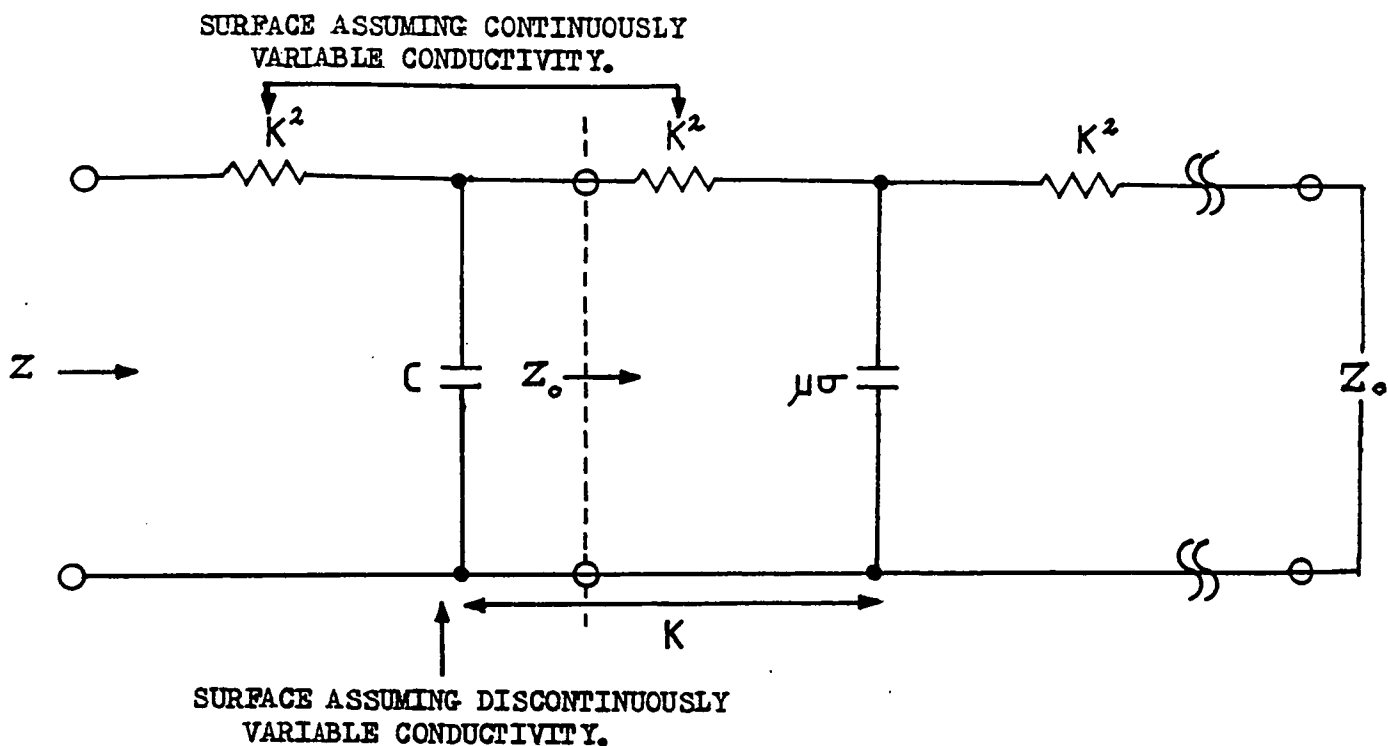
	DISCRETIZATION ERROR (%)		COMPUTATION ERROR (%)
	100 Ω M.	200 Ω M.	100 Ω M.
APPARENT RESISTIVITY	-0.05	-0.20	0.12
PHASE	-1.96	-3.86	-2.05

FIGURE 7.1. THE COMPUTED APPARENT RESISTIVITY OF A HALF-SPACE FOR E-POLARIZATION. THE APPARENT RESISTIVITY OF A 100 OHM-METRE HALF-SPACE WAS COMPUTED USING THE FINITE DIFFERENCE METHOD OF BREWITT-TAYLOR AND WEAVER (1975) ASSUMING A CONTINUOUSLY VARIABLE RESISTIVITY AT THE SURFACE OF THE HALF-SPACE. THE RESISTIVITY OF THE HALF-SPACE WAS THEN VARIED AND THE APPARENT RESISTIVITIES RECALCULATED USING:

- (1) THE FIRST ORDER APPROXIMATION. THIS USED THE METHOD OF SWIFT (1965) AND JUPP AND VCOFF (1975).
- (2) THE FOURTH ORDER APPROXIMATION. THIS USED THE ALTERNATIVE MODIFICATION OF (1) TO FOURTH ORDER.

THE APPARENT RESISTIVITY VALUES WERE AVERAGED OVER 11 POINTS AT THE CENTRE OF THE GRID SUCH THAT NO POINT WAS LESS THAN 3.75 SKIN DEPTHS FROM THE EDGE OF THE GRID. THE ERRORS SHOWN ARE THE STANDARD DEVIATIONS OF THE AVERAGES.

WHEN DERIVATIVES ARE CALCULATED, METHOD (1) GIVES THE DERIVATIVE AT THE START OF THE INTERVAL WHEREAS METHOD (2) GIVES A MEAN VALUE OF THE DERIVATIVE OVER THE THE INTERVAL.



E-POLARIZATION. (CONTINUOUSLY VARIABLE CONDUCTIVITY AT THE SURFACE). $C = \mu\sigma/2$

E-POLARIZATION. (DISCONTINUOUSLY VARIABLE CONDUCTIVITY AT THE SURFACE). $C = \mu\sigma$

H-POLARIZATION. (DISCONTINUOUSLY VARIABLE CONDUCTIVITY AT THE SURFACE). $C = \mu\sigma$

FIGURE 7.2. THE ELECTRIC CIRCUIT ANALOGUE USED TO CALCULATE THE ACCURACY OF THE BREWITT-TAYLOR AND WEAVER FINITE DIFFERENCE FORMULATION AS APPLIED TO A HALF-SPACE OF CONDUCTIVITY σ WITH CONSTANT MESH SPACINGS K .

For E-polarization with a discontinuous variation of resistivity at the conductivity-structure air interface (Brewitt-Taylor and Weaver (1976)) we have :

$$S_A = \frac{4\omega\mu}{k^2} \left| \frac{Z_0 \delta^2}{2\delta^2 + jZ_0} \right|^2 \quad 17$$

$$S_A \approx S \left[1 + \frac{1}{2} \delta \right] \quad \text{WHERE } \delta > h \quad 18$$

$$\phi \approx \pi/4 + \frac{1}{4} \delta \quad \text{WHERE } \delta > h \quad 19$$

For H-polarization as used for the modelling in this study we have:

$$S_A = \frac{S^2 k^2}{\omega\mu} \left| \frac{\delta^2 + jZ_0}{Z_0 \delta^2} \right|^2 \quad 20$$

$$S_A \approx S \left[1 + \frac{1}{8} \delta^4 \right] \quad \text{WHERE } \delta > h \quad 21$$

$$\phi \approx \pi/4 + \left[\frac{k^2}{4\delta^2 - k^2} \right] \quad \text{WHERE } \delta > h \quad 22$$

Similar results may be obtained using an inductor-resistor analogue.

Brewitt-Taylor and Johns (1980) give an accuracy assessment for the lumped network and transmission line approximations for Maxwell's equations using propagation analysis.

Consider now an electromagnetic disturbance entering a half-space. As the wave penetrates to increasing depth in the conductor the higher frequency components of the wave become attenuated more rapidly than the low frequency components. At depth, the most dominant wave frequencies have larger skin depths than at shallower levels. Thus it appears reasonable to increase the vertical mesh spacing with depth. In the case of a half space a logarithmically spaced mesh is suggested by the exponential decay in a homogeneous conductor of the amplitude at any one frequency.

The variation of the mesh spacing however causes each section of the ladder network to possess a slightly different characteristic impedance unless $\delta \gg k/\sqrt{2}$. Hence reflections are set up at each node associated with a change in mesh spacing. Where the spacing is continuously changing the reflections are sufficient to generate errors in the calculated ρ_A value.

7.2.2 THE APPLICATION OF THE RELATIONSHIPS.

The relationships derived above may be used to estimate the mesh spacing required for a given accuracy of apparent resistivity and phase in a uniform resistive block.

They may also be used to ascertain the computational rounding error incurred when calculating the response of a half-space.

CHAPTER VIII

THE APPLICATION OF THE TWO-DIMENSIONAL INVERSION TO THE MAGNETOTELLURIC DATA

8. THE TWO-DIMENSIONAL MODELLING.

The following sections describe the two-dimensional modelling which was conducted using only the data with bias ranges less than those shown in Table (1).

Sections 8.1 TO 8.5 describe the general considerations common to the three iterative series described in subsequent sections 8.6 TO 8.8. Section 8.9 describes the simplification of the model derived from the second series of iterations and the calculation of the error parameters.

8.1. THE NECESSITY FOR TWO-DIMENSIONAL MODELLING.

All the sites at which Magnetotelluric measurements were made in this study showed slight anisotropy indicating that the structure was two or three dimensional. Since however the skew estimates were usually less than 0.2 except at site G (Section 4.1.7 and Figure 4.2) this indicated the presence of only limited three-dimensional effects (section 1.6.1).

While the variation of apparent resistivity and phase responses between the non-anomalous sites is small as is the variation between the associated one-dimensional models, the necessity for two-dimensional modelling has already been shown in Figure (5.2) by the differences between the one-dimensional models.

8.2 THE ASSUMED GEOLOGICAL STRIKE.

It was assumed for the purpose of two-dimensional modelling that the conductivity structure had a strike of 15° east of north at all points along the profile. This direction is along the assumed geological strike of the Moine Thrust. Furthermore it generally lies perpendicular to the gravity and smoothed aeromagnetic gradients in the region of study.

The assumption of invariance in conductivity structure along this line permitted the projection of the site positions onto a line 75° west of north. None of the apparent resistivity and phase responses appeared to be affected by the intrusives in the region of study (Section 4.2 TO Section 4.2.5.3).

8.3 THE DESIGN OF THE FINITE DIFFERENCE MESH.

If a computationally efficient finite difference method, such as that developed by Brewitt-Taylor and Weaver, is used to derive the apparent resistivity and phase responses for a two-dimensional conductivity structure then the number of finite difference nodes must be kept to a minimum.

The largest acceptable mesh spacing may be estimated by considering a half space where the estimates of apparent resistivity and phase are obtained for $h < \delta/4$ where δ is the skin depth (Section 7.2). Also in the case of the half space if $h \ll \sqrt{\delta}$ then the changes in the mesh spacing do not cause large reflections of an incident electromagnetic disturbance (Section 7.2).

However for a half space it is not necessary to adhere to these spacings at large depths for every given frequency, since total reflections of the incident electromagnetic disturbance at depths of 2δ will produce reflected disturbances of only approximately 1% of the amplitude of the disturbance at the surface.

To minimize the number of horizontal meshes the mesh spacings were arranged in nearly linear blocks with only a limited number of discontinuities at which the reflections may occur. However the ratio of mesh sizes between the blocks is greater than between the individual meshes in the continuously varying mesh spacing scheme. As a result the reflections at the block boundaries are greater but fewer in number.

The horizontal mesh spacings were necessarily identical at the surface and at depth. The mesh spacings at the surface were made as large as required by the surface conductivity at the highest frequency used. This resulted in the mesh spacings at depth being smaller than necessary.

Unlike the finite element method the finite difference method necessitates the use of continuous mesh lines throughout the model structure. For this reason the finite element method may be more suitable than the finite difference method for magnetotelluric modelling.

8.4 THE PARAMETERIZATION OF THE TWO-DIMENSIONAL MODELS.

The use of a starting model with a large number of parameters may lead to a structure which requires subsequent simplification. Further the resolution of the small scale parameters of such a model is often inferior to that of the larger scale parameters. On the other hand, an insufficient number of parameters in the initial model may lead to an optimal biased model with a poor fit to the data. It also results in the need to add further parameters for an acceptable fit to the data, and, in subsequent iterations, a considerable change in the optimal biased model. On grounds of efficiency it appears that the model requires to be sufficiently over-parameterized and constrained by an explicit smoothing function, for example by the addition of a smoothing matrix as a-priori data (Twomey 1977, Section 6.2, Section 9.4.2). Alternatively additional parameters have to be added to the model before the insufficiently parameterized model becomes highly biased during the iteration sequence. The iteration used in this study utilized no explicit smoothness function constraints. The only constraints used were those which express a preference for small step lengths and hence minimal amendments to each successive model in the iteration scheme.

A least squares variance fit was required to logarithmic resistivity and linear phase data. The parameter units were chosen so that the linear relationship between the parameters and the data extended over a wide range of values. This was effected by using as parameters logarithmic resistivity and logarithmic depth with the surface as origin. The vertical boundary position parameters were linear length as there appeared to be no horizontal origin acceptable to all the horizontally displaced sites.

It should be remembered however that changes in the depth or horizontal position parameters may change the length of certain other block boundaries and such changes may lead to non-linear changes in the logarithmic resistivity and linear phase responses of the model hence giving rise to a reduced range of linearity for these parameters.

8.5 THE COMPUTATION OF THE JACOBIAN.

The Jacobian for the two-dimensional inversion scheme was obtained by computing partial derivatives. Each iteration adjusted its associated initial model. In order to compute the derivatives a parameter from the initial model was perturbed by unit change and the difference between the initial model response and the perturbed model response taken.

In the case of block resistivities the resistivities themselves were changed.

In the case of the block boundaries consider for example two blocks A and B each at least two mesh spacings wide and separated by a vertical boundary. Suppose we require to move the boundary such that the area of block A is increased. A third block (C) the width of which is only one mesh spacing is introduced so that it lies along the boundary and occupies for example part of the area formerly in block B. Initially blocks B and C have the same resistivity which differs from that of block A. In order that the boundary be moved, the resistivity of block C is changed to that of block A. In the case of non-uniformly spaced grids, the method may also change the width of the transitional resistivity region.

8.6 THE FIRST SERIES OF ITERATIONS.

A series of iterations was carried out to test the routine written by the author on a two-dimensional model with variable block resistivities and block boundaries. The number of parameters was restricted to ascertain whether the method could produce an acceptable model with a few parameters. This series of iterations is described below.

8.6.1 THE DATA.

The data for this series of iterations were taken from five sites A, B, D, F and G. The amplitude and phase data for both polarizations was used at seven frequencies covering the range 0.3Hz. TO 300 Hz. The variance on the log-resistivity data was nominally set at 1.0 log-ohm-metres relative to the variance on the linear phase of 10^0 . No account was taken of the possibility of bias at this stage.

8.6.2 THE INITIAL MODEL AND THE PARAMETERIZATION.

One-dimensional models were available for five sites and these indicated a three layer structure extending continuously from west to east with a resistive block at the centre.

Owing to the similarity between these one-dimensional models and the LISP (Section 1.5.1) and M.O.I.S.T. (Section 1.5.3) seismic models an initial two-dimensional model based upon the structure presented in (Figure 8.1) was used.

Initially a model with a restricted number of parameters was determined along with the Jacobian generated by the parameter perturbations. This however was extended so that each site had two

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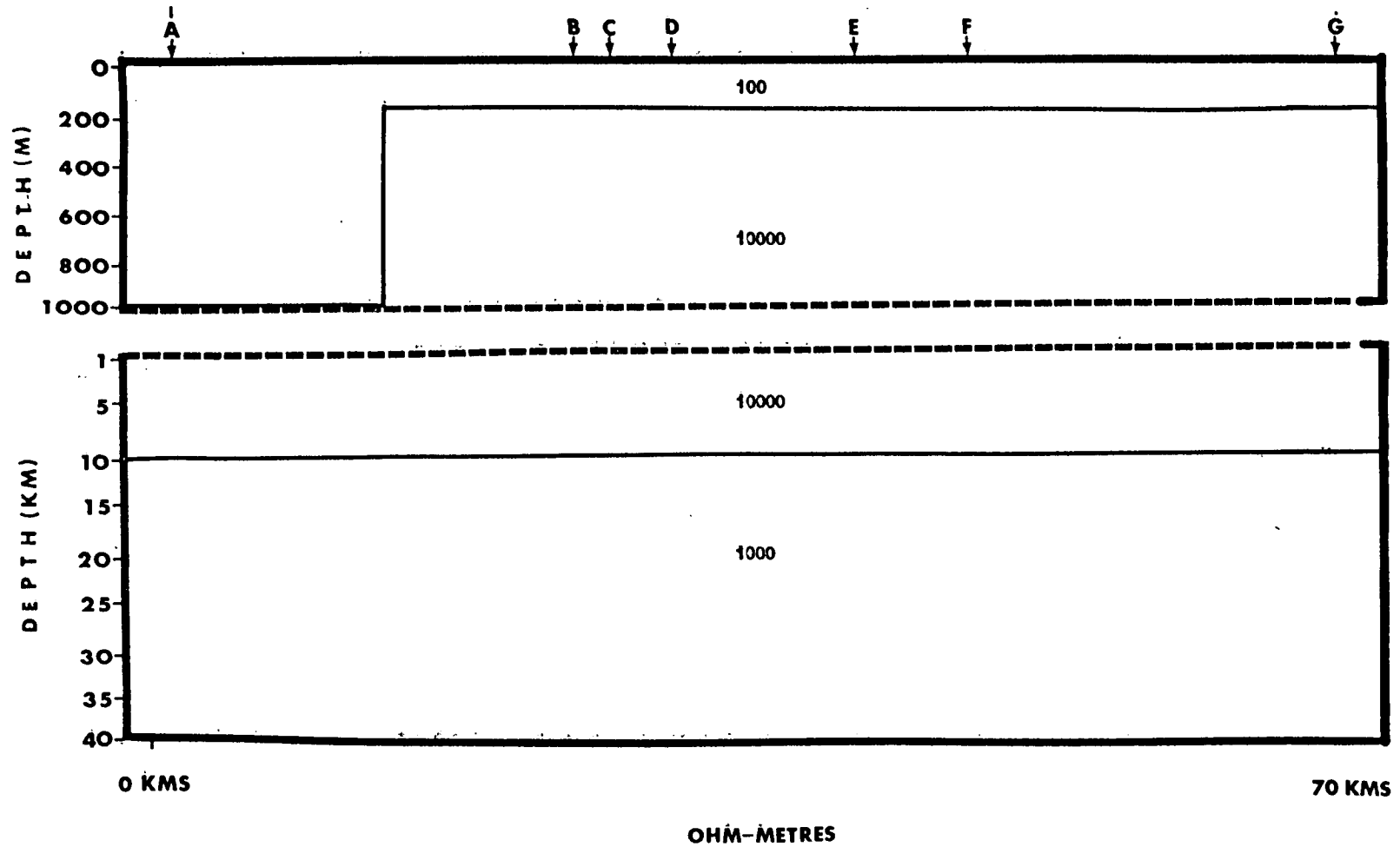


FIGURE 8.1. THE FIRST SERIES OF ITERATIONS. THE INITIAL MODEL.

variable depth parameters. These depth segments each extended laterally to mid-site positions. The block resistivities however were initially assumed to be continuous from west to east on account of the apparent association between the one-dimensional electrical conductivity models and the LISPB and M.O.I.S.T. seismic results.

The separation between the horizontal boundary segments was convenient since the sites were located in regions where there was little possibility of severe non-linearity arising from the generation of vertical boundaries, as the levels of the horizontal boundary segments changed. The range of linearity could thus be assumed to be large, enabling rapid initial convergence of the sum of squares residual with each iteration from an easy starting point.

8.6.3. THE ITERATION.

The step-lengths were limited using the truncation method. Two criteria were used to derive the assumed rank of matrix A. First no element of the step correction vector should assume a value outside the range to which the linearization of the model applied. The second criterion involved the inspection of a plot of the Euclidian length of the step correction vector against the projected residual sum of squares misfit (Figure 8.2). It was found that the rank could be increased so decreasing the residual sum of squares while the Euclidian Norm of the step vector steadily increased. At some critical rank the Euclidian Norm of the step vector would rise sharply with little decrease in the residual sum of squares misfit. The highest rank for A that did not exceed the critical rank but satisfied the linear limit criterion was used to calculate the step vector.

The effect on the predicted residual sum of squares of the addition to the initial model of a number of resistivity block parameters was found to be negligible. A three layer block resistivity initial model was then corrected (using the step correction vector) to produce a second model.

The second model was in turn split into smaller resistivity blocks but this was found to have little effect on the predicted residual sum of squares. Subdivision into two sections of many of the horizontal boundary sections was similarly found to have little effect on the predicted residual sum of squares. The three layer block resistivity second model was then corrected. Three possible correction vectors were selected. The three trial responses for the third model were calculated to test for convergence. The third accepted model was then taken to be

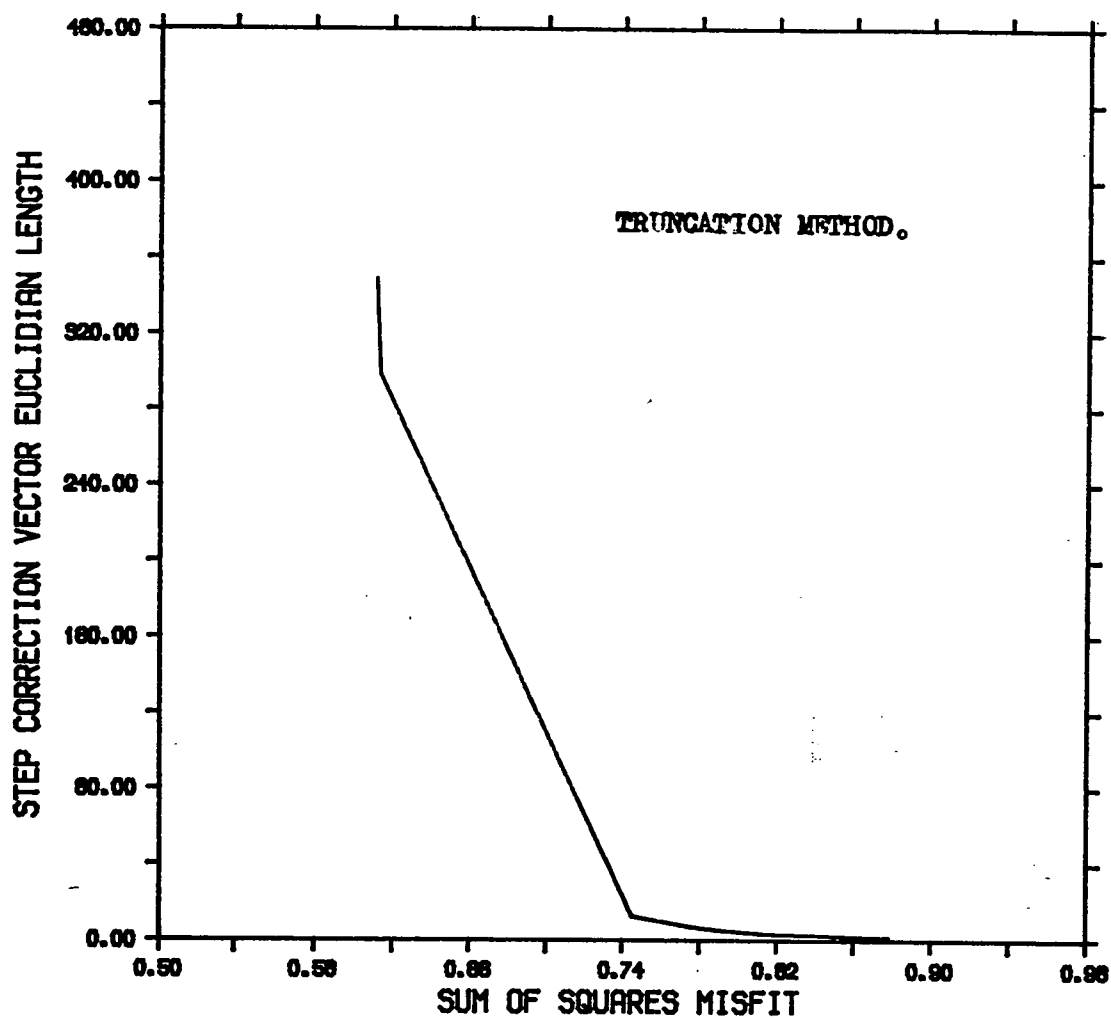


FIGURE 8.2.

that model with the minimum residual sum of squares misfit and is shown in Figure (8.3).

No further parameter additions were made to this model and a set of three step vectors was produced. Following a convergence test the fourth model was taken to be that model with the minimum residual sum of squares misfit and is shown in Figure (8.3).

The step-lengths which permitted convergence of each of models 1 TO 3 were successively shorter. In addition the reductions in the sum of squares residual misfit became smaller as the iterations proceeded. The sum of squares residual misfits for each model are shown in table (8.1).

8.7 THE SECOND SERIES OF ITERATIONS.

The first series of iterations produced models which did not adequately fit the data. The principal reasons were considered to be the finite difference mesh used and the parameterization of the model.

A second series of iterations was thus produced which varied from those of the first series as described below.

8.7.1 THE REGION TO BE MODELLED.

Owing to the computational effort required to produce the Jacobian the use of a finer finite difference mesh (Section 8.4.3) required the region to be modelled to have a smaller lateral extent.

It was thus restricted to the area about the Moine Thrust containing the high resistivity anomaly located at sites D and E. The north-western and south-eastern margins of the two-dimensional structure were taken to be those produced by the first series of iterations.

In this way the modelling area was restricted to the region of higher site density and anomalous structures.

8.7.2. THE DATA.

The data set used in the second series of iterations consisted of that used in the first series of iterations with the following modifications. The data were supplemented by that of site C which extended from 780 Hz. TO 8.0 Hz. Also sites KIN and SHN were added to the data set with frequencies extending from 0.1 Hz. to 1.2×10^{-3} Hz. Data from sites A and G were excluded on account of their remoteness from the central region of interest. In addition the E-polarization data at site E were excluded on account of their unreliability.

The errors on the data were assigned in accordance with table (3.2)

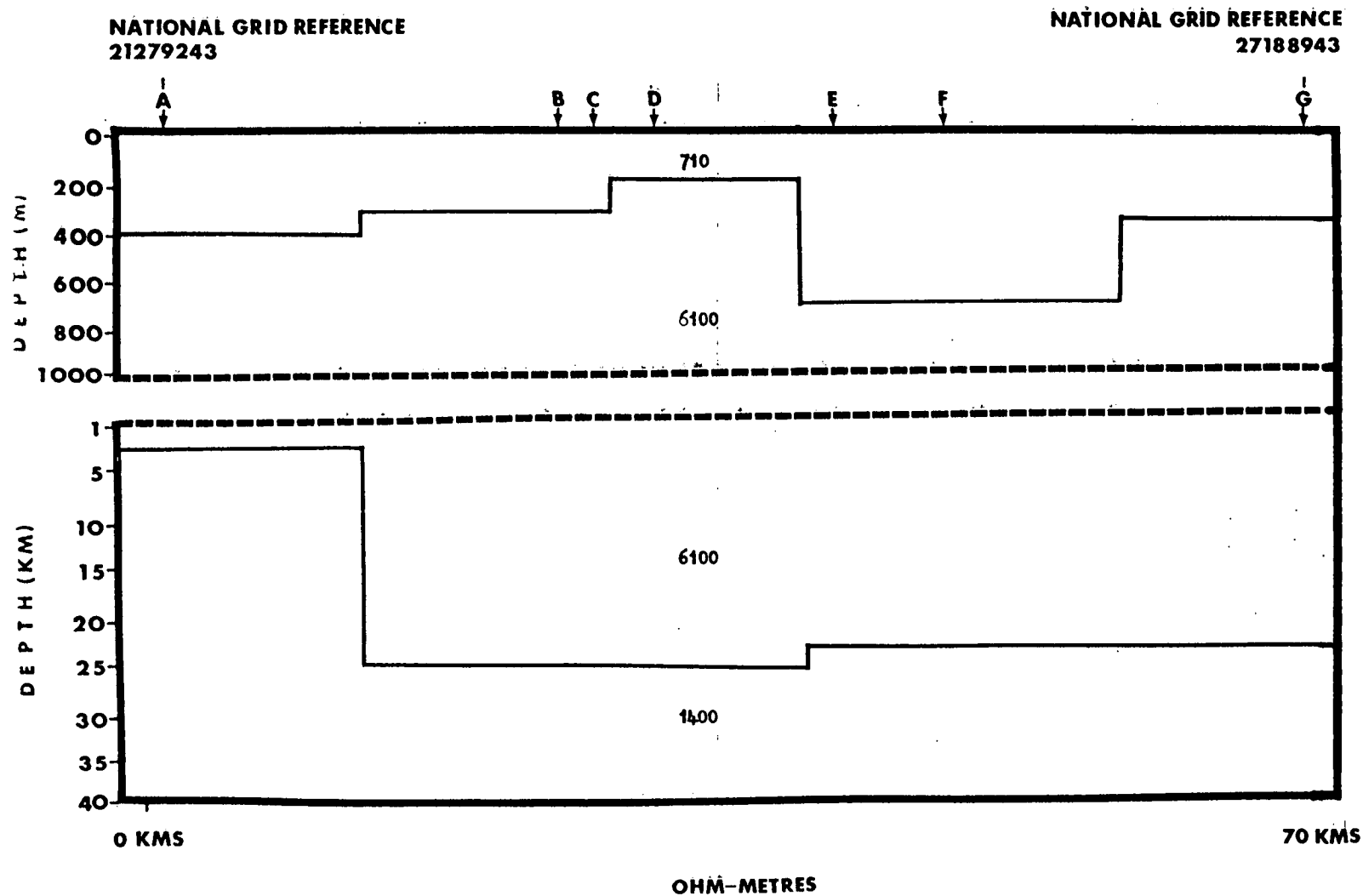


FIGURE 8.3. THE FIRST SERIES OF ITERATIONS. THE FINAL MODEL. THE RESOLUTION OF THE PARAMETERS IS NOT SHOWN.

ITERATION	JACOBIAN	MISFIT	ROOT MEAN SQUARE			ROOT MEAN SQUARE		
			SCALED	MISFIT		MISFIT		
			RHO	PHASE	RHO	RHO	PHASE	RHO
					PHASE			PHASE
					*			
1	1	ACTUAL	0.62	2.35	1.72	0.62	23.50	16.63
1	1	PREDICTED	0.49	0.99	0.80	0.49	9.91	7.02
2	2	ACTUAL	4.37	2.18	3.46	0.44	10.92	7.73
2	2	PREDICTED	3.42	1.95	2.79	0.34	9.77	6.92
3	3	ACTUAL	3.57	1.90	2.86	0.36	9.51	6.73
3	3	PREDICTED	3.34	1.87	2.70	0.33	9.37	6.63

ACTUAL MISFIT :
 THE ACTUAL SUM OF SQUARES MISFIT BETWEEN THE RESPONSES OF THE MODEL AND THE DATA.

LEAST SQUARES MISFIT :
 THE LEAST SQUARES MISFIT BETWEEN THE RESPONSES OF THE MODEL OBTAINED USING THE JACOBIAN AND THE DATA

PREDICTED MISFIT :
 THE PREDICTED MISFIT OBTAINED BETWEEN THE RESPONSES OF THE MODEL OBTAINED USING THE JACOBIAN AND DAMPING AND THE DATA.

NOTES:

 THE OPTIMIZATION USED ONLY THE SCALED RESISTIVITY AND PHASE PARAMETER (*).

 THE PARAMETERS FOR THE FIRST ITERARION WERE SCALED DIFFERENTLY TO THOSE FOR THE SECOND AND THIRD SERIES OF ITERATIONS.

TABLE 8.1. THE FIRST SERIES OF ITERATIONS. SUM OF SQUARES MISFIT.

8.7.3. THE MESH.

The corrections to the third model from the first series of iterations as predicted by the step vector involved many boundary changes which were of sub-mesh separation lengths. Further the coarse mesh size was considered to introduce errors in the calculated responses made by each iteration. For these reasons a new set of meshes was devised to continue the iterative process.

The mesh spacing was made finer. The block resistivities near the surface of the conductivity structure were used in a half-space model to ascertain the mesh spacing that would give an apparent resistivity error not exceeding approximately 20% at the highest frequency used for modelling. This mesh spacing was used near the surface of the conductivity structure. At the greater depths, wider mesh spacings were used to take account of the decreased amplitudes of the higher frequency signals and the higher resistivities found there. The mesh separations were approximately constant within a number of vertical groups to avoid the multiple reflections found with a continuously varying mesh spacing (section 8.3).

8.7.4 THE PARAMETERISATION.

The parameterization was restricted to variable block resistivities. The constraint of a model with three layers extending continuously from north-west to south-east was abandoned and more horizontal block divisions were introduced.

In this way it was considered that regions of anomalous resistivity could be approximately located before the introduction of block boundary parameters.

8.7.5. THE ITERATION.

The initial model was based on the block resistivities and boundaries produced by the first series of iterations (Figure 8.4). However in the second series of iterations only the block resistivities were made variable.

The block resistivity perturbation was fixed at 0.02 log-ohm-meters. The step length of the correction vector was increased until the largest element of the correction vector was 0.2 log-ohm-metres.

Each Jacobian was used for two iterations. After the first iteration, the convergence was tested using forward modelling and an up-dated error vector produced. The second iteration was based upon the up-dated error vector. This allowed over-correction of the model to be

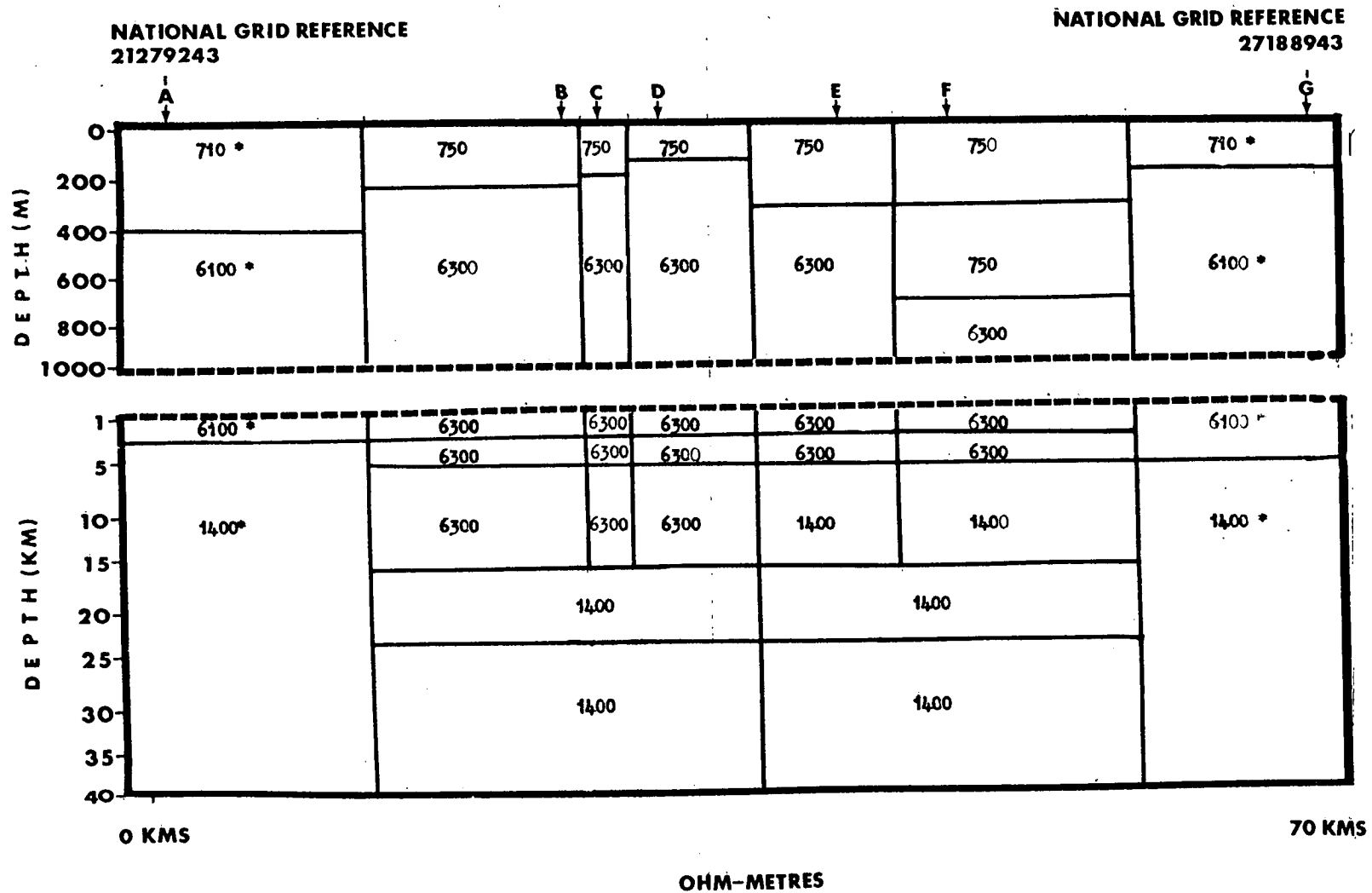


FIGURE 8.4. THE SECOND SERIES OF ITERATIONS. THE INITIAL MODEL.

itself corrected under certain conditions .

Eight iterations were carried out with four Jacobians. The sum of squares residual misfits are shown in table (8.2).

8.7.6. THE ITERATION RESULTS.

The iterations produced a resistive anomaly to the east of the Moine Thrust (Figure 8.5) as found in the one-dimensional models (Figure 5.2). However the resistive structure was less than twice as resistive as that of the one-dimensional models ($1.5 \times 10^5 \Omega \text{M.}$) and extended to depths less than 16.0 Kms.

The fit of the model response to the data is shown in Figure (8.6).

8.8 THE THIRD SERIES OF ITERATIONS.

The modifications to the mesh and parameterization for the second series of iterations were insufficient to effect any considerable improvement in the fit of the model response to the data within eight iterations, except at site D and site E for H-polarization data where a considerable improvement is seen.

It is possible that further improvement in the fit of the model response to the data could be effected by further iterations with or without the introduction of block boundaries as variables. However the first option would admit variables and could not be efficiently implemented without the use of the methods in sections (7.1.1), (7.1.2) and (7.1.3).

It was considered more important to show that only a few iterations with approximately 20 variables would be sufficient to improve the fit of a two-dimensional model response to the data, where the two-dimensional model had been constructed from one-dimensional models. This was on account of the two-dimensional inversions which required large numbers of parameters and iterations also requiring large quantities of computation time. This is considered below.

8.8.1. THE PARAMETERIZATION.

The model space was reparameterized using the mean values of the resistivities and depths obtained from the one-dimensional models for the directions parallel and perpendicular to strike (Figure 8.7). The block resistivities were made variable parameters and the block boundaries were fixed.

ITERATION	JACOBIAN	MISFIT	ROOT MEAN SQUARE SCALED MISFIT			ROOT MEAN SQUARE MISFIT		
			RHO	PHASE	RHO PHASE *	RHO	PHASE	RHO PHASE
1	1	ACTUAL	3.71	1.65	2.89	0.47	11.05	7.75
1	1	LEAST SQUARES	1.41	0.86	1.17	0.32	8.45	5.93
1	1	PREDICTED	3.09	1.68	2.50	0.41	11.22	7.86
2	1	ACTUAL	3.11	1.70	2.52	0.41	11.19	7.85
2	1	LEAST SQUARES	1.35	0.81	1.11	0.31	8.06	5.65
2	1	PREDICTED	2.42	1.66	2.08	0.37	11.18	7.84
3	2	ACTUAL	2.52	1.72	2.16	0.38	11.33	7.94
3	2	LEAST SQUARES	1.28	0.78	1.06	0.30	7.82	5.48
3	2	PREDICTED	2.15	1.56	1.88	0.36	10.52	7.38
4	2	ACTUAL	2.17	1.58	1.90	0.36	10.70	7.50
4	2	LEAST SQUARES	1.28	0.78	1.06	0.30	7.72	5.41
4	2	PREDICTED	1.90	1.39	1.67	0.35	9.69	6.79
5	3	ACTUAL	1.93	1.42	1.70	0.35	10.08	7.07
5	3	LEAST SQUARES	1.29	0.75	1.06	0.33	7.83	5.49
5	3	PREDICTED	1.74	1.27	1.53	0.34	9.76	6.84
6	3	ACTUAL	1.74	1.27	1.53	0.34	9.63	6.75
6	3	LEAST SQUARES	1.29	0.75	1.06	0.33	7.81	5.47
6	3	PREDICTED	1.61	1.13	1.39	0.34	9.25	6.49
7	4	ACTUAL	1.62	1.15	1.41	0.34	9.38	6.58
7	4	LEAST SQUARES	1.36	0.72	1.10	0.34	7.00	4.91
7	4	PREDICTED	1.54	1.03	1.31	0.34	8.36	5.86
8	4	ACTUAL	1.54	1.04	1.32	0.34	8.99	6.31
8	4	LEAST SQUARES	1.36	0.72	1.09	0.34	7.01	4.92
8	4	PREDICTED	1.50	0.93	1.25	0.35	7.93	5.57

ACTUAL MISFIT :

THE ACTUAL SUM OF SQUARES MISFIT BETWEEN THE RESPONSES OF THE MODEL AND THE DATA.

LEAST SQUARES MISFIT :

THE LEAST SQUARES MISFIT BETWEEN THE RESPONSES OF THE MODEL OBTAINED USING THE JACOBIAN AND THE DATA

PREDICTED MISFIT :

THE PREDICTED MISFIT OBTAINED BETWEEN THE RESPONSES OF THE MODEL OBTAINED USING THE JACOBIAN AND DAMPING AND THE DATA.

NOTES:

THE OPTIMIZATION USED ONLY THE SCALED RESISTIVITY AND PHASE PARAMETER (*).

THE FIRST THREE ITERATIONS APPEAR TO ADJUST THE MISFIT WITH RESPECT TO THE DISTRIBUTION OF ERRORS ON THE DATA.

TABLE 8.2. THE SECOND SERIES OF ITERATIONS. SUM OF SQUARES MISFIT.

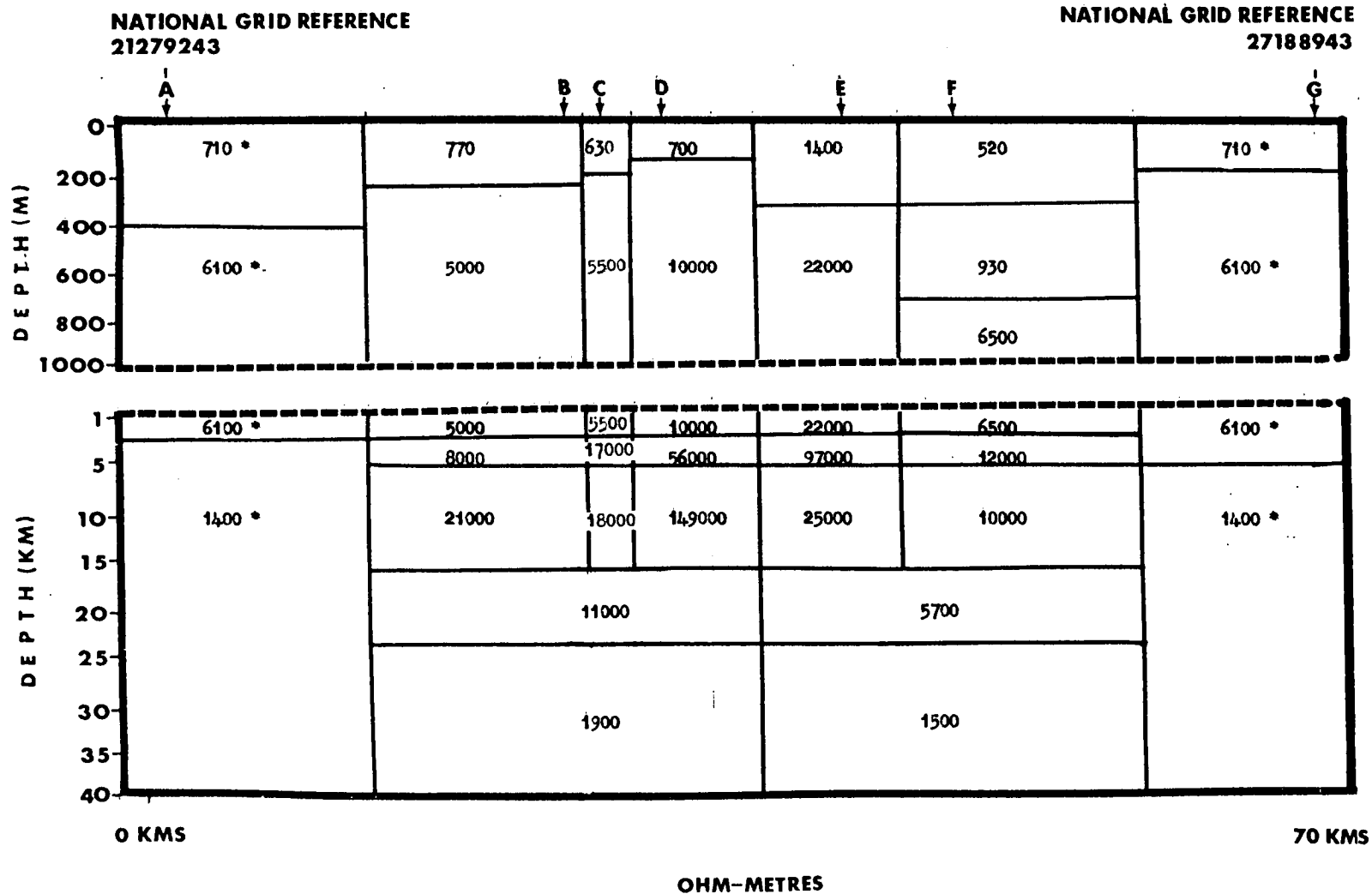


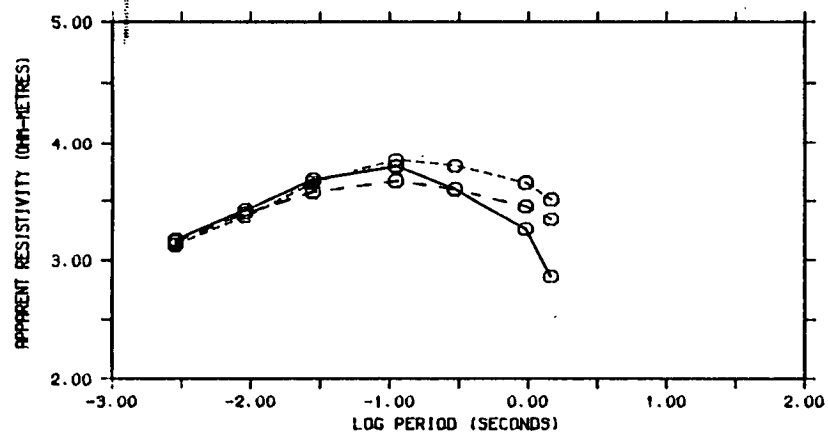
FIGURE 8.5. THE SECOND SERIES OF ITERATIONS. THE FINAL MODEL. THE RESOLUTION OF THE PARAMETERS IS NOT SHOWN.

FIGURE 8.6.

THE SECOND SERIES OF ITERATIONS. THE RESPONSE FUNCTIONS.

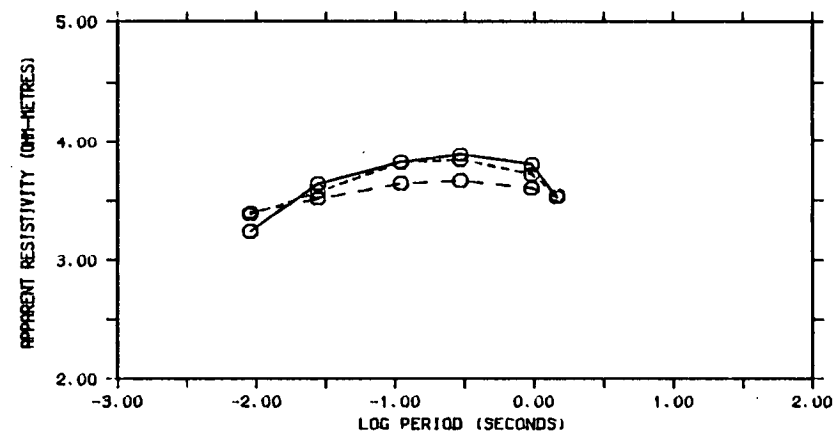
MODEL APPARENT RESISTIVITY RESPONSE

SITE : B E-POLARIZATION



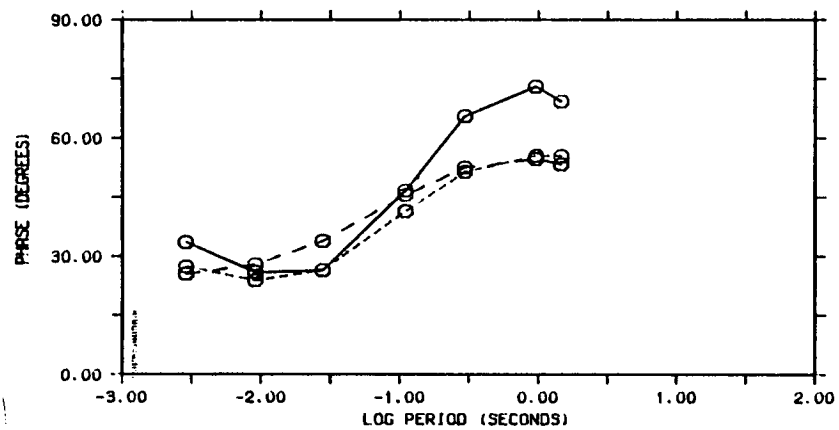
MODEL APPARENT RESISTIVITY RESPONSE

SITE : B H-POLARIZATION



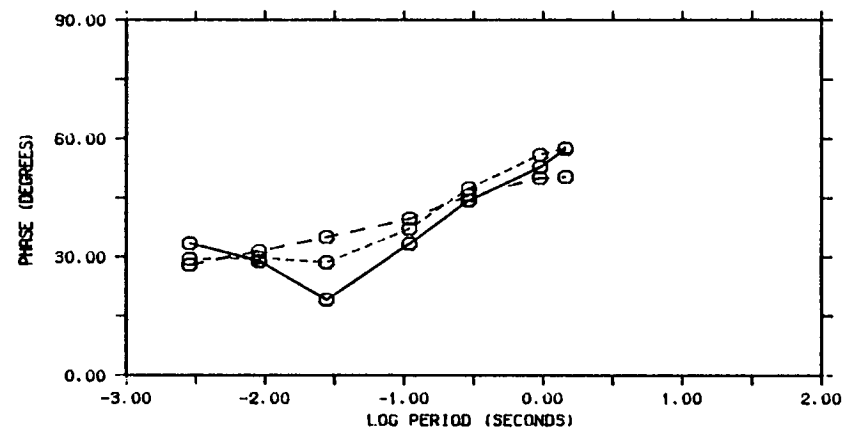
MODEL PHASE RESPONSE

SITE : B E-POLARIZATION



MODEL PHASE RESPONSE

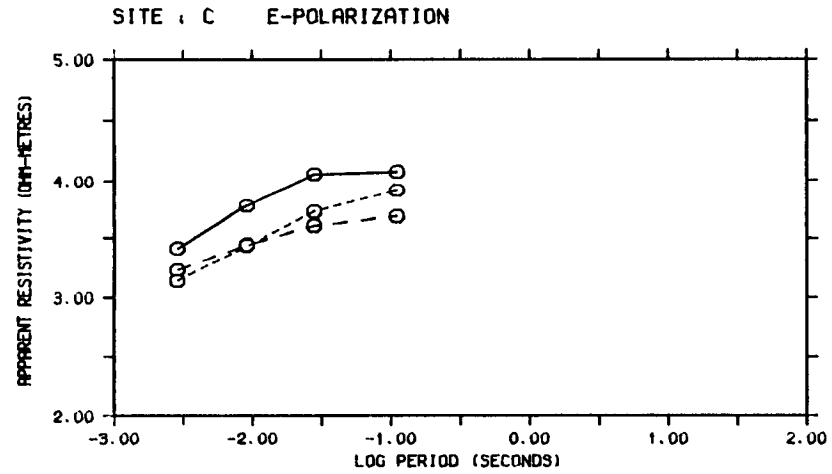
SITE : B H-POLARIZATION



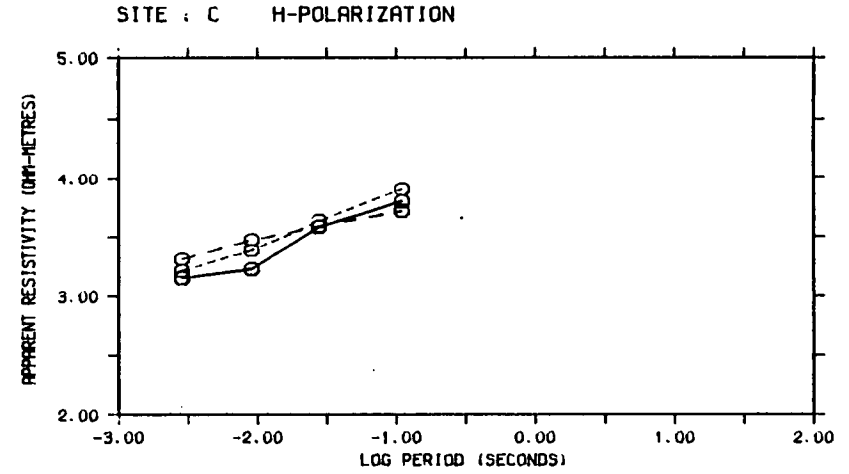
DATA. ——— INITIAL MODEL. - - - - FINAL MODEL. ·····

FIGURE 8.6. (1).

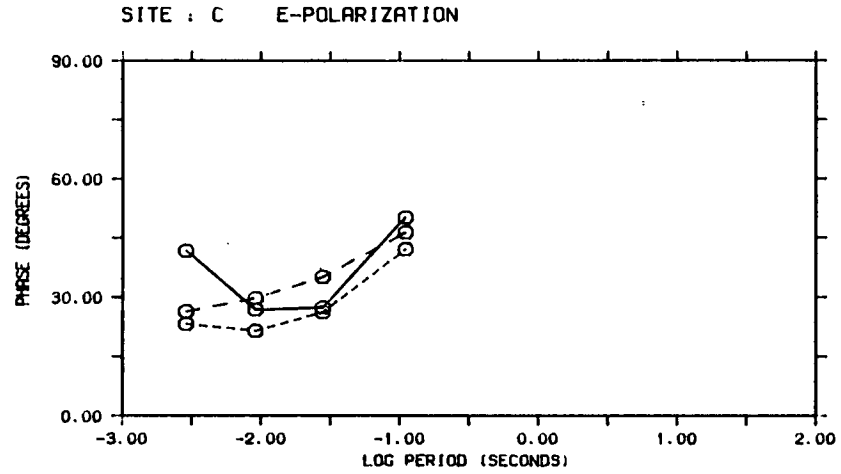
MODEL APPARENT RESISTIVITY RESPONSE



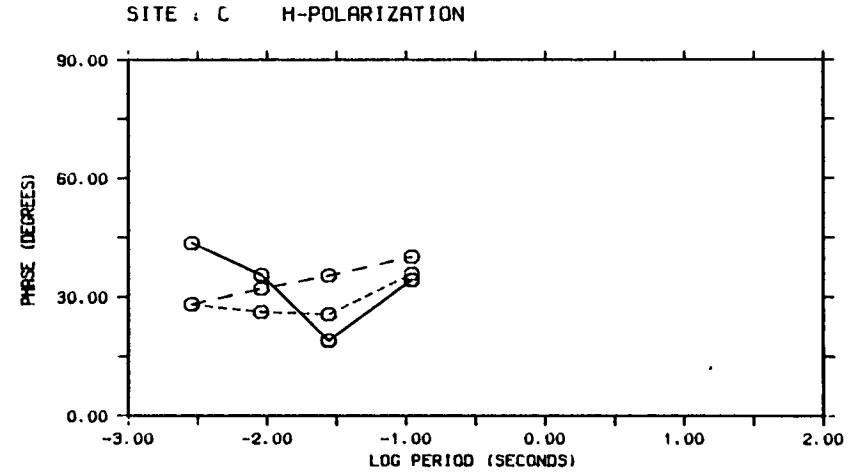
MODEL APPARENT RESISTIVITY RESPONSE



MODEL PHASE RESPONSE



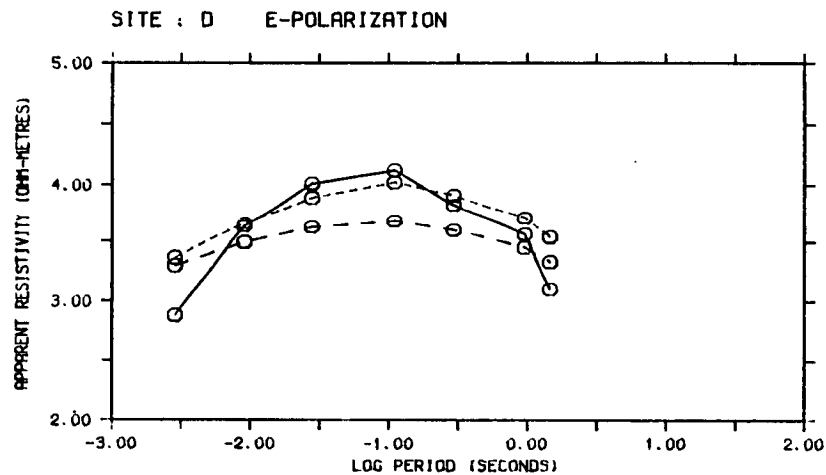
MODEL PHASE RESPONSE



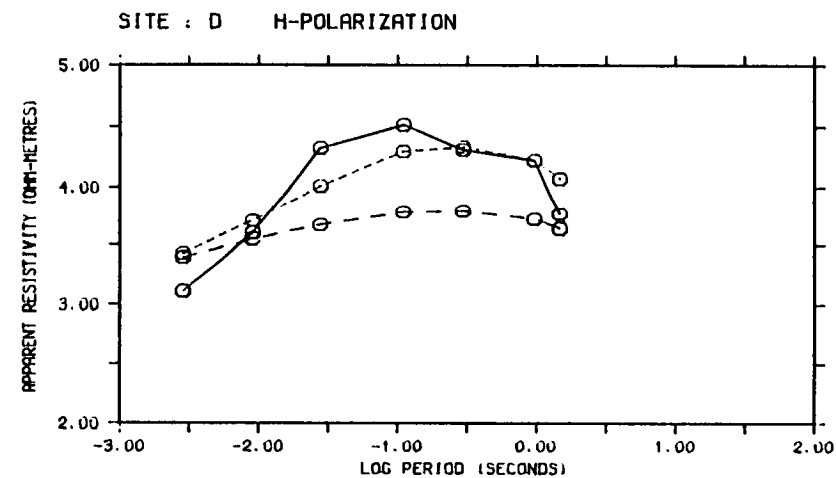
DATA. ——— INITIAL MODEL. - - - - FINAL MODEL. - - - - -

FIGURE 8.6. (2).

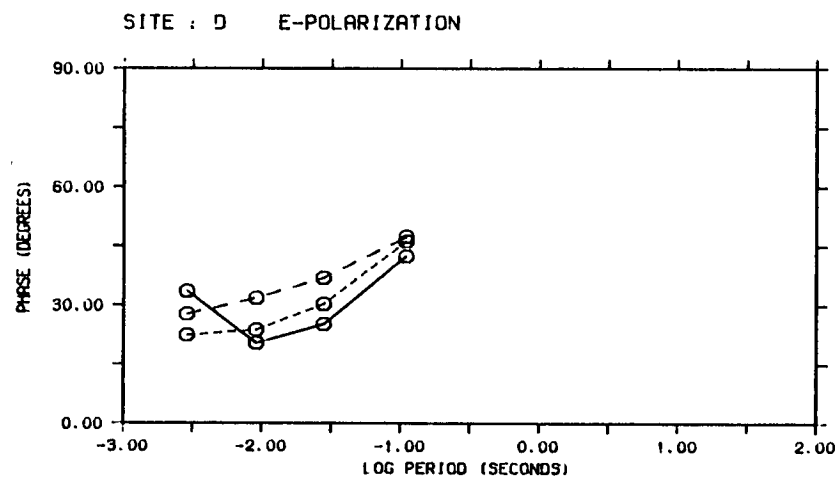
MODEL APPARENT RESISTIVITY RESPONSE



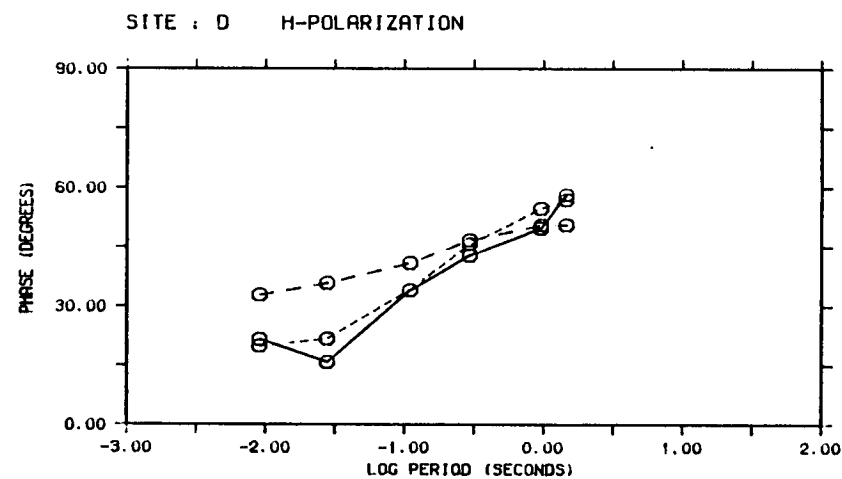
MODEL APPARENT RESISTIVITY RESPONSE



MODEL PHASE RESPONSE



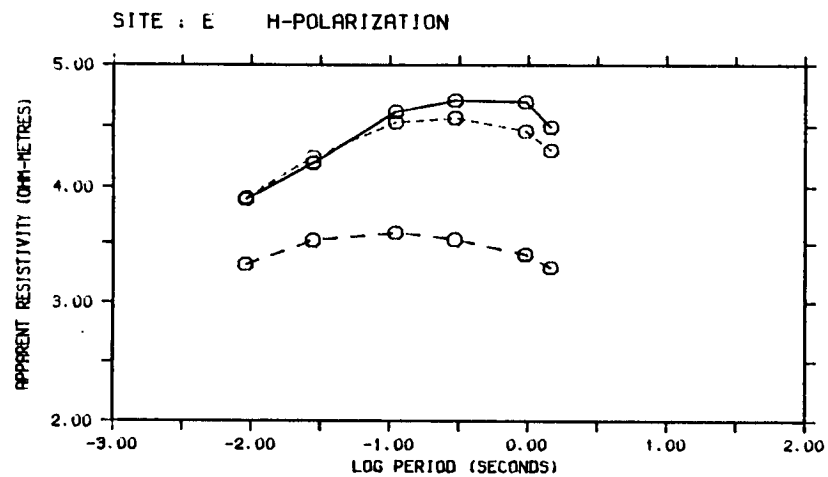
MODEL PHASE RESPONSE



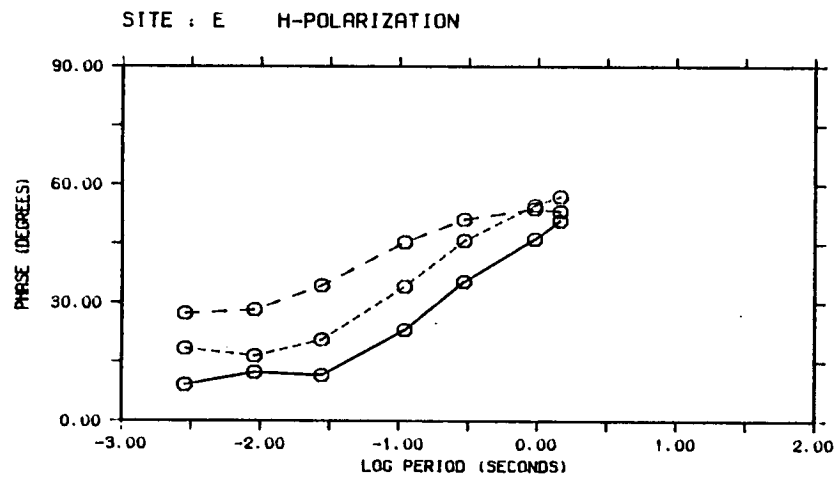
DATA. ——— INITIAL MODEL. --- FINAL MODEL.

FIGURE 8.6. (3).

MODEL APPARENT RESISTIVITY RESPONSE



MODEL PHASE RESPONSE



DATA. ——— INITIAL MODEL. - - - - - FINAL MODEL. - - - - -

FIGURE 8.6. (4).

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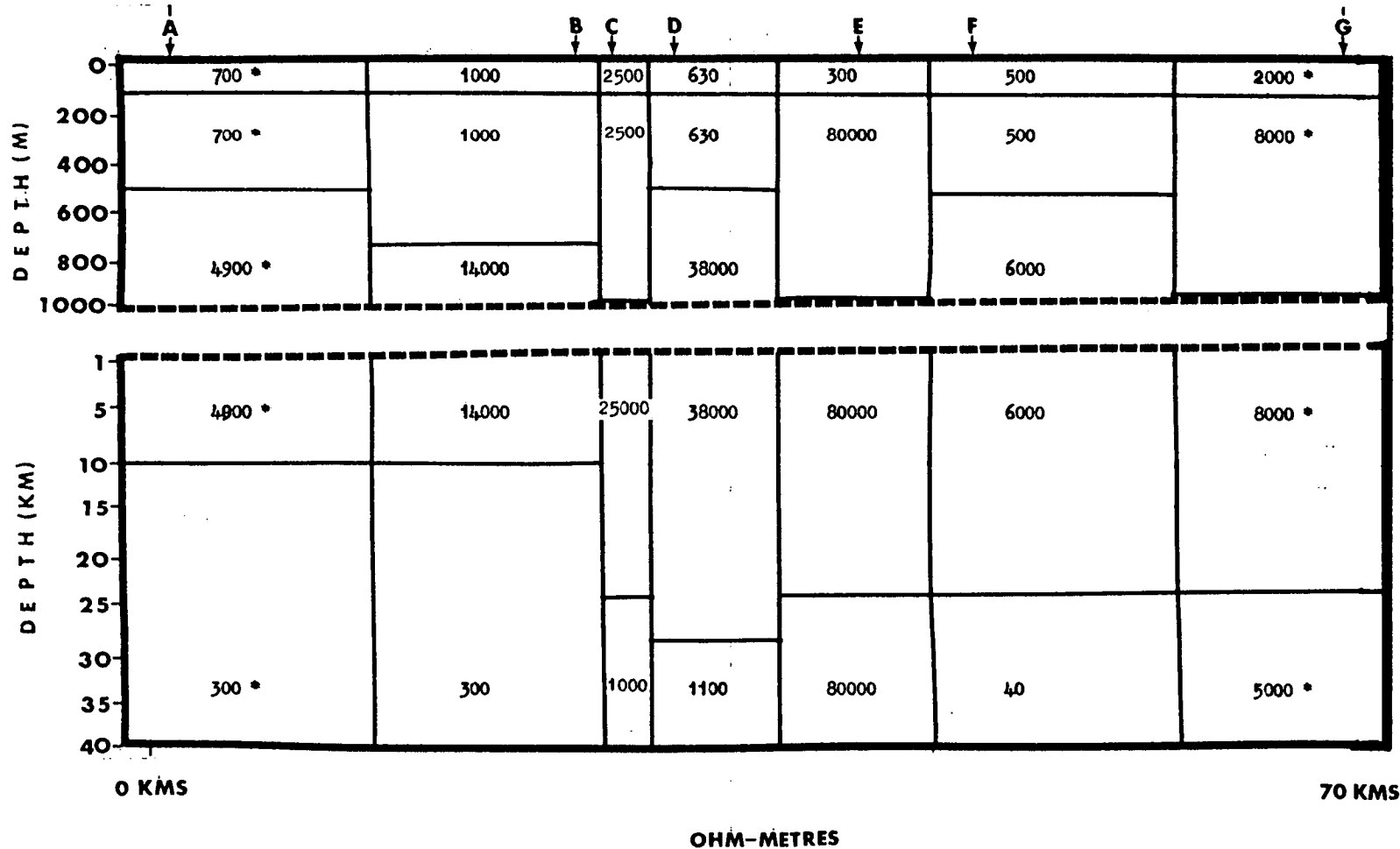


FIGURE 8.7. THE THIRD SERIES OF ITERATIONS. THE INITIAL MODEL.

8.8.2. THE MESH.

The mesh was similar to that used for the second series of iterations with some adjustments for the relocated block boundaries.

8.8.3. THE ITERATION.

Using the initial model of Section (8.8.1) one iteration was conducted which produced residual sum of square misfits as shown in table (8.3).

8.8.4. THE ITERATION RESULTS.

The one-dimensional model responses fit the entire data set well at all sites. However when the one-dimensional structure is modelled in two dimensions with a reduced data set the two-dimensional model responses do not fit this data set. especially at site D and at site E for H-polarization as may be seen by comparison of Figure 5.1 with Figure 8.6.

One iteration was sufficient to show that an improvement in the fit of the two-dimensional model responses to the data could be obtained. Hence on the assumption that the data had been produced by a two-dimensional structure the two-dimensional modelling technique produced in this case a better model than could be obtained by the assembly of adjacent one-dimensional models. The iteration produced a model similar to that of the second series of iterations with a higher resistivity ($2.5 \times 10^5 \Omega \text{M.}$) in the region of site E between 1 Km. and 20 Kms. depth (Figure 8.8).

8.9. THE ERRORS ON THE MODEL PARAMETERS.

The errors on the block resistivities of the second series of iterations were obtained using the methods of section (6.1.7) in conjunction with a parameter rationalization technique described below (Figure 8.9).

Since the errors were linear approximations calculated with a zero damping factor (Section 6.1.7.5) the error is symmetric about the least squares solution (Section 6.1.7.3).

The damping factor and step correction vector elements for the final iteration of the second series of iterations were smaller than those of the other iterative series. The results of the second series of iterations are thus closer to those of the least squares technique than are those of the other iterative series. Hence the calculated errors are more representative of the results from the second series of

ITERATION	JACOBIAN	MISFIT	ROOT MEAN SQUARE			ROOT MEAN SQUARE		
			SCALED		MISFIT	MISFIT		
			RHO	PHASE	RHO	RHO	PHASE	RHO
					PHASE			PHASE
					*			
1	1	ACTUAL	2.54	0.69	1.87	0.39	6.30	4.44
1	1	LEAST SQUARES	1.36	0.77	1.11	0.30	6.37	4.49
1	1	PREDICTED	1.41	0.76	1.14	0.32	6.35	4.48
2	1	ACTUAL	1.51	0.71	1.18	0.31	5.92	4.17

ACTUAL MISFIT :
 THE ACTUAL SUM OF SQUARES MISFIT BETWEEN THE RESPONSES OF THE MODEL AND THE DATA.

LEAST SQUARES MISFIT :
 THE LEAST SQUARES MISFIT BETWEEN THE RESPONSES OF THE MODEL OBTAINED USING THE JACOBIAN AND THE DATA

PREDICTED MISFIT :
 THE PREDICTED MISFIT OBTAINED BETWEEN THE RESPONSES OF THE MODEL OBTAINED USING THE JACOBIAN AND DAMPING AND THE DATA.

NOTES:

THE OPTIMIZATION USED ONLY THE SCALED RESISTIVITY AND PHASE PARAMETER (*).

TABLE 8.3. THE THIRD SERIES OF ITERATIONS. SUM OF SQUARES MISFIT.

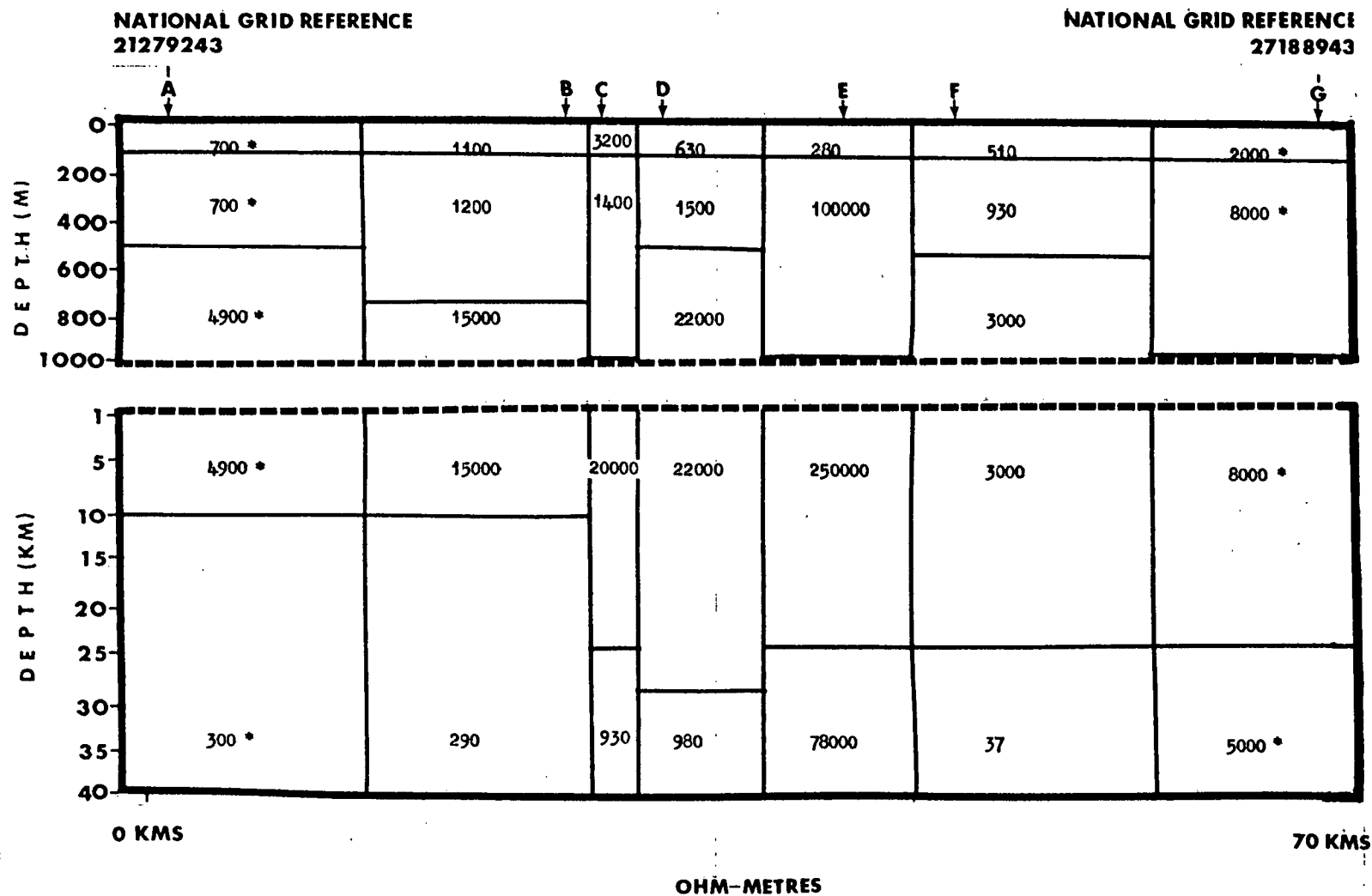


figure 8.8. THE THIRD SERIES OF ITERATIONS. THE FINAL MODEL. THE RESOLUTION OF THE PARAMETERS IS NOT SHOWN.

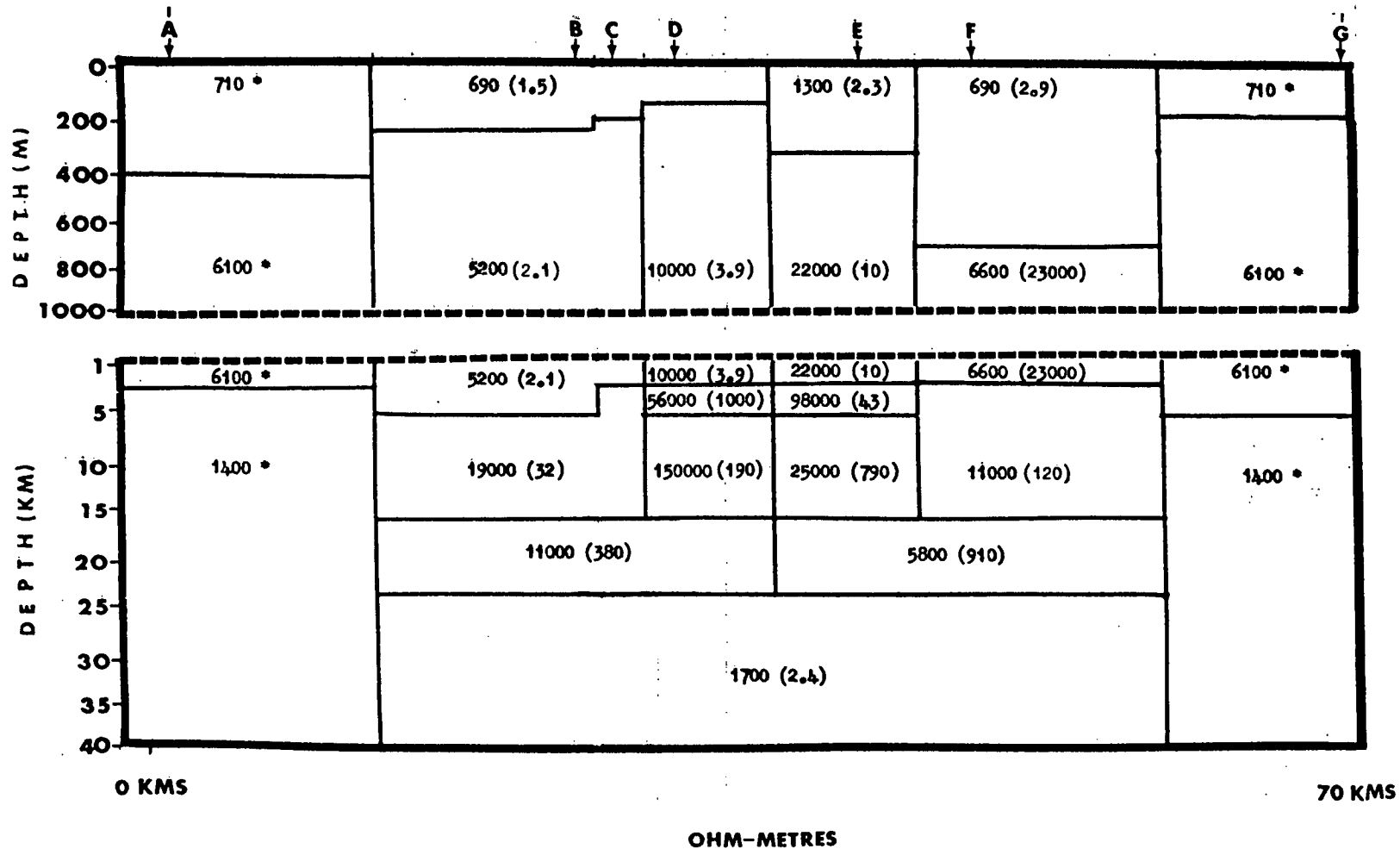


FIGURE 8.9. THE SECOND SERIES OF ITERATIONS. A SIMPLIFIED FINAL MODEL. LINEAR APPROXIMATIONS TO THE ERROR FACTORS ARE SHOWN IN BRACKETS. WHERE THE ERROR FACTORS EXCEED 10 NON-LINEAR EFFECTS ARE LIKELY TO MAKE THE ERROR FACTOR APPROXIMATIONS INACCURATE. ERRORS ARE ONLY CALCULATED FOR THE VARIABLE BLOCK RESISTIVITY PARAMETERS IN THE SECOND SERIES OF ITERATIONS. MINOR DETAILS IN THE BOUNDARIES SHOWN ARE THE RESULT OF THE PARAMETERIZATION AND ARE NOT LIKELY TO BE WELL RESOLVED.

iterations and the error range lies approximately symmetrically about the mean results. Furthermore owing to non-linearities in the two-dimensional model response with respect to the model parameters the Jacobian used in the estimation of the errors should be more accurate (Section 6.1.7.6).

The errors on the model parameters were estimated using two methods. The error on the individual parameters was estimated by setting the maximum residual sum of squares error Q_0 such that :

The Jacobian was that used for the final iteration step and hence the errors may be incorrectly estimated. No iterations were conducted for the error estimations.

Unresolved adjacent parameters of similar values were averaged together by summing the appropriate columns of the Jacobian. The new parameters were estimated and the errors on the parameters calculated for the individual parameters. This differs from maximizing the sum of the parameters $x^T b$ since the amalgamated parameters may only take one value. The Jacobian was that used for the final iteration step and hence the errors may be underestimated. No iterations were conducted for the error estimations.

8.10 THE GENERAL REGIONAL CONCLUSIONS FROM THE TWO-DIMENSIONAL MODELS.

Although all of the iterations are not completely converged, the first and second iteration results appear to indicate that the depth of the base of the resistor at the centre of the profile is not less than that implied in the one-dimensional sections (Figure 5.2).

A comparison of the final simplified model of the second series of iterations with the generalised crustal resistivity models of Hjelt (1987) (Figure 8.10) suggests that a cond crustal model may be used to represent the study region. Although the maximum resistivities from the two-dimensional model appear to exceed those of the cold crust model, the former are associated with large errors (Figure 8.9).

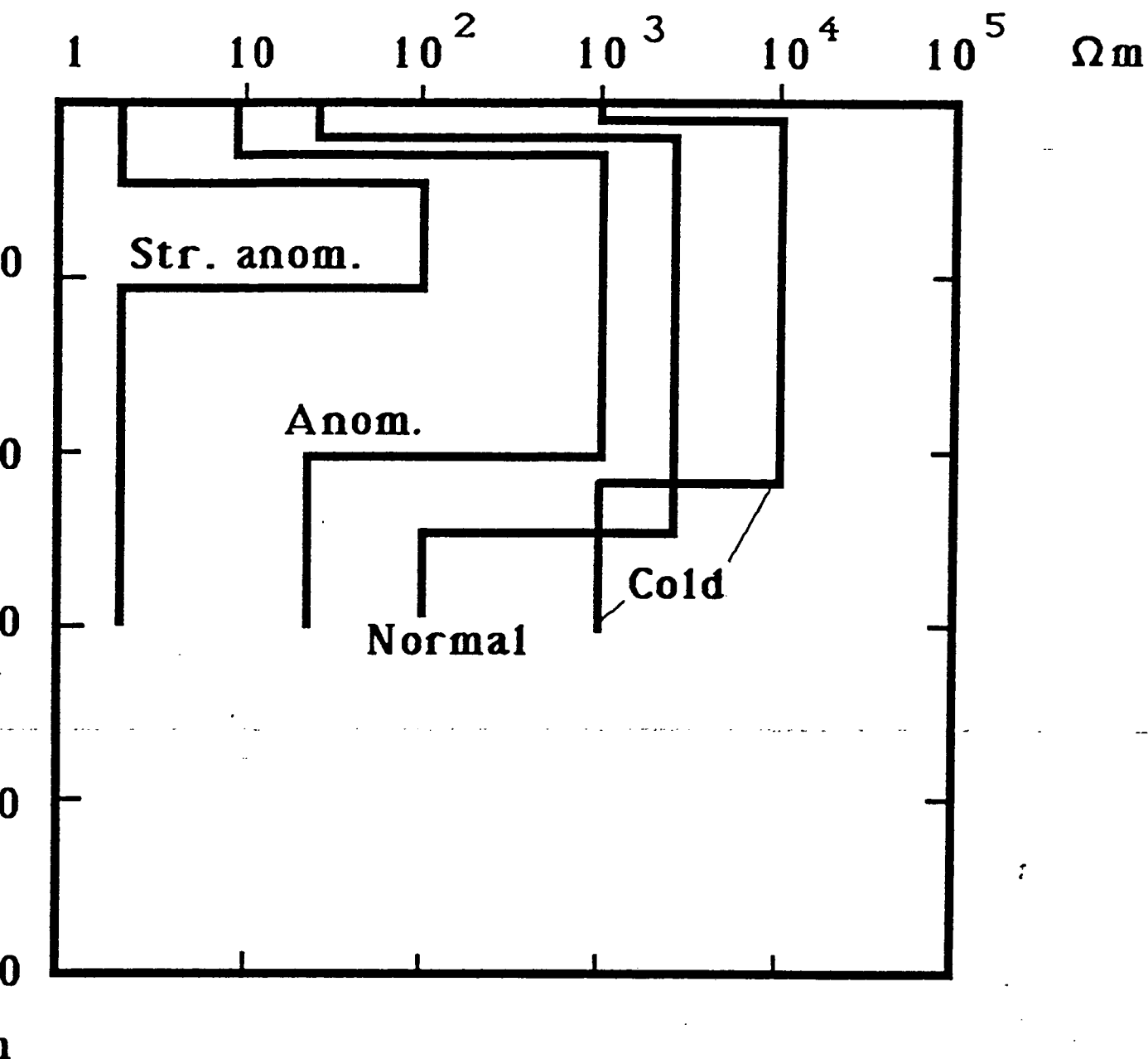


FIGURE 8.10. GENERALISED CRUSTAL RESISTIVITY PROFILES (AFTER HJELT 1987).

THE PROFILES ILLUSTRATED ARE AS BELOW:

- 1) STRONGLY ANOMALOUS CRUST. (STR. ANOM.).
- 2) ANOMALOUS CRUST. (ANOM.).
- 3) NORMAL CRUST. (NORMAL.).
- 4) COLD CRUST. (COLD.).

CHAPTER IX

SUMMARY AND CONCLUSIONS AND SUGGESTIONS FOR FURTHER WORK

9.1. THE REGIONAL STUDY.

Magnetotelluric measurements were made along a profile in the Moine Thrust region of Northern Scotland between National Grid References 21279243 and 27188943 in the frequency range 780 Hz. TO 0.1 Hz. The data were supplemented by those of Mbipom (1980) where the data sets were compatible. They were in the frequency range 0.05 Hz. TO 0.0012 Hz. and from nearby sites along an adjacent profile.

The data were processed in the frequency domain with bias on the data being estimated using the four impedance tensor estimators.

The resistivity structure was modelled using a Hedgehog algorithm. Two-dimensional modelling was subsequently conducted using a biased linear estimation algorithm extended by the author.

- (1) There is no evidence of a resistivity contrast between the Lewisian Foreland and The Moinian Hinterland.
- (2) A crust of resistivity not less than 1×10^4 ohm-metres and extending to a depth of approximately 22 Kms. has been detected at National Grid Reference 23939160. This crustal resistivity value is considerably greater than that obtained at more westerly sites.
- (3) The resistive structure may extend to National Grid Reference 24599013 but not further eastwards than National Grid Reference 25279021. Further observations are required to verify the existence of this feature both owing to the unreliability of the data at National Grid References 24599013 and 25279021 and the need for additional data between National Grid References 23939160 and 25279021.
- (4) The comparison of the models with geological, gravity and aeromagnetic studies appear to yield no obvious similarities.
- (5) The two-dimensional models correspond with the resistivity

profiles of Hjelt (1977) for cold crust.

9.2. THE INVERSION STUDY.

A data set was used to investigate and modify a two-dimensional Magnetotelluric inversion method using singular value truncation and ridge regression iteratively.

A computer programme was written by the author to invert the two-dimensional Magnetotelluric data. Novel block boundary parameters were used and parametric errors were calculated using a linear approximation. Three experimental inversions were conducted. Essential features of these inversions are described below in order of significance.

- (1) An initial model was constructed from a section consisting of adjacent one-dimensional models. The misfit between the model response and the data was calculated. After a single iteration the fit between the model response and the data had improved so that the sum of squares misfit was 79% of the initial value.
- (2) A novel block boundary technique was used with both the block resistivities and block boundaries being variable parameters in the inversion scheme. Although the vertical boundaries did not move substantially (probably owing to the sparsity of the sites in this study) it was found that during a given iteration the movement of the horizontal boundaries considerably aided convergence.
- (3) With the data set and model parameters used it appeared from these experiments (when Jacobian matrices are used twice) that at least ten iterations would be required to produce an acceptable model.

9.3. THE ADDITIONAL INVERSION STUDIES.

The two-dimensional finite difference routine of Brewitt-Taylor and Weaver was modified by the author to allow derivatives to be calculated. The computing time required by this amendment was reduced to a minimum of 0.065 of that required by the unmodified programme.

A novel extension of the modification was made. Instead of calculating the derivative at the beginning of the finite interval by

using a first order approximation, it involved a series expansion to higher orders which allowed a mean derivative to be calculated over the interval. This accounted for non-linearity within the interval and is useful when it is known that certain parameters are incremented more than others during an iteration. It is also advantageous when calculating the larger errors and when calculating the responses of models the parameters of which have been changed substantially.

9.4.1. FURTHER WORK: THE REGIONAL STUDY.

The following suggestions are made for further work.

- (1) The data at sites E and F require verification. If they are valid a higher density of sites is required in the region of the sites in order to improve the resolution of the structure to which the responses are attributable. A large spread resistivity sounding (1 Km. TO 2Kms.) would help verify the presence of the highly resistive region at approximately 600 metres depth between sites D and E.
- (2) A Magnetotelluric sounding is required at the centre of a known or exposed granite body to ascertain directly the resistivity of the granites to establish whether or not a contrast between the granites and the country rocks exist.
- (3) A high resolution broadband Magnetotelluric study over the whole region would necessitate a substantial survey conducted over several months to obtain the high quality data required. Resources for such a study were not available at the time of the study.

9.4.2 FURTHER WORK: THE TWO-DIMENSIONAL INVERSION.

The following suggestions for further work are made.

- (1) The ridge regression should in future studies be used with the modified Brewitt-Taylor algorithm. As the computation time required per iteration is now reduced this will enable more iterations to be made with models incorporating more parameters.

- (2) The use of additional data in the form of additional geophysical data or a geologically preferential model, may be a desirable alternative to ridge regression. The addition of a-priori data with various weightings may be used to produce desirable model features such as a preferred model. Alternatively models without regions of localised high and low resistivity may be produced using a smoothing matrix as a-priori data.

APPENDIX I

THE ALTERNATIVE MODIFICATION OF THE BREWITT-TAYLOR AND WEAVER ALGORITHM (SECTION 7.2)

```

      SUBROUTINE ZOLLRD(NEQN, NC, SEQ, NONZ, LOC1, NEXT, ROWS,
      COEFF,
      +      NBUF,      CBUF,      IBUF,      IERROR)      C
      -----
      C PERFORM REDUCTION STEP OF ZOLLENKOPF SOLUTION.
      COMPLEX COEFF(NC), LEFTJJ, LFACT, DIAG, CBUF(NBUF)
      INTEGER NONZ(NEQN), SEQ(NEQN), ROWS(NC), NEXT(NC),
      LOC1(NEQN),
      + STEP, SMALL, PIVCOL, PIVROW, PIVLOC, ROWR, ROWJ,
      VACANT,
      + OLDVAC, IBUF(NBUF)
      COMMON /CZOLL/ VACANT, MAXVAC, IDISC, IZOLL(7)
      INTEGER NRRR(15000), NCCC(15000), NAAA(15000)
      COMPLEX AAAA(15000)
      COMMON/MATRIX/ NRRR, NCCC, AAAA, K
      COMMON/ITERAT/ INC, IPOL
      COMMON/STORE1/ NAAA
      IF(INC.EQ.1) GO TO 8200
      J=0
      K=0 8000 J=J+1
      NI=LOC1(J)
      IF(NI.NE.0) GOTO 8100
      N2=NONZ(J)
      IF(N2.NE.0) STOP 'N2.NE.0'
      GOTO 8000 8100 K=K+1
      NRRR(K)=ROWS(NI)
      NCCC(K)=J
      NAAA(K)=NI
      NI=NEXT(NI)
      IF(NI.NE.0) GOTO 8100
      IF(J.NE.NEQN) GOTO 8000 8200 DO 8300 I=1,K
      AAAA(I)=COEFF(NAAA(I)) 8300 CONTINUE
      IF(INC.EQ.1) RETURN C C 600P FOR EACH COLUMN OF
MATRUX
      IERROR = 0
      IEND = NEQN - 1
      DO 600 STEP = 1, IEND C FIND COLUMN WITH SMALLEST NUMBER
      OF NONZERO COEFFS.
      ISEQ = SEQ(STEP)
      SMALL = NONZ(ISEQ)
      IPIVOT = STEP
      ISTART = STEP + 1
      DO 10 INDEX = ISTART, NEQN
      ISEQ = SEQ(INDEX)
      IF(SMALL .LE. NONZ(ISEQ)) GO TO 10
      IPIVOT = INDEX
      SMALL = NONZ(ISEQ) 10 CONTINUE C SWAP NEW PIVOT
      COLUMN NAD FIRST UNUSED COLUMN.
      PIVCOL = SEQ(IPIVOT)

```

```

      SEQ(IPIVOT) = SEQ(STEP)
      SEQ(STEP) = PIVCOL
      IF(SMALL .LE. 0) GO TO 600 C FIND DIAGONAL ELEMENT AND
CALCULATE L(J,J)
      LOCJ = LOC1(PIVCOL) 12 IF(ROWS(LOCJ) .EQ. PIVCOL) GO TO
15
      LOCJ = NEXT(LOCJ)
      GO TO 12 15 DIAG = COEFF(LOCJ)
      LEFTJJ = 1. / DIAG
      COEFF(LOCJ) = LEFTJJ C WORK DOWN PIVOT COLUMN
CALCULATING NEW L(R,J)
      LOCJ = LOC1(PIVCOL) 17 IF(ROWS(LOCJ) .NE. PIVCOL)
COEFF(LOCJ) = - LEFTJJ * COEFF(LOCJ)
      LOCJ = NEXT(LOCJ)
      IF(LOCJ .GT. 0) GO TO 17 C LOOP FOR EACH ELEMENT IN
PIVOT COLUMN 25 PIVLOC = LOC1(PIVCOL) 30 PIVROW = ROWS(PIVLOC)
      IF(PIVROW .EQ. PIVCOL) GO TO 500 C CALCULATE FACTOR -
L(R,J) / L(J,J)
      LFACT = - DIAG * COEFF(PIVLOC) C WORK DOWN COLUMN WHOSE
C IS SAME AS CIRRENT R IN PIVOT COLUMN
      LOCR = LOC1(PIVROW)
      ROWR = ROWS(LOCJ)
      LOCR0 = 0
      LOCJ = LOC1(PIVCOL) 40 ROWJ = ROWS(LOCJ)
      IF(ROWR - ROWJ) 100, 200, 300 C TERM IN COLUMN C ONLY,
A(R,C) UNCHANGED SO DO NOTHING. 100 LOCR0 = LOCR
      LOCR = NEXT(LOCJ)
      GO TO 280 C TERM IN BOTH COLUMNS 200 IF(ROWR .EQ.
PIVCOL) GO TO 250 C CALCULATE NEW VALUE OF A(R,C) IN PLACE
      COEFF(LOCJ) = COEFF(LOCJ) + LFACT*COEFF(LOCJ)
      LOCR0 = LOCR
      LOCR = NEXT(LOCJ)
      GO TO 270 C DELETE UNNEEDED COEFF IN PIVOT ROW. 250
NEXTR = NEXT(LOCJ)
      IF(LOCJ0 .GT. 0) GO TO 255
      LOC1(PIVROW) = NEXTR
      GO TO 260 255 NEXT(LOCJ0) = NEXTR 260 NEXT(LOCJ)
= VACANT
      VACANT = LOCR
      NONZ(PIVROW) = NONZ(PIVROW) -1
      LOCR = NEXTR C MOVING ON TO NEXT TERMS. 270 LOCJ =
NEXT(LOCJ) 280 IF(LOCJ .GT. 0) GO TO 290
      ROWR = NEQN + 1
      GO TO 400 290 ROWR = ROWS(LOCJ)
      GO TO 400 C TERM IN PIVOT COLUMN ONLY, INSERT NEW COEFF
IN COL C. 300 IF(VACANT .GT. 0) GO TO 310
      IERROR = 1
      RETURN 310 IF(LOCJ0 .GT. 0) GO TO 320
      LOC1(PIVROW) = VACANT
      GO TO 325 320 NEXT(LOCJ0) = VACANT 325 OLDVAC =
VACANT
      VACANT = NEXT(VACANT)
      NEXT(OLDVAC) = LOCR
      ROWS(OLDVAC) = ROWJ
      COEFF(OLDVAC) = LFACT * COEFF(LOCJ)
      NONZ(PIVROW) = NONZ(PIVROW) + 1
      MAXVAC = MAX0(MAXVAC, VACANT-1)
      LOCR0 = OLDVAC
      LOCJ = NEXT(LOCJ) C ENDS OF LOOPS 400 IF(LOCJ .GT. 0) GO
TO 40 500 PIVLOC = NEXT(PIVLOC)

```

```

      IF(PIVLOC .GT. 0) GO TO 30 C WRITE OUT EQUATION JUST
      PROCESSED TO DESC
      IF(IDISC .GT. 0) CALL ZOLLWR(NEQN, NC, SEQ, LOC1, NEXT,
      ROWS,
      + COEFF, NBUF, CBUF, IBUF, STEP) 600 CONTINUE C PROCESS
      LAST STAGE, ONLY ONE TERM LEFT.
      LOCJ = LOC1(SEQ(NEQN))
      COEFF(LOCJ) = 1. / COEFF(LOCJ)
      IF(IDISC .GT. 0) CALL ZOLLWR(NEQN, NC, SEQ, LOC1, NEXT,
      ROWS,
      + COEFF, NBUF, CBUF, IBUF, NEQN)
      RETURN
      END
      SUBROUTINE ZOLDS2(NEQN, SEQ, RHS, NBUF, CBUF, IBUF) C
-----*
C ZOLLENKOPF MATRIX MULTIPLICATION USING INVERSE MATRIZ FROM
DISC.
      COMPLEX CBUF(NBUF), RHS(NEQN), TEMP,Z(45000),RHS0(3000)
      +
      ,AAAA(15000),RHS1(3000),RHS2(3000),RHS3(3000),RHS4(3000)
      +
      ,RHS5(3000),RHS6(3000),ARHS(3000),ZZ1(100),ZZ2(100),ZZ3(100)
      INTEGER SEQ(NEQN), IBUF(NBUF), STEP, COLUMN,
      ROW,IZ(45000)
      + ,NRRR(15000),NCCC(15000)
      COMMON /CZOLL/ IZOLL(2), IDISC, IBLK1, IBLOCK, LOC
      COMMON /STORE/ Z,IZ
      COMMON/CPROB/NX,NY,NZ,NXP,NYP,NZP,NCPTF,NPROB,NROW,NDIM,LSYM(3)
      COMMON/MATRIX/NRRR,NCCC,AAAA,K
      COMMON/ITERAT/ INC,IPOL
      COMMON/ITERN/ NLEVEL,AITER1,AITER2,MAXITR,NPRINT
      COMMON/STORE2/RHS0,RHS5,RHS6
      COMMON/SIGMAC/ZZ1,ZZ2,ZZ3,SURFAC,YLOC,ZGRID1,ZGRID2,ZGRID3
C
      ITAG1=0
      ITAG2=0
      ITAG3=0
      RES01=1.0E70
      RES02=1.0E70
      NITR=0
      BITER1=AITER1
      BITER2=AITER2
      IF(INC.EQ.0) BITER1=100.0
      IF(INC.EQ.0) BITER2=1.0
      NMIN=NY-1
      IF(IPOL.EQ.1) NMIN=(NY-2)*(NLEVEL-1)+1
      IF(INC.NE.0) GO TO 8100
      DO 8000 I=1,NEQN
      RHS0(I)=RHS(I)
      RHS1(I)=RHS(I)
      RHS3(I)=CMPLX(0.0,0.0) 8000 CONTINUE
      GOTO 8600 8100 DO 8400 I=1,NEQN
      RHS1(I)=RHS5(I)-RHS0(I)+RHS(I)
      RHS3(I)=RHS6(I)
      RHS(I)=CMPLX(0.0,0.0) 8400 CONTINUE
      ITAG1=1
      GOTO 8800 8600 NITR=NITR+1
      LOC = 0
      LOCBUF = 1
      STEP = 0 C FORWARD MULTIPLICATION, LOOP FOR EACH

```

```

EQUATION. 10 STEP = STEP + 1
            COLUMN = - IZ(LOCBUF)
            SEQ(STEP) = COLUMN
            TEMP = RHS(COLUMN)
            RHS(COLUMN) = (0.,0.)
            GO TO 25 20 RHS(ROW) = RHS(ROW) + TEMP *
Z(LOCBUF)
            LOC = LOC + 1 25 LOCBUF = LOCBUF + 1 30 ROW =
IZ(LOCBUF)
            IF(ROW) 10, 40, 20 C REVERSE MULTIPLICATION, SKIP PAST
LAST EQUATION. 40 LOCBUF = LOCBUF - 1 45 IF(IZ(LOCBUF) .GT. 0)
GO TO 40
            STEP = STEP - 1 C LOOP FOR EACH COLUMN OF MATRIX 50
COLUMN = SEQ(STEP)
            TEMP = RHS(COLUMN)
            GO TO 65 60 IF(ROW .NE. COLUMN) TEMP = TEMP +
Z(LOCBUF) * RHS(ROW) 65 LOCBUF = LOCBUF - 1 70 ROW =
IZ(LOCBUF)
            IF(ROW .GT. 0) GO TO 60
            RHS(COLUMN) = TEMP
            STEP = STEP - 1
            IF(STEP .GT. 0) GO TO 50 C C

            IF(INC.EQ.1) GO TO 8800
            DO 8700 I=1,NEQN
            RHS6(I)=RHS3(I)
            RHS5(I)=ARHS(I) 8700 CONTINUE 8800 DO 8900 I=1,NEQN
            RHS4(I)=RHS3(I)
            RHS3(I)=RHS3(I)+RHS(I)
            ARHS(I)=CMPLX(0.0,0.0) 8900 CONTINUE
            DO 9000 I=1,K
            ARHS(NRRR(I))=ARHS(NRRR(I))+AAAA(I)*RHS3(NCCC(I))
9000 CONTINUE
            RES11=0.0
            RES12=0.0
            DO 9100 I=NMIN,NEQN
            RES11=RES11+RHS(I)*CONJG(RHS(I))
            RHS(I)=RHS1(I)-ARHS(I)
            RES12=RES12+RHS(I)*CONJG(RHS(I)) 9100 CONTINUE
            RES11=SQRT(RES11)
            RES12=SQRT(RES12)
            WRITE(10,*) RES11,RES12
            IF(ITAG1.NE.0) RES11=RES01
            RES21=BITER1*RES01
            RES22=BITER2*RES02
            IF(RES12.GT.RES02) ITAG3=1
            IF(RES11.GT.RES21)GOTO 8200
            IF(RES12.GT.RES22)GOTO 8200
            IF((NITR.GE.MAXITR).AND.(INC.NE.0)) GO TO 8200
            RES01=RES11
            RES02=RES12
            ITAG1=0
            GOTO 8600 8200 IF(ITAG3.EQ.1) GO TO 8500
            DO 9200 I=1,NEQN
            RHS4(I)=RHS3(I) 9200 CONTINUE 8500 IF(NPRINT.EQ.0)
GOTO 9400
            DO 9500 I=1,NEQN
            RHS(I)=RHS4(I) 9500 CONTINUE 9400 CONTINUE
            NMAX=NY-2
            DO 9300 I=1,NMAX

```

```

      ZZ1(I+1)=RHS4(I+(NY-2)*(NLEVEL-3))
      ZZ2(I+1)=RHS4(I+(NY-2)*(NLEVEL-2))
      ZZ3(I+1)=RHS4(I+(NY-2)*(NLEVEL-1)) 9300 CONTINUE
      ZZ1(1)=ZZ1(2)
      ZZ1(NY)=ZZ1(NY-1)
      ZZ2(1)=ZZ2(2)
      ZZ2(NY)=ZZ2(NY-1)
      ZZ3(1)=ZZ3(2)
      ZZ3(NY)=ZZ3(NY-1)
      RETURN
END

```

APPENDIX I.

THE INVERSION PROGRAMME USED IN SECTIONS (8.5) TO (8.9).

```

      INTEGER
TEMP1(400),TEMP12(400),TEMP3(400),A1,A3,F,COL(40)
      REAL*8 TEMPR(400),R(400),TEMPRA(400,40),RA(400,40)
      REAL*8 TEMP2(400),TEMP4(400),TEMP5(400)
      REAL*8
TEMP6(400),TEMPM0(400),MODEL0(400),A2,A4,A5,A6
      REAL*8 B1,B2,B3,B4,LM
      REAL*8 A(400,40),B(400),U(400,40),V(40,40)
      REAL*8
TEMP7(400),TEMP8(400),TEMP9(400),TEMP10(40),RADJ(400)
      REAL*8 ADJ,SUMF,TEMP11(400),TEMP13(400),TEMP14(400)
      COMMON /SPLIT/ISUM1,TEMP9
      COMMON/RECORD/ MAX,TEMP1,TEMP3

```

```

      CALL FPRMPT ('DATA RECORD LENGTH : ',21)
      READ(5,*) MAX
      CALL FPRMPT ('SENSITIVITY MATRIX : N : ',25)
      READ (5,*) N
      CALL FPRMPT (' NUMBER OF FREQUENCIES : ',24)
      READ (5,*) F

```

```

      CALL FPRMPT('RHO:0,PHASE:1.RHO AND PHASE:2',29)
      READ(5,*) ITAG C*****READ IN DATA

```

```

      DO 1 I=1,MAX
      READ(52,*) A1,A2,A5,A3,A4,A6
      TEMP1(I)=A1
      TEMP2(I)=A2
      TEMP3(I)=A3
      TEMP4(I)=A4
      TEMP7(I)=A5
      TEMP8(I)=A6 1 CONTINUE

```

C*****AMPLITUDE/PHASE/AMPLITUDE AND PHASE

```

      IF(ITAG.EQ.0)GO TO 180
      IF(ITAG.EQ.1) GO TO 190
      IF(ITAG.EQ.2) GO TO 200 180 DO 160 I=1,MAX
      TEMP3(I)=0 160 CONTINUE
      GO TO 200 190 DO 170 I=1,MAX

```

TEMP1(I)=0 170 CONTINUE 200 CONTINUE

C*****CALCULATE M

```
      ISUM=0
      DO 10 I=1,MAX
      IADD1=0
      IF(TEMP1(I).GT.0) IADD1=1
      ISUM=ISUM+IADD1 10 CONTINUE
      ISUM1=ISUM
      ISUM=0
      DO 20 I=1,MAX
      IADD2=0
      IF(TEMP3(I).GT.0) IADD2=1
      ISUM=ISUM+IADD2 20 CONTINUE
      ISUM2=ISUM
      M=ISUM1+ISUM2
```

C*****RESISTIVITY AND PHASE CONCERTED TO
C*****LOG(RESISTIVITY) AND PHASE C*****READ IN
STANDARD MODEL

```
      DO 30 I=1,MAX
      READ(51,*) B1,B2,B3,B4
      TEMP5(I)=B2
      TEMP6(I)=B3
      READ(50,*) B1,B2,B3,B4
      TEMP13(I)=B2
      TEMP14(I)=B3 30 CONTINUE
```

C*****SET UP STANDARD MODEL

```
      I1=0
      I10=ISUM1
      DO 90 I=1,MAX
      IF(TEMP1(I).LT.1) GO TO 100
      I1=I1+1
      TEMP12(I1)=0
      IF(TEMP1(I).GT.1) TEMP12(I1)=1
      TEMPM0(I1)=DLOG10(TEMP5(I)) 100 IF(TEMP3(I).LT.1) GO
TO 90
      I10=I10+1
      TEMP12(I10)=0
      IF(TEMP3(I).GT.1) TEMP12(I10)=1
      TEMPM0(I10)=TEMP6(I) 90 CONTINUE
```

C*****SET UP ERROR VECTOR

```
      I20=0
      I30=ISUM1
      DO 50 I=1,MAX
      IF(TEMP1(I).LT.1) GO TO 40
```

```

I20=I20+1
  TEMPR(I20)=(DLOG10(TEMP2(I))-DLOG10(TEMP5(I)))
  TEMP11(I20)=TEMP7(I) 40 CONTINUE

  IF(TEMP3(I).LT.1) GO TO 50
I30=I30+1
  TEMPR(I30)=(TEMP4(I)-TEMP6(I))
  TEMP11(I30)=TEMP8(I) 50 CONTINUE

C*****SET UP SENSITIVITY MATRIX

  DO 60 J=1,N
I40=0
  I50=ISUM1
  DO 70 I=1,MAX
    K=J+10
    READ(K,*) B1,B2,B3,B4
    IF(TEMP1(I).LT.1) GO TO 80
I40=I40+1
    TEMPRA(I40,J)=(DLOG10(B2)-DLOG10(TEMP13(I))) 80
IF(TEMP3(I).LT.1) GO TO 70
  I50=I50+1
    TEMPRA(I50,J)=(B3-TEMP14(I)) 70 CONTINUE 60 CONTINUE

C*****COPY TO TEMPORARY MATRIX

N0=N 1000 N=N0
  DO 440 I=1,M
  DO 450 J=1,N
    RA(I,J)=TEMPRA(I,J) 450 CONTINUE
  R(I)=TEMPR(I) 440 CONTINUE

C*****INCREMENTAL ADJUSTMENT OF ERROR VECTOR
C*****AND REALLOCATION OF N

  CALL FPRMPT('INCREMENTAL MODEL CHANGE? ',26)
  READ(5,*) NTAG
  IF(NTAG.LT.1) GO TO 210
  DO 220 I=1,N
  CALL FPRMPT('PERTURBATION VECTOR : ',22)
  READ(5,*) ADJ
  TEMP10(I)=ADJ 220 CONTINUE
  DO 230 I=1,M
  SUMF=0.0
  DO 240 J=1,N
    SUMF=SUMF+TEMPRA(I,J)*TEMP10(J) 240 CONTINUE
  RADJ(I)=SUMF 230 CONTINUE
  DO 250 I=1,M
  R(I)=TEMPR(I)-RADJ(I) 250 CONTINUE
  WRITE(6,260) 260 FORMAT(' PERTURBATION VECTOR')
  WRITE(6,270)(TEMP10(I),I=1,N) 270
  FORMAT(2X,10(F10.4))
  WRITE(6,280) 280 FORMAT(' PERTURBED ERROR VECTOR')
  WRITE(6,290)(RADJ(I),I=1,M) 290 FORMAT(2X,10(F10.4))

```

```

        CALL FPRMPT('NEW N : ',8)
        READ(5,*) N

210 CONTINUE

C*****ADD COLUMNS OF MATRIX, DELETE SUPERFLUOUS COLUMNS
C*****AND REALLOCATE N

420 CALL FPRMPT('AMALGAMATE N VARIABLES : N : ',29)
      READ(5,*) NC
      IF(NC.EQ.0) GO TO 430
      CALL FPRMPT('AMALGAMATE VARIABLES : ',23)
      READ(5,*)(COL(I),I=1,NC)
      I1=COL(1)
      DO 380 I=2,NC
      I2=COL(I)
      DO 390 J=1,M
      RA(J,I1)=RA(J,I1)+RA(J,I2)
      IF(I2.EQ.N) GO TO 390
      NN=N-1
      DO 400 K=I2,NN
      I3=K+1
      RA(J,K)=RA(J,I3) 400 CONTINUE 390 CONTINUE
      N=N-1
      DO 410 J1=2,NC
      COL(J1)=COL(J1)-1 410 CONTINUE 380 CONTINUE
      GO TO 420 C*****DISPLAY INITIAL DATA

430 WRITE (9,110) M,N 110 FORMAT ( ' SENSITIVITY MATRIX : M :
',I4,'N : ',I4)
      DO 120 I80=1,M
      WRITE (9,130) (RA(I80,I120),I120=1,N) 130 FORMAT
(2X,10(F8.4,2X)) 120 CONTINUE
      WRITE (6,140) 140 FORMAT (' ERROR VECTOR')
      WRITE (6,150) (R(I140),I140=1,M) 150 FORMAT
(2X,10(F8.4,2X))

      CONTINUE

C*****ADJUST ROW SCALING FACTORS

      CALL FPRMPT ('VARIANCE MULTIPLIER : ',24)
      READ(5,*) LM
      DO 330 I=1,M
      IF(TEMP12(I).GT.0) GO TO 340
      TEMP9(I)=TEMP11(I)
      GO TO 330 340 TEMP9(I)=LM*TEMP11(I) 330 CONTINUE

C*****ROW SCALE RESISTIVITY AND PHASE MATRICES
C*****AND COPY TO TEMPORARY MATRICES

      DO 350 I=1,M
      MODEL0(I)=TEMPM0(I)/TEMP9(I)
      R(I)=R(I)/TEMP9(I) 350 CONTINUE

```

```

DO 360 J=1,N
DO 370 I=1,M
RA(I,J)=RA(I,J)/TEMP9(I) 370 CONTINUE 360 CONTINUE

CALL SCALE(M,N,RA)

```

```

CALL MISFIT (M,R,F)

CALL GRADIE (M,N,F,RA,R,MODEL0)
CALL MATCH2 (M,N,A,RA,R,F,MODEL0,U,V)

GO TO 1000

```

```

STOP
END

```

```

SUBROUTINE MISFIT(M,M1,F)

INTEGER M,F,S,L
REAL*8
M1(400),SUM,SUMA,SUMP,RSUM,RSUMA,RSUMP,TEMP9(400)
COMMON/SPLIT/ISUM1,TEMP9

SUMA=0.0
RSUMA=0.0
IF(ISUM1.LT.1) SUMA=1.0E10
IF(ISUM1.LT.1) RSUMA=1.0E10
IF(ISUM1.LT.1) GO TO 50
DO 1 I=1,ISUM1
SUMA=SUMA+(M1(I)**2)/FLOAT(ISUM1)
RSUMA=RSUMA+((M1(I)*TEMP9(I))**2)/FLOAT(ISUM1) 1
CONTINUE

50 ISUM3=ISUM1+1
ISUM4=M-ISUM1
SUMP=0.0
RSUMP=0.0
IF(ISUM4.LT.1) SUMP=1.0E10
IF(ISUM4.LT.1) RSUMP=1.0E10
IF(ISUM4.LT.1)GO TO 60
DO 10 I=ISUM3,M
SUMP=SUMP+((M1(I))**2)/FLOAT(ISUM4)
RSUMP=RSUMP+(((M1(I))*TEMP9(I))**2)/FLOAT(ISUM4) 10
CONTINUE

```

```

60 SUM=((SUMA*FLOAT(ISUM1))+(SUMP*FLOAT(ISUM4)))/
   C FLOAT(ISUM1+ISUM4)
   RSUM=((RSUMA*FLOAT(ISUM1))+(RSUMP*FLOAT(ISUM4)))/
   C FLOAT(ISUM1+ISUM4)

   WRITE(6,20)                                20          FORMAT('
DESCRIPTION',50X,'ROW-SCALED',10X,'ROW-DESCALED')
   WRITE(6,30) SUMA,RSUMA 30 FORMAT(' AMPLITUDE MISFIT
VARIANCE',36X,F10.4,10X,F10.4)
   WRITE(6,40) SUMP,RSUMP 40 FORMAT(' PHASE MISFIT
VARIANCE',36X,F10.4,10X,F10.4)
   WRITE(6,70) SUM,RSUM 70 FORMAT(' AMPLITUDE AND PHASE
MISFIT VARIANCE',26X,F10.4,10X,
   C F10.4)
   RETURN
   END
   SUBROUTINE DECODE(M,F,R,MODEL0,IT1,ID,FACTOR,NRR)

   INTEGER F,TEMP1(400),TEMP3(400)
   REAL*8
R(400),MODEL0(400),C1(400),C2(400),NEWMOD(400)
   REAL*8
DEC1(400),DEC2(400),DEC3(400),DEC4(400),FACTOR
   REAL*8
DEC5(400),DEC6(400),DEC7(400),DEC8(400),DEC9(400)
   REAL*8 DEC10(400),DEC11(400),DEC12(400),DEC13(400)
   REAL*8 DEC14(400),TEMP9(400)
   COMMON/SPLIT/ISUM1,TEMP9
   COMMON/ERROR/C1
   COMMON/RECORD/MAX,TEMP1,TEMP3

C*****CALCULATE AMMENDED MODEL

   DO 1 I=1,M
   NEWMOD(I)=(R(I)+MODEL0(I)+C1(I))*TEMP9(I)
   C2(I)=C1(I)*TEMP9(I) 1 CONTINUE

C*****DECODE VECTORS TO INPUT FORMAT

   I10=0
   DO 10 I=1,MAX
   IF(TEMP1(I).LT.1) GO TO 20
   I10=I10+1
   DEC1(I)=NEWMOD(I10)
   DEC5(I)=C2(I10)
   DEC11(I)=TEMP9(I10)
   GO TO 10 20 DEC1(I)=99999.9999
   DEC5(I)=99999.9999
   DEC11(I)=0.0 10 CONTINUE
   I20=ISUM1
   DO 30 I=1,MAX
   IF(TEMP3(I).LT.1) GO TO 40
   I20=I20+1
   DEC2(I)=NEWMOD(I20)
   DEC6(I)=C2(I20)

```

```

DEC12(I)=TEMP9(I20)
GO TO 30 40 DEC2(I)=99999.9999
DEC6(I)=99999.9999
DEC12(I)=0.0 30 CONTINUE

```

C*****DECODE VECTORS TO SITE FORMAT

```

I30=0
ISTEP=MAX/F
DO 50 ISTART=1,ISTEP
DO 60 I=ISTART,MAX,ISTEP
I30=I30+1
DEC3(I30)=DEC1(I)
DEC4(I30)=DEC2(I)
DEC7(I30)=DEC5(I)
DEC8(I30)=DEC6(I)
DEC13(I30)=DEC11(I)
DEC14(I30)=DEC12(I) 60 CONTINUE 50 CONTINUE

```

C*****RECOVER DATA

```

DO 220 I=1,MAX
DEC9(I)=DEC3(I)-DEC7(I)
DEC10(I)=DEC4(I)-DEC8(I)          220          CONTINUE

```

C*****WRITE DECODED VECTORS TO OUTPUT FILES

```

WRITE(7,90)IT1 90 FORMAT(' SINGULAR VALUES TRUNCATED
AFTER ENTRY : ',I4)
IF(NRR.EQ.2) GO TO 120
WRITE(7,110) ID 110 FORMAT('SINGULAR VALUES DAMPED
BY ENTRY : ',I4)
GO TO 140 120 WRITE(7,130) FACTOR 130 FORMAT(' Q(1)*X
: X : ',F10.4) 140 WRITE(7,100) 100 FORMAT(' RHO DATA RHO
MODEL RHO MISFIT RHO ERROR
C PHASE DATA PHASE MODEL PHASE MISFIT PHASE ERROR')
NF=F-1
NS=MAX/2
N1=0
N2=0
N3=0
DO 70 I=1,MAX
IF(N1.GT.NF) N1=0
N1=N1+1
IF(I.GT.NS) GO TO 170
IF(N1.EQ.1) GO TO 150
GO TO 200 150 N2=N2+1
WRITE(7,160) N2 160 FORMAT(' E-POLARIZATION : SITE :
',I4)
GO TO 200 170 IF(N1.EQ.1) GO TO 180
GO TO 200 180 N3=N3+1
WRITE(7,190) N3 190 FORMAT(' H-POLARIZATION : SITE :
',I4)          200          WRITE(7,80)
DEC9(I),DEC3(I),DEC7(I),DEC13(I),DEC10(I),
C DEC4(I),DEC8(I),DEC14(I) 80 FORMAT(2X,8(F10.4,5X))
WRITE(8,210) N1,DEC9(I),DEC3(I),DEC13(I),DEC10(I),
C DEC4(I),DEC14(I) 210 FORMAT (2X,I4,8(F10.4,2X)) 70
CONTINUE

```

RETURN
END

SUBROUTINE MATCH2(M,N,A,RA,R,F,MODEL0,U,V)

INTEGER M,N,F,INDEX
REAL*8 RA(400,40),R(400),A(M,N),U(M,N),V(N,N),Q(40)
REAL*8 U0(400,40),V0(40,40),Q0(40),TOL,MODEL0(400)

DO 800 J=1,N
DO 810 I=1,M
A(I,J)=RA(I,J) 810 CONTINUE 800 CONTINUE
INDEX=1
CALL SVD(M,N,A,U,V,Q,INDEX)

832 CONTINUE

DO 840 J=1,N
DO 850 I=1,M
U0(I,J)=U(I,J) 850 CONTINUE 840 CONTINUE
DO 860 I=1,N
DO 870 J=1,N
V0(I,J)=V(I,J) 870 CONTINUE 860 CONTINUE
CALL SVDA(M,N,U0,V0,Q,R,TOL,F,RA,MODEL0)
RETURN
END

SUBROUTINE RESIDU(M,N,F,RA,B,R,MODEL0)

INTEGER M,N,F
REAL*8
RA(400,40),B(400),R(400),C(400),C1(400),C2(400)
REAL*8 LENGTH,RESIDUE,S,MODEL0(400)
COMMON/ERROR/C1

LENGTH=0
DO 400 I400=1,N
LENGTH=LENGTH+(B(I400))**2 400 CONTINUE
DO 410 I410=1,M
S=0
DO 420 I420=1,N
S=S+(RA(I410,I420))*B(I420) 420 CONTINUE
C(I410)=S 410 CONTINUE

DO 430 I430=1,M
C1(I430)=C(I430)-R(I430) 430 CONTINUE

```

      WRITE (6,440) LENGTH 440 FORMAT (' EUCLIDIAN
LENGTH',F10.4)
      WRITE (6,450) 450 FORMAT ( ' RESIDUE,LINEAR PROJECTED
SUM SQUARED DEVIATIONS')

```

```

      CALL MISFIT (M,C1,F)

```

```

C WRITE (6,460) C460 FORMAT (' LINEAR PROJECTED ERROR VECTOR')
C CALL MISFIT(M,C,F)

```

```

      RETURN
      END

```

```

SUBROUTINE SVDA(M,N,U0,V0,Q,R,TOL,F,RA,MODEL0)

```

```

      INTEGER L(40),LL(40),F
      REAL*8 U0(400,40),V0(40,40),Q(40),R(400)
      REAL*8
      U0T(40,400),V0T(40,40),Q1(40),U01(400,40),V01(40,40)
      REAL*8
      U01T(40,400),V01T(40,40),TOL,RA(400,40),MODEL0(400)
      REAL*8 RHS(40),RHS1(40),SUM

```

```

C*****FIND ORDER OF SINGULAR VALUES

```

```

      DO 1 I=1,N
      LL(I)=0 1 CONTINUE
      DO 10 I=1,N
      S=0.0
      DO 20 J=1,N
      IF(LL(J).GT.0) GO TO 20
      IF(Q(J).GT.S) JI=J
      IF(Q(J).GT.S) S=Q(J) 20 CONTINUE
      LL(JI)=1
      L(I)=JI 10 CONTINUE C*****ORDER SINGULAR VALUES
AND MATRICES

```

```

      DO 30 J=1,N
      K=L(J)
      DO 40 I=1,M
      U01(I,J)=U0(I,K) 40 CONTINUE 30 CONTINUE
      DO 50 J=1,N
      K=L(J)
      Q1(J)=Q(K)
      DO 60 I=1,N
      V01(I,J)=V0(I,K) 60 CONTINUE 50 CONTINUE
C*****TRANSPOSE MATRICES

```

```

      DO 70 I=1,M
      DO 80 J=1,N
      U01T(J,I)=U01(I,J) 80 CONTINUE 70 CONTINUE
      DO 90 I=1,N
      DO 2000 J=1,N
      V01T(J,I)=V01(I,J) 2000 CONTINUE 90 CONTINUE

```

```

C*****OBTAIN UT*B

```

```

DO 2010 I=1,N
  SUM=0.0
  DO 2020 J=1,M
    SUM=SUM+U01T(I,J)*R(J) 2020 CONTINUE
    RHS(I)=SUM 2010 CONTINUE C*****OBTAIN UT*B/L
    DO 2040 I=1,N
      RHS1(I)=RHS(I)/Q1(I) 2040 CONTINUE
      WRITE(6,900) 900 FORMAT(' SINGULAR VALUES')
      WRITE(6,910)(Q1(I),I=1,N) 910 FORMAT(2X,10(F8.4))
      WRITE (6,920) 920 FORMAT(' PARAMETER VECTORS')
      DO 930 I=1,N
        WRITE(6,940)(V01T(I,J),J=1,N) 940
        FORMAT(2X,10(F8.4)) 930 CONTINUE
      WRITE(6,2030) 2030 FORMAT(' ROTATED RIGHT HAND SIDES')
      WRITE(6,240) (RHS(I),I=1,N) 240 FORMAT(2X,10(F12.4))
      WRITE(6,2050) 2050 FORMAT(' TRANSFORMED RIGHT HAND
SIDES ((UT*B)/L)')
      WRITE(6,2060) (RHS1(I),I=1,N) 2060 FORMAT
(2X,10(F12.4)) C WRITE(6,950) C950 FORMAT(' DATA VECTORS') C
DO 960 J=1,M C WRITE(6,970)(U01T(I,J),I=1,N) C970
FORMAT(2X,10(F8.4)) C960 CONTINUE
    CALL INVERS(M,N,Q1,V01,U01T,R,TOL,F,RA,MODEL0,V01T)
    RETURN
  END
SUBROUTINE SCALE(M,N,MX)

  REAL*8 MX(400,40),CVAR(40),SUMV
  COMMON/SCAL/CVAR

  DO 5 I=1,N
    CVAR(I)=1.0 5 CONTINUE

  CALL FPRMPT('NOSCALE?0: COLUMN?1: MANUAL?2:',28)
  READ(5,*) I1
  IF(I1.EQ.0)GO TO 60
  IF(I1.EQ.1)GO TO 70
  IF(I1.EQ.2) GO TO 80

70 CONTINUE
  DO 1 J=1,N
    SUMV=0.0
    DO 10 I=1,M
      SUMV=SUMV+(MX(I,J))**2 10 CONTINUE
    CVAR(J)=DSQRT(SUMV) 1 CONTINUE 50 CONTINUE
    DO 20 J=1,N
      DO 30 I=1,M
        IF(CVAR(J).LT.1.0E-10) CVAR(J)=1.0E-10
        MX(I,J)=MX(I,J)/CVAR(J) 30 CONTINUE 20 CONTINUE
      GO TO 60 80 CONTINUE
      DO 40 I=1,N
        CALL FPRMPT('MX(I,J)/X, X : ',12)
        READ(5,*) CVAR(I) 40 CONTINUE
        GO TO 50 60 CONTINUE
      WRITE (6,90) 90 FORMAT(' M(I,J)/X : X: ')
      WRITE (6,2000) (CVAR(I), I=1,N) 2000
      FORMAT(2X,10(F10.4,2X))
      RETURN
    END
  SUBROUTINE

```

INVERS(M,N,Q1,V01,U01T,R,TOL,F,RA,MODEL0,V01T)

```
      INTEGER M,N,F
      REAL*8
      U01T(40,400),V01(40,40),V02(40,40),P(40,400),Q1(40)
      REAL*8 Q2(40),R(400),V2(40),TOL,SMALL,MIN,SUM,SUM1
      REAL*8
      RA(400,40),MODEL0(400),ERR1(40),ERR2(40),TEMP9(400)
      REAL*8
      SUM2,SUM3,SUMCOL(400),FACTOR,V01T(40,40),C1(400)
      REAL*8 D,L,LSQE,SOL1(40),SOL2(40)
      COMMON/SPLIT/ ISUM1,TEMP9
      COMMON/ERROR/C1      C*****RIDGE      REGRESSION
PARAMETERS,NDIV1,NDIV2 C*****CODE:NRR=0 RESCALE MARGINAL
DATA VARIANCE C*****CODE:NRR=1 MANUAL BY STEPS
C*****CODE:NRR=2 MANUAL CONTINUOUS C*****CODE:NRR=3
RIDGE REGRESSION C*****CODE:NRR=4 OBTAIN RESIDUE
      NDIV1=20
      NDIV2=20
      NLSQ=1
      NRR=1
      NI=0
      IT1=N
      ID=0
      GO TO 2050 240 NLSQ=0
      WRITE(6,3240) 3240 FORMAT(' *****')
      CALL FPRMPT ('OPTION : ',9)
      READ(5,*) NRR
      IF(NRR.EQ.0)GO TO 3180
      IF(NRR.EQ.4) GO TO 3230
      CALL FPRMPT ('TRUNCATE AFTER : ',17)
      READ(5,*) IT1
      NI=0
      IF(NRR.EQ.2) GO TO 3190
      IF(NRR.EQ.3) GO TO 3100
      CALL FPRMPT ('DAMP BY ENTRY : ',16)
      READ(5,*) ID
      IF(ID.EQ.0) GO TO 2050
      D=Q1(ID)
      GO TO 2090 2050 D=0.0
      GO TO 2090 3190 CALL FPRMPT('DAMP BY ENTRY(1)*X : X :
',25)
      READ(5,*) FACTOR
      D=FACTOR*Q1(1)
      GO TO 2090 C*****INCREMENT RIDGE REGRESSION
DAMPING FACTOR 3100 NI=NI+1
      IF(N.LT.2)GO TO 3130
      D=Q1(N)+(FLOAT(NI)*(Q1(1)-Q1(N)))/FLOAT(NDIV1)
      GO TO 2090 3130
D=Q1(N)+(FLOAT(NI)*(Q1(N)-FLOAT(NDIV2)*Q1(N)))/FLOAT(NDIV1)
2090 L=D**2
      DO 2060 I=1,IT1
      Q2(I)=Q1(I)/(Q1(I)**2+L) 2060 CONTINUE
      IT2=IT1+1
      DO 2070 I=IT2,N
      Q2(I)=0.0 2070 CONTINUE
      DO 20 J=1,N
      DO 30 I=1,N
      V02(I,J)=V01(I,J)*Q2(J) 30 CONTINUE 20 CONTINUE
```

```

DO 2000 K=1,M
DO 110 I=1,N
SUM=0.0
DO 120 J=1,N
SUM=SUM+V02(I,J)*U01T(J,K) 120 CONTINUE
V2(I)=SUM 110 CONTINUE
DO 130 I=1,N
P(I,K)=V2(I) 130 CONTINUE 2000 CONTINUE

DO 40 I=1,N
SUM1=0.0
SUM2=0.0
DO 50 J=1,M
SUM1=SUM1+P(I,J)*R(J)
SUM2=SUM2+P(I,J) 50 CONTINUE
SOL1(I)=SUM1
SOL2(I)=SUM1
ERR1(I)=SUM2
ERR2(I)=SUM2 40 CONTINUE
CALL RSCALE(N,SOL2)
CALL RSCALE(N,ERR2) C*****COLUMN SUMS OF
PSEUDOINVERSE MATRIX 3030 DO 3050 J=1,M
SUM=0.0
DO 3060 I=1,N
SUM=SUM+P(I,J) 3060 CONTINUE
SUMCOL(J)=SUM 3050 CONTINUE C*****WRITE TO
RIDGE REGRESSION FILES
IF (NI.LE.0) GO TO 3170
DO 3120 I=1,N
NJ=I+60
WRITE(NJ,*) D,SOL2(I) 3120 CONTINUE
C*****DISPLAY OUTPUT C WRITE(6,250) TOL C250 FORMAT('
TOLERANCE',F6.4)
IF(NRR.EQ.3) GO TO 3150 3170 WRITE(6,280) IT1 280
FORMAT(' SINGULAR VALUES TRUNCATED AFTER ENTRY : ',I4)
IF(NRR.EQ.2) GO TO 3200
WRITE (6,2080) ID 2080 FORMAT(' SINGULAR VALUES DAMPED
BY ENTRY : ',I4)
GO TO 3210 3200 WRITE(6,3220) FACTOR 3220 FORMAT('
Q(1)*X : X : ',F10.4) 3210 WRITE(6,3040) 3040 FORMAT('
PSEUDOINVERSE MATRIX')
DO 3160 I=1,M
J=M-I+1
WRITE(9,3020)(P(K,J),K=1,N) 3020
FORMAT(2X,20(F4.1,2X)) 3160 CONTINUE C WRITE(6,3070) C3070
FORMAT(' COLUMN SUMS FOR PSEUDOINVERSE MATRIX') C
WRITE(6,3080)(SUMCOL(I),I=1,M) C3080 FORMAT(2X,10(F10.6,2X))
WRITE(6,3500) 3500 FORMAT(' COLUMN DESCALED
SOLUTIONS')
WRITE(6,200) 200 FORMAT(' SOLUTIONS')
WRITE(6,210)(SOL2(I),I=1,N) 210
FORMAT(2X,10(F10.6,2X))
WRITE(6,2030) 2030 FORMAT(' SOLUTION ERRORS')
WRITE (6,2040) (ERR2(I),I=1,N) 2040
FORMAT(2X,10(F10.6,2X))
WRITE(6,3600) 3600 FORMAT(' COLUMN SCALED SOLUTIONS')
WRITE(6,3700) 3700 FORMAT(' SOLUTIONS')
WRITE(6,3800)(SOL1(I),I=1,N) 3800
FORMAT(2X,10(F10.6,2X))

```

```

        WRITE(6,3900) 3900 FORMAT(' SOLUTION ERRORS')
        WRITE(6,4000)(ERR1(I),I=1,N)
    4000
    FORMAT(2X,10(F10.6,2X))
    CALL RESIDU(M,N,F,RA,SOL1,R,MODEL0)
    IF(NLSQ.LT.1) GO TO 3400
    LSQE=0.0
    DO 3300 I=1,M
        LSQE=LSQE+C1(I)**2    3300    CONTINUE    3400    CALL
    DECODE(M,F,R,MODEL0,IT1,ID,FACTOR,NRR)
    NRR0=NRR 3150 IF(NI.LE.0) GO TO 240
    IF(NI.GE.NDIV1) GO TO 240
    GO        TO        3100        3230        CALL
    RESOLV(M,N,NRR0,IT1,FACTOR,ID,P,VOLT,R,SOL1,LSQE)
    GO TO 240 3180 CONTINUE
    RETURN
    END

```

SUBROUTINE RSCALE(N,SOL)

```

    REAL*8 SOL(40),CVAR(40)
    COMMON/SCAL/CVAR

```

```

    DO 1 I=1,N
        SOL(I)=SOL(I)/CVAR(I) 1 CONTINUE
    RETURN
    END

```

SUBROUTINE GRADIE(M,N,F,RA,R,MODEL0)

```

    INTEGER M,F
    REAL*8
    RA(400,40),GRAD(400),CHANGE(400),R(400),M1(400)
    REAL*8 MODEL0(400),B(400)
    REAL*8 MIN,MAX,FACTOR,SUM

```

C*****CALCULATE GRADIENT

```

    DO 1 J=1,N
        SUM=0.0
        DO 10 I=1,M
            SUM=SUM+RA(I,J) 10 CONTINUE
        GRAD(J)=SUM 1 CONTINUE
        WRITE(6,40) 40 FORMAT(' GRADIENT VECTOR')
        WRITE(6,50) (GRAD(I),I=1,N) 50 FORMAT(2X,10(F12.4))

```

C*****CALCULATE CHANGE VECTOR 90 CALL FPRMPT('LINEAR
LIMIT : ',15)

```

    READ (5,*) MAX
    IF (MAX.GT.1000)GO TO 100
    MIN=0.0
    DO 20 I=1,N
        IF(GRAD(I).LT.MIN) MIN=GRAD(I) 20 CONTINUE
        IF(MIN.LT.1.0E-10) MIN=1.0E-10
        FACTOR =MAX/MIN
        DO 30 I=1,N
            CHANGE(I)=FACTOR*GRAD(I) 30 CONTINUE
        WRITE(6,60) MAX 60 FORMAT(' LINEAR LIMIT',F12.4)
        WRITE(6,70)(CHANGE(I),I=1,N) 70 FORMAT(2X,10(F12.4))

```

```

      CALL RESIDU(M,N,F,RA,CHANGE,R,MODEL0)
      GO TO 90 100 RETURN
      END

```

```

      SUBROUTINE
      RESOLV(M,N,NRR0,IT1,FACTOR,ID,P,V01T,R,SOL,LSQE)

```

```

      REAL*8 P(40,400),V01T(40,40),R(400),B(40),V(400)
      REAL*8
      UMAX(400),UMIN(400),SOLMAX(40,40),SOLMIN(40,40)
      REAL*8
      SOL(40),SUM1,SUM2,FACTOR,MULTIP,C1(400),MU,RES,LSQE
      COMMON/ERROR/C1

      RES=0.0

      DO 310 I=1,M
        RES=RES+C1(I)**2      310      CONTINUE      290      CALL
FPRMPT('PERTURBATION FACTOR : ',22)
        READ(5,*) MULTIP
        CALL FPRMPT('SINGLE:1,SUM:2,ARBITRARY:3 ',26)
        READ(5,*) NNR
        IF(NNR.EQ.0) GO TO 300
        IF(NNR.EQ.2) GO TO 80
        IF(NNR.EQ.3) GO TO 320

```

```

      C*****SET B FOR SINGLE VARIABLE

```

```

      NP=N
      K=0 70 K=K+1
      DO 60 I=1,N
        B(I)=0.0 60 CONTINUE
        B(K)=1.0
        GO TO 90 80 NP=N
        K=0 100 K=K+1
        DO 110 I=1,N
          B(I)=V01T(K,I) 110 CONTINUE
      GO TO 90 320 NP=1
      K=1
      DO 330 I=1,N
        CALL FPRMPT (' VECTOR ENTRY : ',16)
        READ(5,*) B(I) 330 CONTINUE 90 SUM2=0.0
        DO 10 I=1,M
          SUM1=0.0
          DO 20 J=1,N
            SUM1=SUM1+P(J,I)*B(J) 20 CONTINUE
          V(I)=SUM1
          SUM2=SUM2+(SUM1)**2 10 CONTINUE
          IF(SUM2.LT.1.0E-10) SUM2=1.0E-10
          MU=DSQRT((RES*MULTIP-LSQE)/SUM2)
          DO 30 I=1,M
            UMAX(I)=R(I)+MU*V(I)
            UMIN(I)=R(I)-MU*V(I) 30 CONTINUE
          DO 40 I=1,N
            SUM1=0.0

```

```

SUM2=0.0
DO 50 J=1,M
SUM1=SUM1+P(I,J)*UMAX(J)
SUM2=SUM2+P(I,J)*UMIN(J) 50 CONTINUE
SOLMAX(I,K)=SUM1
SOLMIN(I,K)=SUM2 40 CONTINUE
IF(NNR.EQ.3) GO TO 340
IF(NNR.EQ.2) GO TO 120
IF(K.LT.N) GO TO 70 120 IF(K.LT.N) GO TO 100

```

C*****DISPLAY OUTPUT

```

IF(NNR.EQ.2) GO TO 190
WRITE(6,160) 160 FORMAT(' RESOLUTION SINGLE
VARIABLE')
GO TO 180 190 WRITE(6,170) 170 FORMAT (' RESOLUTION
: LINEAR SUM')
GO TO 180 340 WRITE(6,350) 350 FORMAT (' RESOLUTION
: ARBITRARY LINEAR SUM') 180 WRITE(6,200) RES,MULTIP 200
FORMAT(' RESIDUE : ',F10.4,2X,'PERTURBATION FACTOR : ',F10.4)
IF(NNR0.EQ.2)GO TO 210
WRITE(6,130) IT1,ID 130 FORMAT(' TRUNCATE AFTER :
',I4,2X,'DAMP BY ENTRY : ',I4)
GO TO 150 210 WRITE(6,140) IT1,FACTOR 140 FORMAT('
TRUNCATE AFTER : ',I4,2X,'Q(1)*X : X : ',F10.4) 150
WRITE(6,280) 280 FORMAT(' SOLUTION VECTOR')
WRITE(6,260)(SOL(I),I=1,N) 260
FORMAT(2X,10(F8.4,2X))
WRITE(6,270) 270 FORMAT (' RANGE')
DO 220 J=1,NP
WRITE(6,230)(SOLMAX(I,J),I=1,N) 230
FORMAT(2X,10(F8.4,2X))
WRITE (6,240)(SOLMIN(I,J),I=1,N) 240
FORMAT(2X,10(F8.4,2X))
WRITE(6,250) 250 FORMAT(' ') 220 CONTINUE
GO TO 290 300 RETURN
END

```

SUBROUTINE SVD(M,N,A,U,V,Q,INDEX) C\$\$ CALLS NO OTHER ROUTINES C SINGULAR VALUE DECOMPOSITION) FOR ALGO PROGRAM SEE WILKINSON+REINSCH C HANDBOOK FOR AUTOMATIC COMPUTATION VOL 2 - LINEAR ALGEBRA, PP140-144 C TRANSLATED FROM ALGOL BY R.L.PARKER C THE MATRIX A(M,N) IS DECOMPOSED. SINGULAR VALUES IN Q, PRE-MATRIX IN C POST-MATRIX IN V. INDEX MAY BE 1,2,3 OR 4. IF 1, FIND U,V. IF 2, F C ONLY U. IF 3, FIND ONLY V. IF 4, FIND NEITHER. IN ALL CASES, THE ARRA C MUST BE SUPPLIED AS IT IS USED AS WORKING SPACE FOR THE ROUTINE. C

```

REAL*8 A(M,N),C,E(200),EPS,F,G,H,Q(N),S,TOL
REAL*8 U(M,N),V(N,N),X,Y,Z

```

```

TOL=1.0E-77
EPS=1.0E-15
DO 1100 I=1,M
DO 1100 J=1,N
1100 U(I,J)=A(I,J) C HOUSEHOLDER REDUCTION TO BI-DIAGONAL
FORM
G=0.0

```

```

      X=0.0
      DO 2900 I=1,N
      E(I)=G
      S=0.0
      L=I+1
      DO 2100 J=I,M
2100  S=U(J,I)**2 + S
      IF (S .LT. TOL) GO TO 2500
      F=U(I,I)
      G=-DSIGN(DSQRT(S),F)
      H=F*G - S
      U(I,I)=F - G
      IF (L.GT.N) GO TO 2501
      DO 2400 J=L,N
      S=0.0
      DO 2200 K=I,M
2200  S=U(K,I)*U(K,J) + S
      F=S/H
      DO 2300 K=I,M
2300  U(K,J)=U(K,J) + F*U(K,I)
2400  CONTINUE
      GO TO 2501
2500  G=0.0 C
2501  CONTINUE
      Q(I)=G
      S=0.0
      IF (L.GT.N) GO TO 2601
      DO 2600 J=L,N
2600  S=U(I,J)**2 + S
2601  IF (S.LT.TOL) GO TO 2800
      F=U(I,I+1)
      G=-DSIGN(DSQRT(S),F)
      H=F*G - S
      U(I,I+1)=F - G
      IF (L.GT.N) GO TO 2651
      DO 2650 J=L,N
2650  E(J)=U(I,J)/H
2651  CONTINUE
      IF (L.GT.M) GO TO 2850
      DO 2700 J=L,M
      S=0.0
      IF (L.GT.N) GO TO 2700
      DO 2670 K=L,N
2670  S=U(J,K)*U(I,K) + S
      DO 2690 K=L,N
2690  U(J,K)=U(J,K) + S*E(K)
2700  CONTINUE
      GO TO 2850
2800  G=0.0
2850  Y=DABS(Q(I)) + DABS(E(I))
      IF (Y .GT. X) X=Y
2900  CONTINUE C C ACCUMULATION OF RIGHT-HAND TRANSFORMS (V) C
      GO TO (3000,3701,3000,3701 ),INDEX
3000  CONTINUE
      DO 3700 IBACK=1,N
      I=N+1-IBACK
      IF (G .EQ. 0.0) GO TO 3500
      H=U(I,I+1)*G
      IF (L.GT.N) GO TO 3500
      DO 3100 J=L,N

```

```

3100 V(J,I)=U(I,J)/H
      DO 3400 J=L,N
        S=0.0
        DO 3200 K=L,N
3200   S=U(I,K)*V(K,J) + S
        DO 3300 K=L,N
3300   V(K,J)=V(K,J) + S*V(K,I)
3400 CONTINUE
3500 CONTINUE
      IF (L.GT.N) GO TO 3601
      DO 3600 J=L,N
        V(J,I)=0.0
3600 V(I,J)=0.0
3601 V(I,I)=1.0
      G=E(I)
      L=I
3700 CONTINUE
3701 CONTINUE C C ACCUMULATION OF LEFT-HAND TRANSFORMS
      GO TO (4000,4000,4701,4701 ),INDEX
4000 CONTINUE
      DO 4700 IBACK=1,N
        I=N+1-IBACK
        L=I+1
        G=Q(I)
        IF (L.GT.N) GO TO 4101
        DO 4100 J=L,N
4100   U(I,J)=0.0
4101 IF (G.EQ. 0.0) GO TO 4500
        H=U(I,I)*G
        IF (L.GT.N) GO TO 4401
        DO 4400 J=L,N
          S=0.0
          DO 4200 K=L,M
4200   S=U(K,I)*U(K,J) + S
          F=S/H
          DO 4300 K=I,M
4300   U(K,J)=U(K,J) + F*U(K,I)
4400 CONTINUE
4401 CONTINUE
        DO 4550 J=I,M
4550   U(J,I)=U(J,I)/G
        GO TO 4700
4500 CONTINUE
        DO 4600 J=I,M
4600   U(J,I)=0.0
4700 U(I,I)=U(I,I) + 1.0 C C DIAGONALIZATION OF BI-DIAGONAL
FORM
4701 EPS=EPS*X
      DO 9000 KBACK=1,N
        K=N+1-KBACK C TEST F-SPLITTING
5000 CONTINUE
        DO 5100 LBACK=1,K
          L=K+1-LBACK
          IF (DABS(E(L)).LE. EPS) GO TO 6500
          IF (DABS(Q(L-1)) .LE. EPS) GO TO 6000
5100 CONTINUE C CANCELLATION OF E(L), IF L.GT. 1
6000 C=0.0
          S=1.0
          L1=L - 1
          DO 6200 I=L,K

```

```

      F=S*E(I)
      E(I)=C*E(I)
      IF (DABS(F) .LE. EPS) GO TO 6500
      G=Q(I)
      Q(I)=DSQRT(F*F + G*G)
      H=Q(I)
      C=G/H
      S=-F/H
      GO TO (6050,6050,6200,6200 ),INDEX
6050 CONTINUE
      DO 6100 J=1,M
      Y=U(J,L1)
      Z=U(J,I)
      U(J,L1)=Y*C + Z*S
      U(J,I)=-Y*S + Z*C
6100 CONTINUE
6200 CONTINUE C TEST F-CONVERGENCE
6500 Z=Q(K)
      IF (L .EQ. K) GO TO 8000 C SHIFT FROM BOTTOM 2 X 2
MINOR
      X=Q(L)
      Y=Q(K-1)
      G=E(K-1)
      H=E(K)
      F=((Y-Z)*(Y+Z) + (G-H)*(G+H))/(2.0*H*Y)
      G=DSQRT(F*F + 1.0)
      F=((X-Z)*(X+Z) + H*(Y/(F + DSIGN(G,F))-H))/X C NEXT Q-R
TRANSFORMATION
      C=1.0
      S=1.0
      LPLUS=L + 1
      DO 7500 I=LPLUS,K
      G=E(I)
      Y=Q(I)
      H=S*G
      C=G*G
      Z=DSQRT(F*F + H*H)
      E(I-1)=Z
      C=F/Z
      S=H/Z
      F=X*C + G*S
      G=-X*S + G*C
      H=Y*S
      Y=Y*C
      GO TO (7100,7201,7100,7201 ),INDEX
7100 DO 7200 J=1,N
      X=V(J,I-1)
      Z=V(J,I)
      V(J,I-1)=X*C + Z*S
      V(J,I)=-X*S + Z*C
7200 CONTINUE
7201 Z=DSQRT(F*F + H*H)
      Q(I-1)=Z
      C=F/Z
      S=H/Z
      F=C*G + S*Y
      X=-S*G + C*Y
      GO TO (7300,7300,7500,7500 ),INDEX
7300 DO 7400 J=1,M
      Y=U(J,I-1)

```

```

      Z=U(J,I)
      U(J,I-1)=Y*C + Z*S
      U(J,I)=-Y*S + Z*C
7400  CONTINUE
7500  CONTINUE
      E(L)=0.0
      E(K)=F
      Q(K)=X
      GO TO 5000 C CONVERGENCE
8000  IF (Z .GE. 0.0) GO TO 9000 C Q IS MADE NON-NEGATIVE
      Q(K)=-Z
      GO TO (8100,9000,8100,9000 ),INDEX
8100  DO 8200 J=1,N
8200  V(J,K)=-V(J,K)
9000  CONTINUE
      RETURN
      END

```

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