P-07-88

Oskarshamn site investigation

Comparison between measurements of Total Dissolved Solids and Transient Electromagnetic Soundings in the regional model area

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April 2007

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ISSN 1651-4416 SKB P-07-88

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Keywords: TEM, TDS, Fluid resistivity, Saline groundwater, Ground geophysics.

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Abstract

Data on total dissolved solids (TDS) and fracture specific fluid resistivity have been compiled in a voxel model describing TDS to a depth of 1,000 metres in the Laxemar-Simpevarp area. This model has been compared with layered earth models from transient electromagnetic measurements (TEM), which have been performed over the regional model area of the Oskarhamn site investigation. The TEM models describe the ground as a simple two-layer model with an electrically conductive lower layer, corresponding to an interface of a more intensly saline water body. The depth to the layer interface has been compared with TDS-data where the two types of data have been collected close to each other. It was found that the TEM layer interface corresponded to TDS in the range 4,000 to 10,000 mg/l. An isosurface of the voxel model corresponding to TDS of 4,000 mg/l was extrapolated to the west of the Laxemar area. It was found that this surface coincided fairly well with the layer interfaces of TEM models in the western part of the regional model area that is not sampled by deep boreholes and hence TDS-data from depth.

Calulations made on the basis of empirical models/relationships and measurements on samples show that the bulk resistivity of rock is dominated by surface conduction effects at fluid resistivities above around 1 Ω m. This has the effect that the bulk resistivity is only weakly dependent on TDS in near-surface (low-salinity) rock in the Simpevarp area. In more saline environments, e.g. at greater depth in the investigated area, the bulk resistivity becomes more or less directly proportional to fluid resistivity and is thus more sensitive to variations in TDS. It is therefore reasonable to envisage that the depth to conductive rock, as experienced by the TEM soundings, correspond roughly to the depth where surface conduction becomes subordinate to regular electrolytic conduction in the rock pores. This depth will be a function of the porosity, grain size, texture and mineral composition of the rock. However, the geology of at least the western and central parts of the regional model area is dominated by granitoids of the Trans-Scandinavian Igneous belt and the factors above are expected to be fairly uniform.

Sammanfattning

Mätdata för lösta fasta ämnen (TDS) och elektrisk konduktivitet för vatten från sprickor har sammanställts till en voxel-modell som beskriver TDS till ett djup av 1 000 meter i Laxemar-Simpevarps-området. Denna modell har jämförts med modeller av lagrad jord från transienta elektromagnetiska mätningar (TEM), vilka har utförts över det regionala modellområdet för Oskarhamns platsundersökning. TEM-modellerna beskriver marken med en enkel tvålager-modell med ett elektriskt konduktivt undre lager. Djupet till lagergränsen har jämförts med TDS-data i de fall där bägge typerna av mätningar har gjorts i närheten av varandra. Gränsytan i TEM-modellerna svarade i dessa fall mot värden på TDS i intervallet 4 000 till 10 000 mg/l. En iso-yta från voxelmodellen svarande mot ett TDS-värde på 4 000 mg/l extrapolerades västerut från Laxemarområdet. Denna yta överenstämde väl med lagergränserna för de TEM-modeller som ligger i västra delen av det regionala modellområdet där djupa borrhål och därmed TDS-data från djupet saknas.

Empiriska beräkningar och mätningar på bergprover visar att bulkresistiviteten för berg domineras av ytkonduktivitet för vätskeresistiviteter över ca 1 Ω m. Detta har som effekt att bulkresistiviteten är endast svagt beroende av TDS i ytnära (låg salinitet) berg i Oskarshamnsområdet. I mer salina miljöer, t ex på större djup, blir bulkresistiviteten mer eller mindre linjärt beroende av vätskeresistiviteten och därmed känslig för variationer i TDS. Det är därför rimligt att anta att djupet till lågresistivt berg, som det upplevs av TEM-sonderingarna, svarar ungefär mot det djup där vanlig elektrolytisk ledning börjar dominera över ytkonduktivitet. Detta djup är en funktion av porositet, kornstorlek, textur, och mineralsammansättning hos berggrunden. Geologin i åtminstone den västra och centrala delen av det regionala modellområdet domineras av Smålandsgranit och faktorerna ovan torde vara relativt enhetliga.

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1 Introduction

This document reports the results of the compilation of information from measurements of total dissolved solids in ground water, fluid resistivity in boreholes and models constricted by transient electromagnetic soundings. The work was carried out in accordance with activity plan AP PS 400-05-066. In Table 1-1 the controlling documents for performing this activity are listed. Both activity plan and method descriptions are SKB's internal controlling documents.

Seven TEM soundings were performed in the western part of the regional model area in Simpevarp during September 2005 /1/. Furthermore, five TEM soundings previously performed in a method test project /2, 3/ have been included, although the data quality from the soundings performed within the method test in the Laxemar area were quite poor. The soundings have resulted in two-layer models with an electrically conductive lower layer at a depth below surface ranging from 500 metres in the eastern Laxemar area to almost 1,600 metres in the westernmost part of the regional model area. The positions of the TEM soundings and the depths to the conducting layer in the models are shown in Figure 1-1.

The conductive substratum was interpreted to be due to saline groundwater at depth. Salinity of the groundwater is known to increase with depth from measurements of TDS and fluid resistivity in boreholes. However, TDS increases gradually and not abruptly as in the TEM models. The TEM soundings do not have the resolving power to produce a reliable model with gradually decreasing resistivity with depth due to salinity. The purpose of the present project is therefore to try to correlate the TEM models with TDS data from boreholes to find out, approximately, the TDS-level corresponding to TEM model layer interfaces.

The work gives input parameters to the regional geohydrological model of the Oskarshamn site investigation.

Table 1-1.	Controlling	documents	for the	performance	of the	activity.
					•••••	

Activity plan	Number	Version
Transient elektromagnetisk sondering i Laxemar och regional omgivning	AP PS 400-05-066	1.0



Figure 1-1. Map showing the position of cable loop transmitters used for the TEM soundings 2005 (black polygons labelled 1 to 7) and for the method tests (green polygons labelled A to E). The depths (in metres) to conductive rock in the TEM models are indicated for each transmitter loop.

2 Objective and scope

The presence of saline ground-water at large depth might influence the regional ground-water flow and is hence an important parameter in the assessment of the geohydrological situation in the site investigation area. The depth to, and the nature of the transition to saline groundwater at depth is investigated by sampling and logging in deep boreholes in the candidate area. There are however no deep boreholes in the regional surroundings to the west of the Laxemar subarea. The depth to saline water is also assumed to increase with distance from the coast-line which makes borehole investigations difficult away from the coast. The purpose of this work is to compare results from deep TEM soundings with measurements of TDS in boreholes. This might give an idea about the approximate TDS-level that corresponds to electrically conductive rock in the TEM models. That information will aid the conceptual model development and construction of a regional groundwater model outside the area covered by deep boreholes. A supra-regional flow model have already been made /4/ but further large-scale flow modelling will be made and the data provided in this report will be useful for that modelling.

3 Equipment

3.1 Description of equipment and interpretation tools

The presented work is a pure desktop study. The software listed below was used.

Modelling of TEM data:

• EM Vision v 2.1 (Encom Technology).

Creation of voxel model and 3D-visualization:

- Profile Analyst v 6.0 (Encom Technology).
- Voxler v 1.0 (Golden Software).

Preparation of maps:

- MapInfo Professional v 7.8 (MapInfo Corp.).
- Discover v 8.0 (Encom Technology).
- Surfer v 8.0 (Golden Software).
- ArcGIS 9 (ESRI).

Calculations, data processing and creation of graphs:

- MathCAD 2001i Professional (Mathsoft Engineering & Education Inc.).
- Grapher v 6.0 (Golden Software).
- MS Excel (Microsoft Corporation).

4 Execution and results

4.1 General

TEM soundings of good quality have not been possible to perform in the Laxemar-Simpevarp local model area due to interference from the major electric power lines running through the area from the power plants at Simpevarp. On the other hand, deep boreholes on the mainland are located in the Laxemar subarea only. This means that coincident high quality information about TDS and TEM is not available for comparisons anywhere in the Simpevarp area. Three TEM soundings from a method test /2, 3/ were made in the area covered by boreholes but only one of these was of reasonably good quality. The layered models of these soundings have however been compared with TDS- and fluid resistivity data from nearby boreholes. Two TEM soundings of good quality were made just west of the Laxemar subarea. These are not directly comparable to TDS-data in boreholes since the distance to such holes is too large. The TDS-data have therefore been compiled into a voxel model together with fluid resistivity data and this model has been extrapolated to the TEM sounding locations.

4.2 Compilation of TDS data

During the site investigations, water samples are collected in boreholes during and after drilling with different methods. The chemical composition and, generally, the electrical conductivity are analyzed. Depending on the purpose with the samples, the number of analyzed chemical components varies. From these samples the TDS can be estimated from the sum of ions or a mathematical relation between electrical conductivity and TDS. The latter based on a large number of samples taken before and during construction of the nearby Äspö Hard Rock Laboratory, in boreholes on Äspö island and surrounding areas /5/, see below.

$$WS = C \frac{4.67}{0.741}$$

WS = Water salinity (mg/L), C = Electrical conductivity at 25°C (mS/m).

In this study samples considered representative (i.e. small contents of drilling fluid, in the database represented as; representative and less representative samples) in the hydrogeochemical model vesion Laxemar 2.1 have been used /6/. Generally TDS based on sum of ions have been used, but in a few cases TDS(El.Cond) have been used.

The TDS-data for boreholes in the Laxemar subarea are plotted versus elevation (based on midpoint of the sampled section) in Figure 4-1. A generally increasing trend with depth can be seen. The TDS-data also show a quite large dynamic range, covering values of almost three orders of magnitude. Data from holes at Laxemar (KLX01, 02, 03, 04, 05, 06, 08 and percussion holes), Simpevarp (KSH01A, 02, 03 and percussion holes), Ävrö (KAV01, 04A and percussion holes) and Äspö (KAS02, 03, 04, 06 and percussion holes) were included in the model together with some samples of sea water and near surface groundwater.



Figure 4-1. Measured TDS versus elevation from boreholes in the Laxemar subarea.

4.3 Compilation of fluid resistivity data

Measurements of fluid resistivity give indirect information about TDS. The resistivity of the borehole fluid is routinely logged together with other geophysical logs. These measurements are however performed quite shortly after the completion of the drilling and the borehole fluid is therefore mixed with flushing water during the measurements. The boreholes have also been logged with the Posiva Flow-log (PFL) / 7, 8, 9, 10, 11, 12, 13, 14, 15/. The fluid resistivity is then measured during pumping and more reliable fluid resistivity data can then be acquired. The resistivity of the fluid extracted from single fractures is also measured during PFL-logging. The resistivity values are then allowed to settle during a period of pumping and the final values can be regarded as quite reliable and unaffected by flushing water or water from other depths in the hole.

Only fracture specific fluid resistivity data have been used in the following modelling of data. Data from boreholes KLX02, 03, 04, 05, 06, 07A, 08, 10 and KSH02) were included. The resistivity was corrected for temperature. TDS was thereafter estimated with the help of the formula below from Crain's Petrophysical Handbook:

$$WS = \frac{400000}{(1.8t + 32)^{0.88} / \rho}$$

WS = Water salinity (mg/L NaCl), t = temperature (°C) and ρ = resistivity (Ω m).

The calculated value does not take into account the actual ionic composition of the water. The error introduced in using the above formula as an estimate for TDS is however small compared to other uncertainties in this study. The estimated TDS from fracture specific resistivity measurements can be seen in Figure 4-2. The overall pattern is quite similar to the TDS-values in Figure 4-1. Values from KSH02 are generally higher than for the other holes, reflecting the near-shore position on the Simpevarp peninsula of KSH02.

4.4 Creation of voxel model

The data described in Sections 4.3 and 4.4 were merged and entered into the program Voxler (Golden Software). The input data are displayed in a 3D-plot in Figure 4-3. A three-dimensional regular grid (voxel model) was interpolated with simple inverse distance weighting. The grid node spacing was 100 m in the horizontal directions and 40 m in the vertical direction TDS-values increase rapidly with depth whereas lateral variations are gentler. A vertical:horizontal anisotropy of 1:8.75 was therefore introduced in the interpolation weighting. Finally, a gentle smoothing was performed on the model. The resulting model is presented in Figure 4-4. Iso-surfaces can be generated from voxel models. Figure 4-5 shows such surfaces corresponding to TDS-values of 2,510, 6,310 and 15,850 mg/L. The surfaces are fairly steep close to the coast-line, indicating quite saline water at moderate depth in the eastern part of the model area.



Figure 4-2. Estimated TDS versus elevation based on fracture specific fluid resistivity values from PFL-logging.



Figure 4-3. 3D-plot showing the input data for the creation of a voxel model. The symbols represents measured TDS-values or TDS estimated from fracture specific electric conductivity measurements in boreholes. The vertical scale is exaggerated. View from the southwest.



Figure 4-4. Voxel model showing logarithm of TDS in the Laxemar-Simpevarp area. Hydrography and roads are also shown. The vertical scale is exaggerated. View from the southwest.



Figure 4-5. Iso-surfaces generated from the voxel model in Figure 4-4. The surfaces correspond to TDS-values of 2,510, 6,310 and 15,850 mg/L respectively. Traces of some of the deep boreholes are shown in grey (L2 = KLX02 etc). Hydrography and roads are also shown. The vertical scale is exaggerated.

4.5 Comparison with TEM models

Figure 4-6 shows the position of TEM transmitter loops and the lateral extent of the TDS voxel model. Three soundings (loops A, B and C) were made in the method test /2, 3/ within the area covered by the model. However, due to the noise introduced by power lines in this area, the data quality is not very good for these loops, especially loops B and C. Also, these data were acquired in a way that does not meet the standards of the SKB method description for TEM soundings. A direct comparison of the results from these soundings and the TDS model should therefore be treated with some caution.

TDS-values were extracted from the voxel model for positions corresponding to the centres of loop A, B and C and the depths indicated in Figure 4-6 for those loops. The results are listed in Table 4-1. These results indicate that the TEM model interface might correspond to TDS-values ranging from approximately 4,000 to 11,000 mg/L.

Table 4-1. TDS-values extracted from voxel-model at positions corresponding to TEM layer interfaces (see Figure 4-5).

Loop	TDS at TEM model layer interface (mg/	L)
A	3,974	
В	11,104	
С	9,350	



Figure 4-6. Map showing the position of cable loop transmitters used for the TEM soundings 2005 (black polygons labelled 1 to 7) and for the method tests (green polygons labelled A to E). The depths to conductive rock in the TEM models are indicated for each transmitter loop. The blue, labelled contours represent a polynomial surface fitted to the depth to conductive rock estimated from soundings 1 to 7. The colour-scale map shows log(TDS) at a depth of 680 metres according to the voxel model.

Six of the TEM models for loops to the west of the area covered by the voxel model (loops 1–5 and 7) relies on data of higher quality than the ones listed in Table 4-1. However, since these measurements were performed outside the area covered by the voxel model, a direct comparison is not possible. Planar surfaces were interactively fitted to the western part of iso-surfaces generated from the voxel model of the kind shown in Figure 4-5. The general pattern is that such planes dip approximately 4.5° with an azimuth of 195°, i.e. the dip is towards WNW. The log(TDS)-value corresponding to such a plane that approximately fits the TEM-model interfaces of loops 1, 2 and 3 (Figure 4-5) is 3.6 (\approx 4,000 mg/L). The dip of the plane is also consistent with the polynomial surface that has been fitted to the TEM-model interfaces of loops 1 to 7 (Figure 4-6) /1/. The approximate dip of that polynomial surface was 4.1° with an azimuth of ~ 200°. The orientation of iso-surfaces of the voxel model and the polynomial approximation of TEM models is thus more or less the same. A reasonable estimate for the effective TDS-value that corresponds to a TEM-model interface is thus around 4,000 mg/L. For reference, the contours of the polynomial surface and the TEM loops are shown together with some features in the structural part of the Site Descriptive Model version 2.1 in Figure 4-7.

The polynomial surface fitted to layer interfaces in TEM models /1/ is shown in a 3D plot together with an iso-surface of the voxel model that can be seen as an approximate continuation of the polynomial surface (Figure 4-8). The TDS-value corresponding to the iso-surface is \approx 4,000 mg/L.

(The equation of the polynomial surface is: $depth = -12690582.972022 + 2.012643215325 \cdot RT90North + 8.1183435464148 \cdot RT90East -1.2875675380181E-006 \cdot RT90North \cdot RT90North).$



Figure 4-7. Same as Figure 4-6 (without roads) with the addition of some features in the structural part of the Site Descriptive Model version 2.1.



Figure 4-8. 3D-view from SSE showing a TDS iso-surface ($\approx 4,000 \text{ mg/L}$) from the voxel model to the right. A polynomial surface fitted to TEM model layer interfaces is shown to the left. Traces of some of the deep boreholes are shown in grey (L2 = KLX02 etc). The vertical scale is exaggerated.

4.6 Construction of resistivity model from TDS data

An attempt to construct a vertical resistivity column out of TDS-data is presented below. There is no way to do this in an exact manner. Rock properties like texture, porosity and fracture frequency varies in the rock volume. Also, there is not enough experimental data to describe the variation of resistivity as a function of salinity, temperature and pressure. The discussion below should therefore only be regarded as a conceptual attempt to see if the the TEM sounding data are compatible with modelled TDS-variations with depth in the subLaxemar area.

The resistivity of most rock forming minerals is so high that these minerals can be regarded as perfect insulators at normal temperatures. The resistivity completely depends upon current paths in water-filled pores of the rock. A common way to describe the relation between porosity, fluid resistivity and the bulk resistivity of the rock is through the empirical Archie's law /16/:

 $\sigma = \sigma_w \cdot \phi^m$

Where

(Equation 1)

- σ = bulk conductivity (reciprocal to resistivity)
- σ_w = conductivity of pore fluid
- ϕ = fraction of pore space
- m = empirical constant that describes the effective length of current paths and their effective cross-sectional area

Archie's law has been shown to work well for porous rock, e.g. moderately compacted sedimentary rocks. However, a phenomenon called surface conductivity occurs at the interface between the pore fluid and the solid minerals. The surface charge of the minerals (generally negative) attracts ions of opposite charge and a thin electric double layer is formed. The electric resistivity within this layer is considerably less than in the rest of the pore fluid. This has a very large effect on the resistivity of low porosity, crystalline rocks especially in low-saline environments. Fine-grained rocks containing e.g. mica, chlorite and similar minerals therefore tend to have lower resistivity than coarser rock with the same porosity. The surface conductivity is not as dependent upon ion concentration as the conductivity of the fluid. The normal electrolytic conductivity is dependent upon the effective cross-sectional area of current paths and their average length (described by *m* above). Contrary to this, surface conductivity depends upon the effective surface of the pores and the average length of such connected surfaces. It is therefore very difficult to express surface conductivity and its dependence on fluid resistivity with a simple empirical formula. However, only for the purpose of testing the compatibility of the TDS-model with results from TEM-soundings the following modified version of Archie's law is proposed:

$$\sigma = \sigma_w \cdot \phi^m + a \cdot (\sigma_w + b)^k \cdot \phi^n$$

(Equation 2)

Where the second term represents surface conductivity. A fairly good agreement with petrophysical data /17, 18, 19, 20/ is achieved if the empirical constants *m*, *a*, *b*, *k* and *n* are set to 1.85, 0.08, 1.5, 0.8 and 1.5 respectively. It should however be noted that petrophysical measurements have been performed for just a few values of σ_w .

Figure 4-9 shows the conductivity calculated of both terms in Equation 2 as a function of fluid resistivity. According to this, surface conduction dominates for fluid resistivities above around 1 Ω m whereas normal electrolytic conduction dominates in more saline environments. This has the consequence that the resistivity of near-surface rock in low salinity environments is only moderately dependent upon fluid resistivity. At deeper levels, where the resistivity of the pore fluid is less than around 1 Ω m, it is expected that the bulk resistivity of the rock is more or less linearly dependent of the fluid resistivity and hence sensitive to increased levels of TDS.



Figure 4-9. Surface conductivity and electrolytic conductivity (Archie's law) as a function of fluid resistivity calculated with Equation 2. The porosity was set to 1.1%. This is higher than the normal intra-granular porosity for the area but also takes into account water-filled fractures.

4.7 Calculation of synthetic TEM response

The TDS voxel model was extrapolated to the position of loop 2 in Figure 4-6 using the dip and azimuth of a planar surface described in Section 4-5. This resulted in a vertical resistivity column of Figure 4-10 when the Equation 2 in Section 4.6 was used to convert TDS to resistivity. It is not possible to calculate the response to the TEM system for such a gently varying resistivity model. Instead, a model corresponding to the dashed line in Figure 4-10 was used as an approximation. The synthetic response to this model for the instrument setup of loop 2 can be seen in Figure 4-11 together with field data. The correspondence is quite good, at least for channels with low noise levels in the field data.



Figure 4-10. The solid line shows resistivity versus depth for the rock beneath TEM loop 2 (Figure 4-6). TDS-values were extrapolated to this position from the voxel model and converted to resistivity with Equation 2. The dashed line shows a layered model used to calculate a synthetic TEM response for TEM loop 2.



Figure 4-11. The solid line shows the TEM response of the layered model in Figure 4-9 to the instrument setup of TEM loop 2. The symbols represent the corresponding field data.Data away from the curve represents noisy channels.

5 Discussion and conclusions

The comparison between TEM sounding results and TDS measurements in boreholes is not straight-forward. A number of factors must be considered:

- TEM sounding data of high quality are only available to the west of the Laxemar subarea where no TDS data from deep boreholes are available
- The TEM soundings cannot resolve the gradual increase in TDS that we see in the boreholes. Instead, the TEM soundings result in two-layer models with a sharp resistivity gradient at the layer interface.
- The depth to a conductive sub-stratum in the TEM models has an error limit of around ± 100 metres for the stations with good data.
- The dependence between bulk resistivity of a rock mass and TDS is complex. The texture, grain size, fracture frequency, alteration and temperature influence this relationship.

The resistivity of crystalline rock is only weakly dependent on the resistivity of the pore water fluid as long as surface conductivity dominates the electric conduction. It is known from petrophysical measurements that this is the case in fresh water conditions. Borehole resistivity logging in KLX01 also supports the assumption that the bulk resistivity of the rock is fairly independent of depth for the uppermost few hundred metres of the hole, in spite of a gradual increase in TDS. Unfortunately the resistivity loggings of the new boreholes in the area have been performed just shortly after the completion of the boring, when the borehole fluid has not been in equilibrium with the fluid in the surrounding rock. It is therefore difficult to correctly estimate the rock resistivity from the logging data of those holes.

At higher salinity, volume electrolytic conduction dominates over surface conduction. This means that the bulk resistivity of rock is more or less linearly dependent on pore fluid resistivity in high salinity environments. This has the effect that the resistivity of the rock is expected to decrease fairly quickly below a certain depth.

The best resolved model parameter in electro-magnetic soundings is the depth to a conductive layer. It is therefore reasonable to assume that the TEM sounding models approximately will indicate the decrease in resistivity that will result from the fact that volume electrolytic conduction dominates below some depth. Since the geological environment in the Simpevarp area is fairly uniform we can also assume that this will correspond to roughly the same TDS value in different parts of the area. Unfortunately, the transition process from surface conduction to volume electrolytic conduction is poorly supported by borehole logging data and laboratory petrophysical data. From petrophysical data we know that surface conduction dominates at TDS-values below 600 mg/L (pore-fluid resistivity $\approx 10 \ \Omega m$). Petrophysical data also indicate that volume electrolytic conduction has great influence at TDS-values above around 18,000 mg/L.

The extrapolation of the voxel TDS model to the TEM sounding models to the west and the extrapolation of TEM modelling results to the deep boreholes in the east give similar results when TEM model interfaces and TDS data are compared. In both cases we end up with a TDS value of around 4,000 mg/L corresponding to the TEM model interface. This value is compatible with, but poorly constrained by the petrophysical data. The indicated TDS-value corresponds to a fluid resistivity of around 1.8 Ω m (depending on temperature).

The TDS-value that has been indicated to correspond to the TEM layer interface has fairly wide error limits. However, when compared to the very large dynamic range of TDS-values that has been recorded in the boreholes, the uncertainty does not seem great. Also, the general dip of the salinity gradient is consistent between the TEM models and the TDS voxel model. A gently increased depth to saline groundwater with increasing distance from the coast-line is thus supported by both types of data in a similar way.

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