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Two-Dimensional Occam Model of COPROD2 Data—First Order Description of Resolution and Variance

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A two-dimensional Occam model of crustal electrical conductivity is derived based on data from 35 magnetotelluric stations on a profile in Saskatchewan, Canada. The model is discussed in relation to a first order description of the resolution and variance of the model parameters.

Prior to the two-dimensional Occam's inversion, the data are analysed with respect to underestimated data errors. The analysis is based on separate D^+ inversions of the E- and H-polarization responses and a procedure for adjusting the data errors is presented.

The main features of the model are the presence of two conductive structures with vertically integrated conductivity exceeding 30,000 S and 100,000 S respectively. In addition to these main features, some minor conductive structures are inferred.

1. Introduction

As part of a comparative study on the two-dimensional inversion of magnetotelluric data (JONES, 1993), this paper contributes some results related to the description of resolution and variance of the parameters used for two-dimensional models. The dataset used for this study consists of 35 magnetotelluric response functions obtained along a 407 kilometre east-west profile in Canada. Detailed information on the data set can be found in JONES and SAVAGE (1986). Interpretation of the results together with discussions on general data characteristics can also be found in JONES (1988), JONES and CRAVEN (1990) and DEGROOT-HEDLIN (1991a). The main emphasis in this paper is on some technical aspects related to two-dimensional inversion of magnetotelluric data. No attempts are made to enter into a detailed discussion on the geological interpretation of the model. For this I refer to the paper of JONES (1993) and references therein.

A common procedure in the interpretation of geophysical data is to partition the inversion problem into two steps. The first involves the definition of an optimum model and the construction of this particular model. The second step involves the statistical problem of ascribing uncertainties to the model parameters. For the inversion of magnetotelluric data above a two-dimensional Earth structure, efficient algorithms are available to find a resistivity model which, in some sense, is defined as optimum. The purpose of this paper is to take a step towards a statistical description of the optimum model, which, for the data studied here, is found by using the two-dimensional Occam algorithm of DEGROOT-HEDLIN and CONSTABLE (1990). Furthermore, I shall discuss the importance of having realistic data errors for the inversion. A modification to the two-dimensional Occam inversion for which determinant data are used at high frequencies, instead of the usual E- and H-polarization data, is also introduced. The advantage of using determinant data is a reduction in the computational problems resulting from overparameterizing the inversion grid to seek well-fitting, smooth models.

2. Inversion Procedure

For detailed information on Occam's inversion in two dimensions, I refer to the original paper of DEGROOT-HEDLIN and CONSTABLE (1990). Here, I shall only outline the basic principles in order to aid the description of how a slightly modified Occam's inversion was employed and how the resolution and variance were calculated.

In short, the optimum model in the Occam's inversion is defined as the model which has a maximally smooth variation in resistivity subject to the criterion that it fits to a statistically reasonably tolerance. The statistical judgement is based on the usual least-squares criteria, i.e. the sum of squared differences between measured and model responses weighted by the corresponding data errors. The two-dimensional model is parameterized by means of rectangular prisms, each having uniform conductivity. Calculation of model responses and derivatives is based on a finite element scheme for which a finite element grid is created such that each prism in the model can be built up from a subset of the finite element cells.

It is necessary to overparameterize the inversion grid so that obtaining a misfit at a prescribed level is not prohibited by a parameterization which is too coarse. Limitations on computer memory, in combination with the broad frequency range and large number of stations for the COPROD2 dataset, makes this requirement difficult to accomplish, even after a reduction of data for which every third frequency is used. Especially, it is difficult to obtain a width of the regularization blocks within the upper part of the model fine enough to allow the model response functions at high frequencies to deviate significantly from locally one-dimensional response functions. As noted by DEGROOT-HEDLIN (1991a), the COPROD2 high frequency response is essentially one-dimensional and inversion in terms of locally one-dimensional upper structures might give a satisfactory approximation to the measured response functions at high frequencies. deGroot-Hedlin applied a hybrid inversion scheme in which the results from one-dimensional Occam's inversions were used to estimate the resistivity distribution within the upper part of the two-dimensional model. These resistivities were then kept fixed in the final two-dimensional Occam's inversion for estimation of the regional structure. I have used a slightly different approach where determinant data are used in the two-dimensional Occam's inversion for the high frequency part simultaneously with the usual E- and H-polarization data for the lower frequencies. This procedure is not as computationally efficient as the procedure used by DEGROOT-HEDLIN (1991a) since two-dimensional response calculations are needed even for the high frequencies. However, use of determinant data has the advantage that the requirement of having locally one-dimensional data can be relaxed and that the definition of the smoothness function is retained for the whole model.

In terms of model parameter vector $\mathbf{m}$ and data vector $\mathbf{d}$, the iterative solution to the non-linear inverse problem is written (Eq. 13 of DEGROOT-HEDLIN and CONSTABLE, 1990):

$$\begin{aligned} \mathbf{m}_{i+1} &= [\mu(\boldsymbol{\delta}_y^T\boldsymbol{\delta}_y + \boldsymbol{\delta}_z^T\boldsymbol{\delta}_z) + (\mathbf{W}\mathbf{J}_i)^T(\mathbf{W}\mathbf{J}_i)]^{-1}(\mathbf{W}\mathbf{J}_i)^T\mathbf{W}\hat{\mathbf{d}}_i \\ &= \mathbf{H}\hat{\mathbf{d}}_i \end{aligned} \quad (1)$$

with

$$\hat{\mathbf{d}}_i = \mathbf{d} - F[\mathbf{m}_i] + \mathbf{J}_i\mathbf{m}_i \quad (2)$$

where $\boldsymbol{\delta}_y$ and $\boldsymbol{\delta}_z$ are the roughening matrices, $\mathbf{W}$ the diagonal weighting matrix, $\mathbf{J}_i$ and $F[\mathbf{m}_i]$ the Jacobian and model response respectively for model i and μ is the Langrange multiplier. $\mathbf{H}$ denotes the inverse matrix. Non-linearity of the inverse problem makes calculation of model parameter uncertainties cumbersome. Therefore, the parameter uncertainties presented in this paper are based on an assumption of local linearity such that the method developed for linear problems as described by JACKSON (1972) can be applied. Thus, the variance $\mathrm{var}(m_k)$ of parameter m_k is found from

$$\mathrm{var}(m_k) = \sum_{j=1}^{n} H_{kj}^2 \tag{3}$$

where H_{kj} are the elements of the matrix $\mathbf{H}$ and n is the total number of data.

The resolution matrix $\mathbf{R}$ is defined as

$$\mathbf{R} = \mathbf{HJ}. \tag{4}$$

It is well known from one-dimensional inversion of magnetotelluric data that uncertainty calculations based on assumptions of linearity can be misleading. Similar problems must be expected for two-dimensional inversions and some caution should be used when interpreting these calculations. I suggest these results be used mainly as a guide to where no information is available in the two-dimensional model, i.e. parameters with high variances and low values of the corresponding diagonal element in the resolution matrix. Such regions should appear with very smooth resistivity variations in the two-dimensional model. However, regions with smooth variation in resistivity are not necessarily regions for which we have limited information about the resistivity.

Overparameterization inevitably leads to low resolution. The concept of trade-off between resolution and variance predicts that maximizing the degree of overparameterization, as should be done to achieve maximally smooth models, results in decreasing the resolution and decreasing the variance of the solution. Clearly, the process of discretizing the Earth model into a very fine block structure to obtain a smooth well-fitting model conflicts with a general wish to maintain some degree of resolution of the model parameters. This problem is described in detail for the one-dimensional case by OLDENBURG (1983) and WEIDELT (1985). For a one-dimensional structure, the magnetotelluric impedance measured at a finite number of frequencies does not impose bounds on the conductivity at any particular depth, whereas conductivity averages over a finite depth range might be constrained provided that the depth range is chosen properly in relation to the frequency range of the data. Similarly, for the two-dimensional case, spatial conductivity averages might be expected to be well resolved provided that the size of the cross-section (or number of adjacent regularization blocks) for which the average is calculated is sufficiently large.

3. Significance of Data Errors

The assumption of independence of data errors and that data errors follow a Gaussian distribution often precludes achieving a statistically reasonable fit during both one- and two-dimensional inversion of magnetotelluric data. Two explanations for this discrepancy are: a) local deviations for the assumed dimensionality of geoelectric structure exist in the data set and, b) the data errors have been wrongly estimated. The COPROD2 observations are no exception to this rule, and a discussion of these problems can be found in DEGROOT-HEDLIN (1991a). Whatever the reason for this discrepancy, adjustments of data errors are needed in order to take full advantage of the smoothing properties in the Occam's inversion and still achieve a statistically reasonable fit to the observations. As long as these adjustments have the effect of increasing estimates of data errors, the influence on the inversion result is an increase of the smoothness of the model. Thus *these* data error adjustments do not introduce more structure into the final model.

DEGROOT-HEDLIN (1991a) used a minimum error cutoff such that estimated data errors below this error level were set to this particular minimum value. I have scaled the errors by using a procedure described in BELAY and RASMUSSEN (1992) which is based on separate one-dimensional D^+ inversions (PARKER, 1980, 1983) of the E- and H-polarization data at each station. The frequency dependent scaling factors α_i at the ordered frequencies $[f_1, f_2, \ldots, f_i, \ldots, f_N]$ are found from analyzing the data misfit within narrow frequency bands $[f_{i-n_a}, \ldots, f_i, \ldots, f_{i+n_a}]$

$$\alpha_i = \sqrt{\frac{Q_i}{2(2n_a + 1)}} \tag{5}$$

where

$$Q_i = \begin{cases} \sum_{j=i-n_a}^{j=i+n_a} \frac{|\hat{C}_j - C_j|^2}{\sigma^2} & \text{for } i = n_a + 1, \ldots, N - n_a - 1; \\ Q_{n_a+1}, & \text{for } i < n_a + 1; \\ Q_{N-n_a-1}, & \text{for } i > N - n_a - 1. \end{cases} \tag{6}$$

N is the number of complex data, C_i is the measured response function with estimated variance σ_i^2, and $\hat{C}_i$ is the corresponding one-dimensional model response. A value of $n_a = 2$ was used for calculation of the scaling factors but data at all available frequencies were used for the D^+ inversions. For a Gaussian noise distribution and with $\hat{C}_i$ denoting the true solution, the expectation value for Q_i is 2 times the number of complex data used in the summation, i.e. $2(2n_a+1)$, and the scaling factors would be close to 1. Since D^+ inversions gives the best possible one-dimensional fit to the data, scaling of data errors as described above is not expected to result in significant suppression of data features compatible with a one-dimensional structure. A general evaluation of possible suppression of two-dimensional features is at present not possible. However, as discussed later, this does not seem to be of much importance in the particular case of inverting the COPROD2 data set.

4. Modelling

Due to limitations of available computer memc. y, some reduction of the original data set was necessary prior to the inversion. I have included E- and H-polarization apparent resistivity and phase data in the range 0.05 s–910 s at every third of the available frequencies, but the vertical magnetic field data was excluded. In total, 1448 data were used in the inversion.

The width of the regularization blocks in the upper crust was controlled mainly by the station locations such that the vertical block boundaries are defined by the midpoint between two adjacent stations. Refinement of the grid spacing was made at locations which indicated highly conductive structures.

The maximum period for the inversion of determinant data was selected as 30 s. This choice was based on a comparison between the corresponding penetration depth within the upper conductive layer and the width of the regularization blocks at the top of the two-dimensional model. An average resistivity within the upper part of the structure of about 3 Ωm gives a penetration depth of 5 km which is about equal to the largest distance between station positions and the vertical boundary of the corresponding regularization blocks.

An attempt to invert for a normalized root mean square (RMS) misfit value of 1.00, i.e. fit the data to 68% confidence limits, was unsuccessful since the final model gave a minimum RMS value of 1.34.

A possible reason for the problems of obtaining an RMS value of 1.00 or less might be related to the presence of some residual static shifts in the data. The data used in the inversion had been corrected for static shifts, as described in JONES (1988), but the assumptions made when doing these corrections might not have been fully adequate. The initial static shift corrections were based on one-dimensional inversions and the assumption of a uniform resistivity of the second layer throughout the profile. The assumption of a uniform resistivity is a very strong constraint considering the total length of about 400 km of the profile and it seems reasonable to allow for some residual static corrections. An Occam's inversion (DEGROOT-HEDLIN, 1991b) in which invertible residual static shift parameters were introduced with the constraint that the sum of

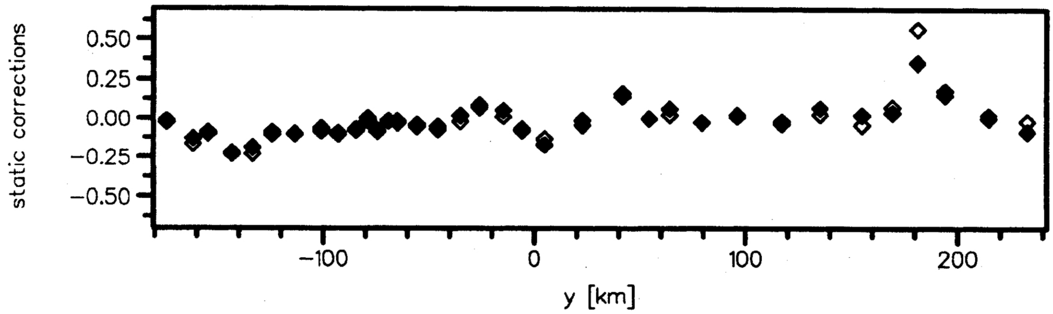

Fig. 1. Residual static shift parameters in $\log_{10}$ units with filled symbol denoting the E-polarization static shift parameters and open symbol denoting the H-polarization static shift parameters. The horizontal coordinate axis refers to distance east of Macoun in Saskatchewan.

TE and TM shift parameters should equal zero, gave an RMS of 1.12. The residual static shift parameters, shown in Fig. 1 in the $\log_{10}$ domain are fairly small with the exception of the station at location +181.2 km which has residual static shift parameters comparable to the maximum initial static shift corrections (see JONES, 1988). The station with maximum residual static shift parameters are located at the TOBE anomaly and the initial static shift corrections might have been influenced by this highly conductive upper crustal structure.

Another possible contribution to the large RMS values when inverting the data with data errors scaled as described above is that separate D^+ inversions of E- and H-polarization data give better RMS values compared to the expectation value of the data residuals based on the true two-dimensional solution. In order to study this possibility, I have calculated the response functions at the 35 sites and frequencies for a model found from a two-dimensional Occam's inversion of the COPROD2 data without any scaling of data errors, added gaussian noise to these computed response functions and finally performed D^+ inversions on these. The RMS values for all D^+ inversions were smaller than the RMS values based on the true two-dimensional model response. Thus, the D^+ models are fitting to noise features within the data. The average of the RMS values for the D^+ inversions was 0.86 which suggests that an additional scaling of the data errors for the COPROD2 data by multiplication with $\frac{1}{0.86} \cong 1.2$ is reasonably if we choose an RMS value of 1.00 as misfit criteria in the two-dimensional Occam's inversion. However, the RMS values of 1.12 and 1.34 for the previous two-dimensional models, with and without residual static shift corrections respectively, imply that residual static shifts corrections are needed in order to obtain an RMS of 1.00 with this additional scaling factor.

The normalized data residuals r_i defined as

$$r_i = \frac{d_i - \hat{d}_i}{\sigma_i} \tag{7}$$

where d_i and $\hat{d}_i$ are the measured and model response respectively with associated data error σ_i at data number i are shown in Fig. 2 for the final model. The data residuals are shown for all 29 available frequencies within the frequency range covered by the 11 frequencies used in the inversion. The RMS value based on data from the 11 frequencies used in the inversion is 1.00 whereas the RMS value found from a forward model calculation for all 29 frequencies is 1.53. Some trends are evident in the data residuals. At stations close to the NACP anomaly (stations

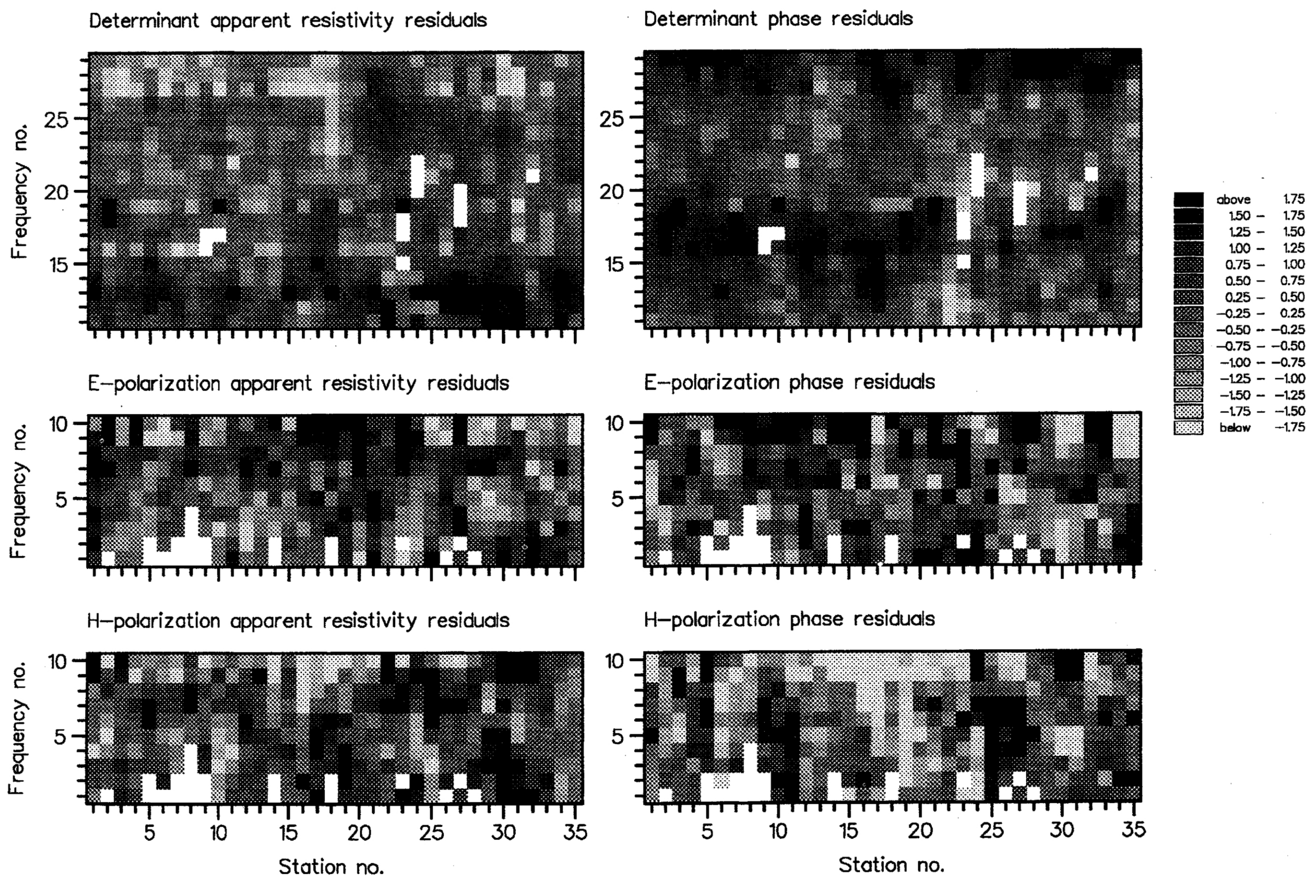

Fig. 2. Normalized data residuals. Station numbering 1 to 35 is from west to east. Frequency numbering 1 to 29 is from low frequency to high frequency. Only data with frequency numbers 1, 2, 5, 8, 11, 14, 17, 20, 23, 26 and 29 were used in the inversion and data which appear as unshaded regions in the diagrams were omitted in the calculations.

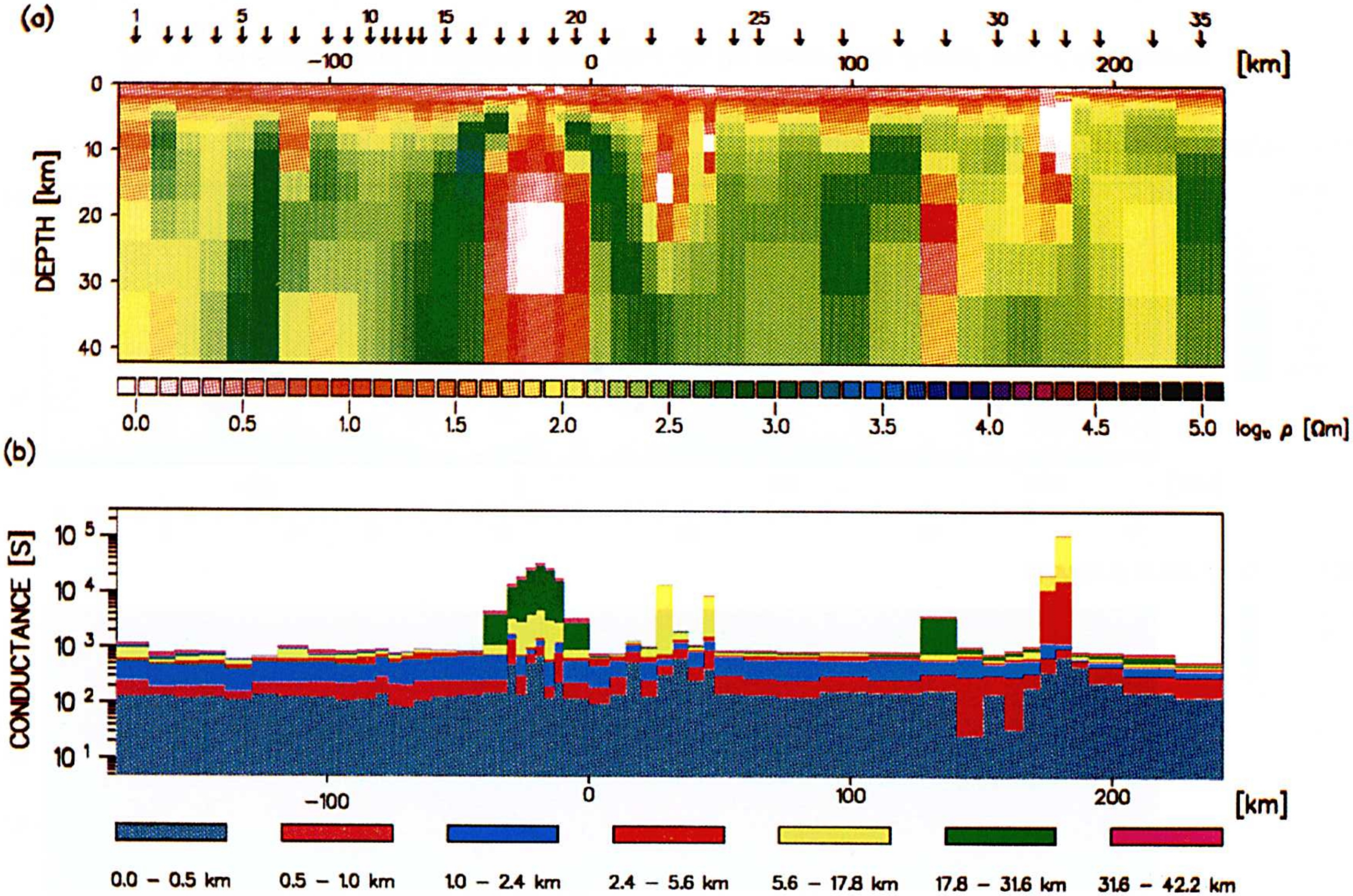

Fig. 3. (a) The two-dimensional model with station locations marked with vertical arrows. The horizontal coordinate axis refers to distance west of Macoun in Saskatchewan. (b) Vertically integrated conductivity (conductance) displayed as cumulative conductance functions for various depth levels.

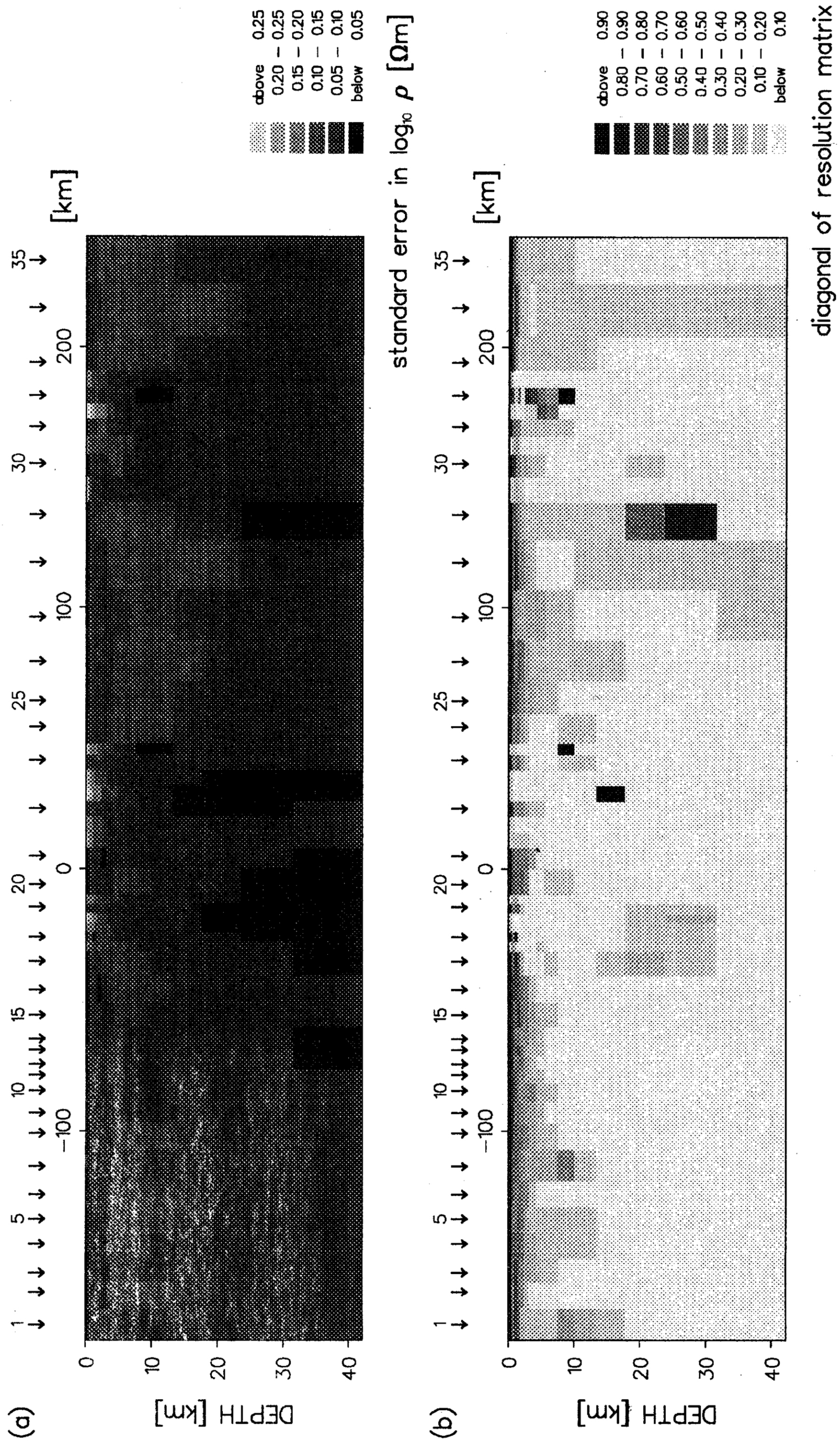

Fig. 4. (a) Standard error in resistivity ($\log_{10}$ units) and (b) corresponding diagonal term of the resolution matrix.

13–23) large negative values of the H-polarization phase residuals can be observed, which might indicate the presence of significant three-dimensional structures. Although no vertical magnetic data were included in the inversion, a comparison between measured and model response tipper functions shows a fairly good agreement between these. Only the station at location +54.4 km show a systematic deviation between measured and model response tipper functions.

The final model is shown in Fig. 3a. Below the conductive Williston sedimentary basin, five highly conductive regions (at horizontal locations −20, +30, +45, +135 and +180 km) are found which are separated from each other by medium to high resistivity rocks. A general result from one-dimensional inversion of magnetotelluric data is that the resistivities often are rather poorly resolved whereas the integrated conductivity is much better resolved. Thus, it might be an advantage to visualize also the two-dimensional model in terms of vertically-integrated conductivity. This quantity is displayed in Fig. 3b for various depth levels. The structures with high conductivity can be seen as peaks in the integrated conductivity of more than an order of magnitude above the normal level of approximately 1,000 S for the entire crust. The major contribution to this normal level is from within the upper 5 km of the crust, i.e. the Williston basin. The most conductive rocks are found for the TOBE anomaly at location +180 km for which the integrated conductivity exceeds 100,000 S for the upper and middle crust. The TOBE structure is a fairly narrow upper crustal structure and does not seem connected to the conductive lower crustal structure about 50 km to the west. Also the NACP anomaly at location −20 km shows extreme values of the integrated conductivity with more than 30,000 S for the entire crust. The two conductive upper and middle crustal structures to the east at locations +30 km and +45 km are separated from the main NACP structure by more resistive rocks and the integrated conductivity within the region separating these structures is close to the normal level of 1,000 S.

The variances and corresponding diagonal terms of the resolution matrix are an integral part of the model and they should be used in the interpretation of the final model. These quantities are shown in Figs. 4a and 4b. In general, the diagonal of the resolution matrix is dominated by fairly low values and high values are found only within the upper part of the two-dimensional model and at a few isolated regions. Low values of the resolution matrix elements must be expected since overparameterization is attempted in order to obtain smooth models. As discussed previously, the low values of the diagonal terms of the resolution matrix indicate that the size of the regularization blocks in most cases are too small to allow the average conductivity within the blocks to be well resolved.

The parameters with corresponding high values of the resolution matrix coincide with low parameter values (highly conductive) and, in some cases, low standard error. However, highly conductive parameter values are not necessarily associated with high resolution. The dependence on the size of the regularization prisms is clearly seen in the somewhat higher resolution for the conductive structure at location +130 km as compared to the resolution for the NACP structure for which a smaller size of the prisms was used.

The highly conductive structures associated with the NACP anomaly are separated by resistive blocks with high standard deviation and rather low resolution. However, the fact that these resistive blocks are present in the model indicates that these are necessary to explain the data since Occam's inversions are supposed to suppress unnecessary structure.

Inspection of variance and resolution calculations indicate that a conductive structure (not shown in the figures) which are indicated in the model at a depth between 42 km and 75 km at location −125 km to −100 km might be well resolved. The structure (two prisms) has a vertically integrated conductivity of 1,000 S and the diagonal elements of the resolution matrix are 0.7 and 0.4 and the standard errors are less than $0.1 \log_{10}$ units.

5. Summary and Conclusion

The COPROD2 data set is clearly no exception to the general experience of magnetotelluric data interpretation in that it is almost impossible to find a data set where one or two-dimensional models can be considered acceptable with a reasonable certainty from a statistical point of view. Progress in obtaining more realistic descriptions of the estimated data errors has been made recently (see e.g. CHAVE and THOMSON, 1989) which might lead to an elimination of improper description of data errors and reduce the problem of finding acceptable models to the limitations imposed by the numerical modelling schemes. The extent to which these problems in the interpretation of the COPROD2 data are caused by poorly estimated data errors, or due to the presence of three-dimensional structures, is difficult to evaluate. Thus, unless the possibility of obtaining a two-dimensional model is rejected, a scaling of data errors is necessary in order to make use of the techniques developed for two-dimensional inversion.

Modification of estimated data errors is certainly not a very satisfactory procedure because it involves a process in which the risk of suppressing important data features is attempted, balanced against the risk of fitting to noise in the data. Justification of the method for scaling of data errors as presented in this paper is obviously related to the question of how well the E- and H-polarization responses can be approximated by the D^+ models.

In order to take full advantage of the smoothing properties of the two-dimensional Occam's inversion, it is of general importance that a sufficiently fine regularization mesh is used. Due to limitations on computer memory, this requirement can be difficult to accomplish when the data cover a broad frequency range. Especially, it becomes difficult to have sufficiently narrow regularization blocks in which case the model responses at high frequencies resemble locally one-dimensional responses. An inversion for which determinant data are used for the high frequency data simultaneously with the usual E- and H-polarization data at the long periods is suggested to extend the frequency range in the inversion.

Modelling of the COPROD2 data seems to indicate that some residual static corrections are required in addition to the static corrections presented by JONES (1988). However, the residual static corrections are fairly small for most of the stations and the differences between resistivities for models derived with and without residual static corrections are smaller than, or comparable to, the estimated standard errors on the resistivities. The presence of spatially separated bodies with high conductivity below the NACP anomaly is required by the data.

The main emphasis in this paper has been on some technical aspects related to two-dimensional inversion of magnetotelluric data. No attempts have been made to enter a discussion on the geological interpretation of the model. For this I refer to the paper of JONES (1993) and references therein.

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