



**SKB**

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**TECHNICAL  
REPORT**

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**Description of groundwater chemical  
data in the SKB database GEOTAB  
prior to 1990**

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April 1992

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DESCRIPTION OF GROUNDWATER CHEMICAL DATA IN THE SKB  
DATABASE GEOTAB PRIOR TO 1990

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April 1992

This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

Information on SKB technical reports from 1977-1978 (TR 121), 1979 (TR 79-28), 1980 (TR 80-26), 1981 (TR 81-17), 1982 (TR 82-28), 1983 (TR 83-77), 1984 (TR 85-01), 1985 (TR 85-20), 1986 (TR 86-31), 1987 (TR 87-33), 1988 (TR 88-32), 1989 (TR 89-40) and 1990 (TR 90-46) is available through SKB.

**Description of groundwater chemical data  
in the SKB database GEOTAB  
Prior to 1990**

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## INTRODUCTION

Groundwater chemical investigations are one of the research areas in SKB's research and development program for the final disposal of spent nuclear fuel.

Since 1985 a specially designed integrated system consisting of a mobile field laboratory and a down-hole measuring probe is used for the chemical characterization of deep groundwater. The groundwater chemical analyses are performed in the field laboratory and  $E_h$  and pH are measured in situ by the down-hole probe.

The chemical data obtained from the specific site investigations are stored in the GEOTAB database on the VAX computer at SKB.

The description of chemical data handling given in this paper concerns the period after 1985.

### 1.1. Historical overview

Prior to 1983: The mobile field laboratory was not yet constructed. The analytical work was done by consulting laboratories. Two or three different laboratories were engaged. In this way, independent analyses were obtained. All field measurements and laboratory results were registered manually in a VAX computer using the database management system DATATRIEVE (DTR). The GEOTAB database was not planned yet, and the only purpose of the registration was to calculate the physical parameters from electrode readings and to simplify the handling of data. The data tables from this period are now revised and included in GEOTAB.

may - december 1984: The performance of the mobile field laboratory was tested. The measured electrode readings were registered by "CHEMMAC", a forerunner to the computer in the field laboratory. The registrations were copied to floppy disks and transferred to DTR for further treatment. The chemical analyses were registered manually in DTR together with control analyses from an independent laboratory.

may 1985 and forward: All the measurements and analyses in the mobile field laboratory were registered by a computer in the field laboratory. The computer also calculated the concentrations from registered readings, dilutions, calibration factors, control standards etc. The data files from the field laboratory were copied to floppy disks and sent to IVL, a consulting company for environmental research, where the files were transferred to DTR.

1987 and forward: The final reduced amount of measurements and analytical data are transferred to the database GEOTAB within one month after the termination of the measurements for a borehole section. The complete DTR files are archived on tape at SKB.

## 1.2. Overview of data flow

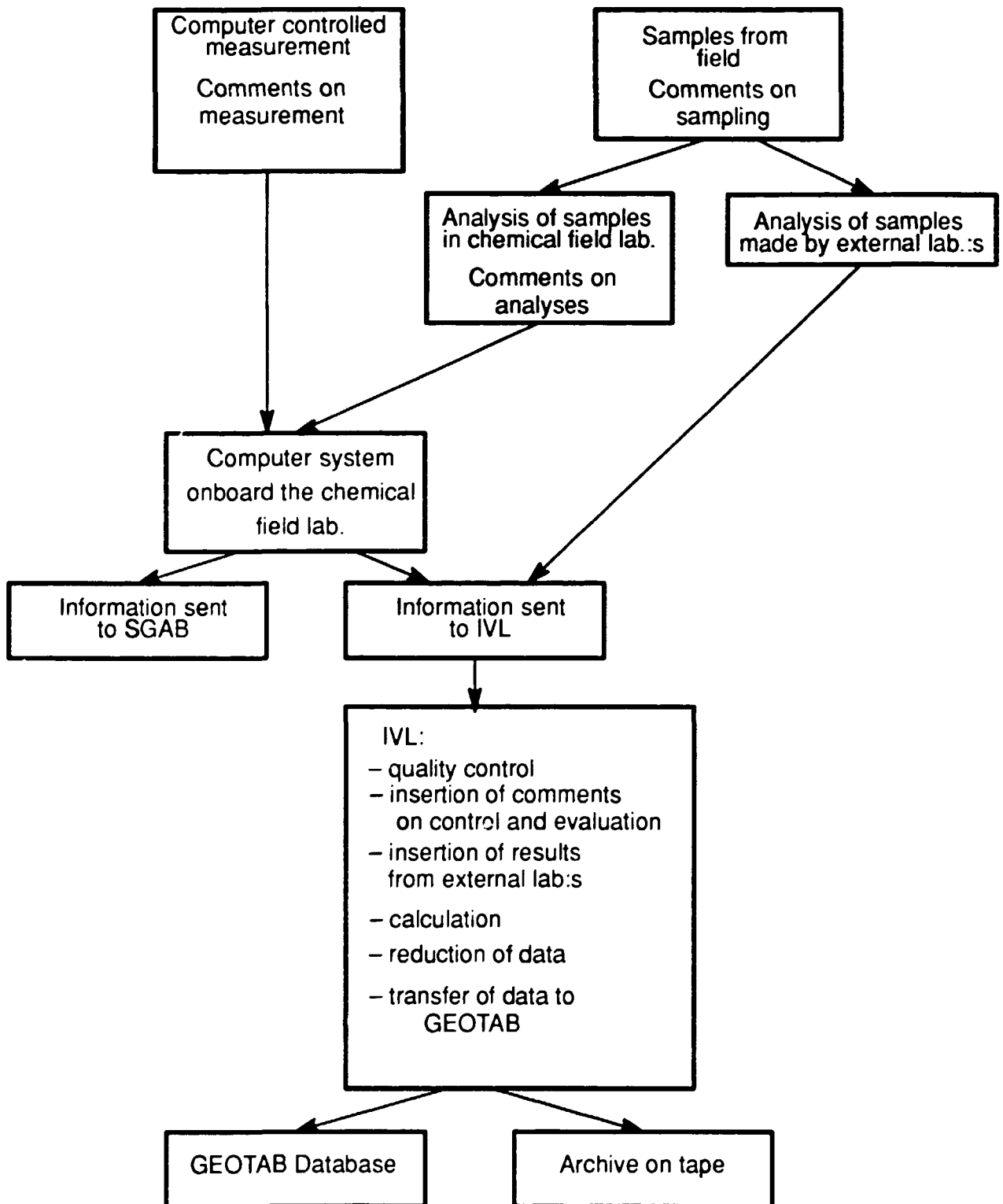


Figure 1.1. A schematic overview of the flow of data from the source to the GEOTAB database or to archives on tape.

The data obtained from chemical investigations of deep groundwater can be divided into three types:

- Results from computer controlled on-line measurements in the mobile field laboratory
- Chemical analyses in the mobile field laboratory
- Analyses performed by external laboratories

The treatment of primary data, from the field laboratory and external laboratories, ie. calculations, quality control and reduction of the data, as well as the final transfer to the database GEOTAB, is performed by IVL. The chemical data group in GEOTAB is called CHEMICAL. It contains the final checked and reduced data.

The total collection of analytical results, measured data and calibrations are archived on tape at SKB.

## 2. COMPUTER CONTROLLED ON-LINE MEASUREMENTS

### 2.1. Introduction

The computer controlled, on-line measurements includes:

- Potentiometric measurements, ie. pH,  $E_h$  and  $pS^{2-}$
- Electrical conductivity measurements
- Oxygen measurements
- Temperature measurements

The measurements are performed by two different parts of equipment in the mobile field laboratory. One part is a down-hole probe which makes in situ measurements in packed off water conductive sections of the borehole. The other part of equipment is located on the surface and consists of a measuring cell through which the water is pumped. Each piece of equipment contains one or two pH electrodes, three different  $E_h$  electrodes (gold, platinum and glassy carbon), a reference electrode, an ionselective sulphide electrode and one or two temperature probes. The surface cell also contains probes for measuring oxygen and electrical conductivity. The measurements are performed continuously at certain time intervals during the pumping and sampling period. A PDP 11 computer controls the measurements.

The readings from the different electrodes and probes are registered by the computer in the mobile field laboratory.

Calibration measurements on well defined solutions are performed before and after each measuring cycle in a borehole section. If the measuring cycle is longer than two weeks, additional calibrations are performed. The calibrations are registered in separate calibration files.

Two sets of calibration files will be created, one set for the down-hole electrodes and one set for the flow through cell electrodes at the surface. Each set contains one file for each calibration solution.

Comments from the laboratory staff on the measurements and calibrations are registered in information files corresponding to the data files.

### 2.2. Calculation of physical parameters from electrode readings

The following electrodes are used for the measurements:

- pH - pressure compensated glass electrode
- $E_h$  - gold, platinum and glassy carbon electrodes
- $pS^{2-}$  - silver/silversulphide electrode
- pressure compensated reference electrode

The calibration constant  $E^0$  for each electrode has to be known in order to calculate the physical parameters pH, pS and  $E_h$  from the electrode readings. In order to obtain the  $E^0$ -values, calibration measurements are performed in solutions where pH, pS and  $E_h$  are well defined.

The calibration solutions/buffers are:



Phthalate buffer (pH 4) + quinhydrone for pH and  $E_h$  measurements.

Phosphate buffer (pH 7) + quinhydrone for pH and  $E_h$  measurements.

Carbonate buffer (pH 10) for pH measurements only.

Sulphide solution 0.01 mol/l and 0.05 mol/l for  $pS^{2-}$  measurements.

### 2.2.1. Calculation of pH from electrode readings

Nernst's equation gives:

$$E = E^0 + (RT/nF) \ln[H^+] \quad (1)$$

The potential  $E$  (mV) is measured in the different buffer solutions where pH is known. pH has different temperature dependence in different pH-buffers. The temperature dependence is included in the expression used for calculating  $E^0$ .

$$E^0(\text{pH } 4) = E_{\text{meas}}(\text{pH } 4) + \text{pH}(10 \text{ } ^\circ\text{C}) * (R/F) \ln 10 * KT \quad (2)$$

$$E^0(\text{pH } 7) = E_{\text{meas}}(\text{pH } 7) + (R/F) \ln 10 * KT * (\text{pH}(0 \text{ } ^\circ\text{C}) - 0.0025 * T) \quad (3)$$

$$E^0(\text{pH } 10) = E_{\text{meas}}(\text{pH } 10) + (R/F) \ln 10 * KT * (\text{pH}(0 \text{ } ^\circ\text{C}) - 0.0125 * T) \quad (4)$$

where:

$KT$  = measured temperature in Kelvin

$T$  = measured temperature in Celsius

The three  $E^0$ -values obtained from measurements in each one of the the three buffer solutions should coincide. Differences of up to  $\pm 10$  mV are however acceptable.

The average  $E_0$  value is used in the calculation of pH in the groundwater:

$$\text{pH} = (E^0(\text{pH}) - E_{\text{meas}}) / (\ln 10 * KT * R/F) \quad (5)$$

### 2.2.2. Calculation of $E_h$ from electrode readings

For the redox electrodes measured against the reference electrode the potential is given by:

$$E = E^0Q - E^0\text{Ag}^+/\text{Ag} + RT/nF (-\ln[\text{Ag}^+]_{\text{ref}} + \ln[\text{H}^+]_{\text{soln}}) \quad (6)$$

The calibration constant  $E^0$  is given by the difference between theoretical  $E_h$  in the calibration solution and the measured electrode reading.  $E_h$  is temperature dependent. The second terms in the expressions below corrects for the temperature dependence.

$$E^0(\text{pH } 4) = E_h(\text{pH } 4, 0 \text{ } ^\circ\text{C}) - 1.518 * T - E_{\text{meas}}(\text{pH } 4) \quad (7)$$

$$E^0(\text{pH } 7) = E_h(\text{pH } 7, 0 \text{ } ^\circ\text{C}) - 1.953 * T - E_{\text{meas}}(\text{pH } 7) \quad (8)$$

The two values obtained for  $E^0$  may not differ more than 20 mV. The average  $E^0$  is used in the calculation of  $E_h$  in the groundwater.

$$E_h = E^0 + E_{\text{meas}} \quad (9)$$

### 2.2.3. Calculation of pS from electrode readings

The sulphide electrode potential in a sulphide solution is determined by the reaction:



The electrode potential can be expressed as:

$$E = E^0\text{S} - \frac{RT}{nF} \ln [\text{S}^{2-}] = E^0\text{S} - \ln 10 \frac{R}{2F} * \text{pS}^{2-} * T \quad (11)$$

The  $E^0$ -value is obtained from calibration measurements in two different solution (0.01 M and 0.05 M sulphide solution).

The free sulphide concentration  $[\text{S}^{2-}]$  in the solution depends on the total sulphide concentration  $[\text{S}_{\text{tot}}] = [\text{S}^{2-}] + [\text{HS}^-]$  and on pH. If  $\log K_{\text{HS}} \gg \text{pH}$  then  $[\text{HS}^-] \sim \text{S}_{\text{tot}}$  and

$$\text{pS}^{2-} = \text{pS}_{\text{tot}} - \text{pH} + \log K_{\text{HS}} \quad (12)$$

$\text{pS}_{\text{tot}}$  is constant in each solution and  $\log K_{\text{HS}} = 14$ , but pH varies with the temperature.

The temperature is removed outside in the right term in equation (11). The resulting factors ( $\text{KS}_{.01}$  and  $\text{KS}_{.05}$ ) for the 0.01 M and the 0.05 M calibration solutions respectively are given below. The temperature dependence of  $\text{pS}^{2-}$  is included.

$$\text{KS}_{.01} = \ln 10 \frac{R}{2F} * \text{pS}^{2-} = 0.0992 * (\text{pS}^{2-} - (10 \text{ C}) + 0.01 * T) \quad (13)$$

$$\text{KS}_{.05} = \ln 10 \frac{R}{2F} * \text{pS}^{2-} = 0.0992 * (\text{pS}^{2-} - (10 \text{ C}) + 0.036 * T) \quad (14)$$

The  $E^0$ -values for the two solutions should coincide and are obtained from:

$$E^0(0.01) = E_{\text{meas}} - (\text{KS}_{.01} * T) \quad (15)$$

$$E^0(0.05) = E_{\text{meas}} - (\text{KS}_{.05} * T) \quad (16)$$

The average value is used for calculation of  $\text{pS}^{2-}$  from the electrode readings in the groundwater measurements.

The expression for  $\text{pS}^{2-}$  will be:

$$\text{pS}^{2-} = (E_{\text{meas}} - E^0) / ((\ln 10 * R/2F) * T) = \quad (17)$$

$$= (E_{\text{meas}} - E^0) * 10.08/T$$

2.3. Data Flow

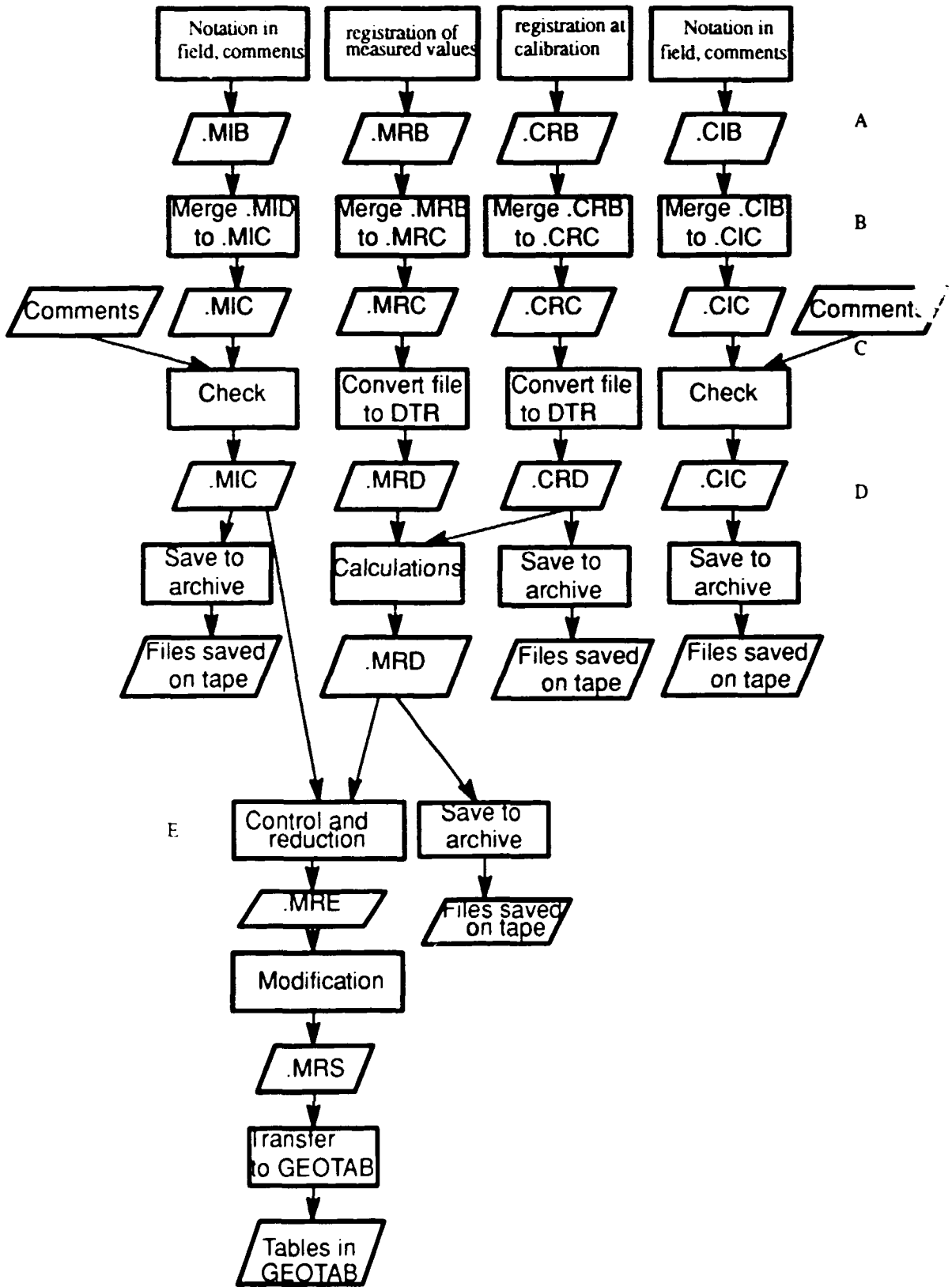


Figure 2.1. A schematic presentation of the data flow

A - The data files registered in the mobile field laboratory have the file name extensions:

.MIB - Information file, comments on measurements

.MRB - Raw data file, measurements

.CRB - Raw data file, calibrations

.CIB - Information file, comments on calibrations

These files are transferred to a floppy disk and sent to IVL, usually once a week.

B - Several of the data files above, usually one week of measurements, are merged into:

.MIC - merged .MIB files

.MRC - merged .MRB files

.CRC - merged .CRB files

.CIC - merged .CIB files

The data files are copied to a VAX computer.

C - The ASCII files .MRC and .CRC are converted to index sequential files of DTR file type.

The computer program CMREAD.EXE is used for the conversion.

.MRD - converted .MRC files

.CRD - converted .CRC files

D - Calibration data (.CRD and .CIC)

The following information from the .CIC file is included in the .CRD file where it is used for calculations:

- corrections for discrepancies in the temperature readings
- conductivity measuring range
- theoretical conductivity of calibration solution

Calculation of  $E^0$  - values for pH and  $E_h$  electrodes are carried out in the .CRD file using the computer program FLOPPCR.DEF.

The calibration file .CRD is printed out and checked.

Comments by IVL on the calibrations are included in the .CIC file.

All calibration information files .CIC from one borehole are merged into one file which is saved on tape in an archive at SKB.

All calibration data files .CRD from one borehole are merged into one file which is saved on tape in an archive at SKB.

D - Measurement data (.MRD and .MIC)

The calibration constants from the .CRD file (an average for the most stable period), and also the conductivity measuring range obtained from the information file .MIC are included in the measurement file .MRD.

Calculations of Eh, pH and pS are performed using the appropriate  $E^0$ -values from the calibration file .CRD and the computer program FLOPPMR.DEF. The .MRD file is printed out and controlled. Comments by IVL on the measured data are included in the .MIC file.

All the data files .MRD for one borehole section are merged into one file with  $E^0$  values included. The total .MRD file is saved on tape at SKB.

The complete information file .MIC is saved on tape at SKB.

E – Reduction and transfer (.MRE and .MRS)

The borehole section file .MRD is copied. The copy file .MRE is subjected to a reduction of data.

The .MRD-file generally contains one registration per hour from all the connected electrodes and probes. Stable readings are usually not obtained in the beginning of a pumping period or just after a calibration.

The file is reduced by keeping a maximum of three readings per twenty-four hours, by omitting instable periods and by rejection of obviously erroneous readings that can be caused by, for instance, a badly working electrode. The reduced file has the extension .MRE.

The file .MRS is a modification of the reduced file .MRE to fit the format in GEOTAB. The computer program FLOPPMRS:DEF defines the file format and also calculates the physical parameters.

The .MRS file is converted into two ASCII files, which corresponds to the tables REDOX and PHETC under the method WATER in GEOTAB.

The datafiles are transferred via a communication link (Datel short distance) from the VAX computer at IVL to GEOTAB on the SKB VAX computer.

### 3. ANALYTICAL DATA FROM SKB:s FIELD LABORATORY

#### 3.1. Introduction

The major components and redox sensitive trace components are analysed by spectrophotometry, titrimetry, potentiometry and ion chromatography in the mobile field laboratory. One sample a day is analysed during a sampling period. The readings, dilutions, calibration factors, control standards etc are registered in a data file and the concentrations of the different constituents are calculated by the computer. Comments on the different analyses are saved on information files.

The equipment in the mobile field laboratory and the analytical methods are described in the reports SKB TR 86-16 and AR 86-14. All the analyses are performed at least twice. The repeated analyses are numbered from 1 to 5 in the data file registered at the mobile laboratory. These numbers are kept until the reduction of data prior to the transfer to GEOTAB.

3.2. Data flow

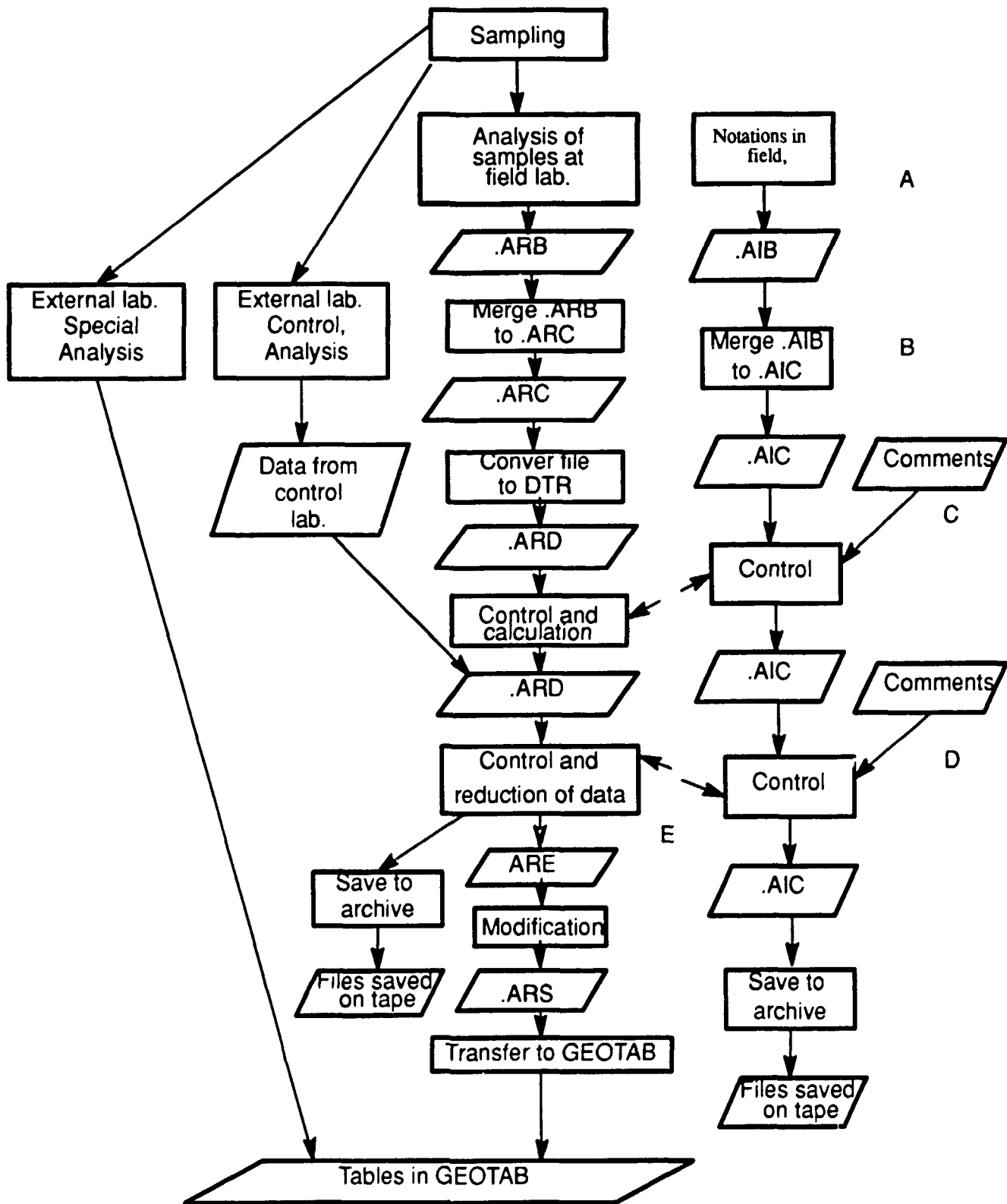


Figure 3.1. A schematic presentation of the data flow

- A The data files registered in the mobile field laboratory have the file name extensions:

.ARB – Result file, analytical data

.AIB – Information file, comments on analyses

These files are transferred to a floppy disk and sent to IVL, usually once a week.

- B Several .A\*B files, usually one week of analyses are merged into:

.ARC – merged .ARB files

.AIC – merged .AIB files

These data files are copied to a VAX computer.

- C – The .ARC files are converted to DTR file type using the computer program ARREAD.EXE.

.ARD – converted .ARC file .

- D The file structure is defined by the computer program FLOPPAR.DEF. This computer program also contains the equations for calculation of charge balance and relative charge balance errors. Except for the calculated analytical results the file also contains control functions such as control factors and results from blank samples. This gives information on the analytical performance in the mobile field laboratory.

When the sampling in a borehole section is terminated, the weekly files are merged together in one section file .ARD. Results from control analyses are numbered from 6 and upwards and included in the .ARD file. A judgement on the quality of the analyses and the most representative analytical values are performed, based on control functions in the mobile laboratory, charge balance and agreement between the analytical results from the mobile laboratory and the control analyses.

An average value or the most representative value for each analysed parameter and each sample is included in the section file .ARD. This chosen analytical value is given the number 0 in the file. Comments on the analytical performance and choice of "most representative value" by Sif Laurent are included in the information file .AIC.

The .ARD file will contain several analytical values for the same parameter which are numbered as follows:

No. 1 – 5 repeated analyses in the mobile laboratory

No. 6 – control analyses by external laboratories

No. 0 the chosen value, which can be an average value or the most representative value

The complete section files .ARD and .AIC are saved on tape in SKB archives.

- E REDUCTION AND TRANSFER (.ARE and .ARS)

The section file .ARD is copied. The copy .ARE is used for the reduction of data. After reduction the file will only contain the chosen concentration



values (average or most representative).

The file .ARS is obtained by modification of the reduced file .ARE using the computer program FLOPPARS.DEF.

The .ARS file will only contain the chosen concentration values.

The .ARS file is converted into two ASCII files which corresponds to the tables MAIN and REM belonging to the method WATER in the GEOTAB database. The concentrations of the major components (mg/l) are recalculated to mequiv/l and the charge balance and relative error are calculated. The calculated values are transferred into an ASCII file which corresponds to the table EQUIV in the database.

The datafiles are transferred via a communication link (datel short distance) from the VAX computer at IVL to GEOTAB on the SKB VAX computer.

#### 4. ANALYTICAL DATA FROM EXTERNAL LABORATORIES

##### 4.1. Introduction

The chemical analyses performed by other laboratories can be divided into two types:

- Control analyses of the major components and some important trace components
- Special analyses which requires specialized laboratories

Control samples are sent to an external lab. once a week for an independent check of the results from the field. Since January 1989 the cations, one sample a day, are also analysed by ICP-measurements at the Department Of Inorganic Chemistry, Royal Institute of Technology.

The special analyses includes isotope determinations, gas analyses and analyses of particulate matter caught on filters. The special sampling is normally performed once a week or once per section. Carbon isotope determinations, on carbon dioxide and carbonate are used for dating the groundwater by the carbon-14 method.

##### 4.2. Data flow

The presentation of the flow of data from external laboratories is included in Fig. 3.1. page 11.

- A,B The analytical results obtained from external laboratories are sent to Sif Laurent IVL for registration.
- C,D Control analyses are included in the .ARD file. These analyses can be separated from the analyses carried out in the field laboratory by their laboratory numbers starting from 6 and upwards.
- E Results from special analyses are registered directly in the database GEOTAB. The tables are ISOTOPE, RRUT, GAS and PARTIC in the method SPECAN . The responsible laboratory is given in "flyleaf" SPECANF.

## 1. APPENDIX – DESCRIPTION OF FILE TYPES: ON-LINE MEASUREMENTS

## 1.1. Description of file type .MIB

The file type .MIB is an ASCII file from the field laboratory with registration of comments on measurements.

Description of file format:

.MIB is a ASCII file with 6 different columns with description as follows:

row 1 – row 5

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss
HEADING	16	10	name of heading parameter
SEQNO	26		sequence number
VALUE	28	20	content of heading parameter

row 6

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss

row 7 – row 15

comment

row 16

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss

row 17 – row 26

comment

Example of file type .MIB

```

89-09-11 10:47: BHID           1      KAS02
89-09-11 10:47: BHNIV        1      130
89-09-11 10:47: BHOMR        1      Äspö
89-09-11 10:47: ANSV         1      kgn
89-09-11 10:47:
start av testmätning

89-09-11 10:47:
stoppa testmätning

```

## 1.2. Description of file type .MRB

The file type .MRB is an ASCII file from the field laboratory with registration of computer controlled on-line measurements

Description of file format:

.MRB is a ASCII file with 6 different columns with description as follows:

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss
PCODE	16	10	parameter code
SEQNO	26	1	sequence number
VALUE	33	*	measured value, mobile laboratory

Possible parameters:

pcode	format	comment
EAUB	NUM(9,4)	gold electrode reading in borehole section (mV)
ECB	NUM(9,4)	glassy carbon electrode reading in borehole section (mV)
EPTB	NUM(9,4)	platinum electrode reading in borehole section (mV)
EPTIB	NUM(9,4)	reading, extra platinum electrode, in borehole section (mV)
EREFB	NUM(9,4)	reference electrode reading, borehole section (mV)
EPHB	NUM(9,4)	glass electrode reading in borehole section (mV)
EPHIB	NUM(9,4)	glass electrode #1, reading, borehole section (mV)
ETB	NUM(9,4)	water temperature reading in borehole section
EAUY	NUM(9,4)	gold electrode reading in flow through cell at the surface (mV)
ECY	NUM(9,4)	glassy carbon electrode reading in flow through cell at the surface (mV)
ECIY	NUM(9,4)	reading, extra glassy carbon electrode, flow through cell at the surface (mV)
EPTY	NUM(9,4)	platinum electrode reading in flow through cell at the surface (mV)
EPTIY	NUM(9,4)	reading, extra platinum electrode, flow through cell at the surface (mV)
EREF1Y	NUM(9,4)	reference electrode #1, reading in flow through cell at the surface (mV)
EREF2Y	NUM(9,4)	reference electrode #2, reading in flow through cell at the surface (mV)
EREFIY	NUM(9,4)	reference electrode #1, reading in flow through cell at the surface (mV)
EPHY	NUM(9,4)	glass electrode reading in flow through cell at the surface (mV)
EPHIY	NUM(9,4)	glass electrode #1, reading in flow through cell at the surface (mV)
EKONDY	NUM(9,4)	electrical conductivity reading in flow through cell at the surface

EO2Y	NUM(9,4)	oxygen probe reading in the flow through cell at the surface
Q	NUM(9,4)	water flow rate (ml/min)
ET1Y	NUM(9,4)	water temp. reading #1 in the flow through cell at the surface
ET2Y	NUM(9,4)	water temp. reading #2 in the flow through cell at the surface
EPSB	NUM(9,4)	sulphide electrode reading in borehole section (mV)
EPSY	NUM(9,4)	sulphide electrode reading in flow through cell at the surface (mV)
EPS1Y	NUM(9,4)	reading, extra sulphide electrode in flow through cell at the surface (mV)
VLARMB	NUM(9,4)	not used
VLARMTS	NUM(9,4)	not used
TRYCK1	NUM(9,4)	pressure registrations, to be treated by SGAB
TRYCK2	NUM(9,4)	pressure registrations, to be treated by SGAB
TRYCK3	NUM(9,4)	pressure registrations, to be treated by SGAB
TRYCK4	NUM(9,4)	pressure registrations, to be treated by SGAB

Example of file type .MRB ( from org. file lx019102.mrb )

90-10-17 10:51	EO2Y	1	6.6960
90-10-17 10:51	EKONDY	1	66.6040
90-10-17 10:51	Q	1	-7.3254
90-10-17 10:51	ET1Y	1	18.3660
90-10-17 10:51	ECY	1	-352.7000
90-10-17 10:51	EPTY	1	-362.4000
90-10-17 10:51	EPHY	1	-113.7000
90-10-17 10:51	EAUY	1	-353.5000
90-10-17 10:51	EREF1Y	1	277.1000
90-10-17 11:53	EO2Y	2	2.5060
90-10-17 11:53	EKONDY	2	66.5200
90-10-17 11:53	Q	2	67.9985
90-10-17 11:53	ET1Y	2	19.1980
90-10-17 11:53	ECY	2	-353.5000
90-10-17 11:53	EPTY	2	-362.8000
90-10-17 11:53	EPHY	2	-113.2000
90-10-17 11:53	EAUY	2	-354.3000
90-10-17 11:53	EREF1Y	2	277.9000
90-10-17 12:53	EO2Y	3	6.9840
90-10-17 12:53	EKONDY	3	66.4480
90-10-17 12:53	Q	3	61.2033
90-10-17 12:53	ET1Y	3	19.7220
90-10-17 12:53	ECY	3	-353.8000
90-10-17 12:53	EPTY	3	-362.5000
90-10-17 12:53	EPHY	3	-112.6000
90-10-17 12:53	EAUY	3	-354.7000
90-10-17 12:53	EREF1Y	3	278.4000
90-10-17 13:53	EO2Y	4	4.7080
90-10-17 13:53	EKONDY	4	66.4480
90-10-17 13:53	Q	4	55.5676
90-10-17 13:53	ET1Y	4	19.8680
90-10-17 13:53	ECY	4	-355.8000

### 1.3. Description of file type .CRB

The file type .CRB is an ASCII file from the field laboratory with calibration registrations.

One file is created for each one of the calibration measurements. The file type .CRB is identical to the .MRB file type.

Description of file format:

.CRB is a ASCII file with 6 different columns with description as follows:

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss
PCODE	16	10	parameter code
SEQNO	26	1	sequence number
VALUE	33	*	measured value, mobile laboratory

Only a few parameters in a .CRB file are relevant to a particular calibration measurement.

Possible parameters, calibration

pcode	format	comment
EAUB	NUM(9,4)	gold electrode reading, borehole probe, calibration solution (mV)
ECB	NUM(9,4)	glassy carbon electrode reading, borehole probe, calibration solution (mV)
EPTB	NUM(9,4)	platinum electrode reading, borehole probe, calibration solution (mV)
EPTIB	NUM(9,4)	reading, extra platinum electrode, calib. soln., borehole probe (mV)
EREFB	NUM(9,4)	reference electrode reading, borehole probe, calibration solution (mV)
EPHB	NUM(9,4)	glass electrode reading, borehole probe, calibration solution (mV)
EPHIB	NUM(9,4)	glass electrode #1, reading, borehole probe, calibration solution (mV)
ETB	NUM(9,4)	temperature reading in calib. soln, borehole probe
EAUY	NUM(9,4)	gold electrode reading in flow through cell at the surface, calibration solution (mV)
ECY	NUM(9,4)	glassy carbon electrode reading, flow through cell at the surface, calib. soln (mV)
ECIY	NUM(9,4)	reading, extra glassy carbon electrode, calib. soln., surface cell (mV)
EPTY	NUM(9,4)	platinum electrode reading in flow through cell at the surface, calib. soln. (mV)
EPTIY	NUM(9,4)	reading, extra platinum electrode, calib. soln., surface cell (mV)
EPHY	NUM(9,4)	glass electrode reading in flow through cell at the surface, calibration soln. (mV)

EPHIY	NUM(9,4)	glass electrode #1, reading in flow through cell at the surface, calib. soln. (mV)
EREF1Y	NUM(9,4)	reference electrode #1, reading in flow through cell at the surface, calib. soln. (mV)
EREF2Y	NUM(9,4)	reference electrode #2, reading in flow through cell at the surface, calib. soln. (mV)
EREF1Y	NUM(9,4)	reference electrode #1, reading in flow through cell at the surface, calib. soln. (mV)
EKONDY	NUM(9,4)	electrical conductivity reading, flow through cell at the surface, calib. soln.
EO2Y	NUM(9,4)	oxygen probe reading in calib. soln., flow through cell at surface
Q	NUM(9,4)	water flow rate (ml/min)
ET1Y	NUM(9,4)	temp. reading #1 in calib. soln., flow through cell at the surface
ET2Y	NUM(9,4)	water temp. reading #2 in calib. soln., flow through cell at the surface
EPSB	NUM(9,4)	sulphide electrode reading, borehole probe, calibration solution (mV)
EPSY	NUM(9,4)	sulphide electrode reading, calib. soln., flow through cell at the surface (mV)
EPS1Y	NUM(9,4)	reading, extra sulphide electrode, calib. soln., surface cell (mV)

Example of file type .CRB ( from org. file lx0001.crb )

90-10-30 11:03 ETB	1	20.7580
90-10-30 11:03 EPHB	1	-157.1000
90-10-30 11:03 ECB	1	108.3000
90-10-30 11:03 ECIB	1	159.2000
90-10-30 11:03 EPTB	1	138.5000
90-10-30 11:03 EAUB	1	145.5000
90-10-30 11:03 VLARMB	1	3197.3000
90-10-30 11:03 EREFB	1	-140.9000
90-10-30 11:04 ETB	2	20.7480
90-10-30 11:04 EPHB	2	-158.6000
90-10-30 11:04 ECB	2	107.0000
90-10-30 11:04 ECIB	2	152.0000
90-10-30 11:04 EPTB	2	133.4000
90-10-30 11:04 EAUB	2	138.5000
90-10-30 11:04 VLARMB	2	3197.4000
90-10-30 11:04 EREFB	2	-135.7000
90-10-30 11:04 ETB	3	20.72400
90-10-30 11:04 EPHB	3	-159.6000
90-10-30 11:04 ECB	3	106.2000
90-10-30 11:04 ECIB	3	145.3000
90-10-30 11:04 EPTB	3	129.5000
90-10-30 11:04 EAUB	3	135.0000
90-10-30 11:04 VLARMB	3	3196.9000
90-10-30 11:04 EREFB	3	-131.7000

#### 1.4. Description of file type .CIB

The file type .CIB is an ASCII file from the field laboratory with comments on calibrations. The file also contains parameters needed for calculation of electrical conductivity (KONDK and KONDSKALA)

Description of file format:

.CIB is an ASCII file with 6 different columns with description as follows:

row 1 – row 5

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss
HEADING	16	10	name of heading parameter
SEQNO	26	1	sequence number
VALUE	28	20	content of heading parameter

row 6

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss

row 7 – row 15

comment

row 16

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss

row 17 – row 26

comment

Example of file type .CIB

```

89-09-11 10:47: BHID          1      AS02
89-09-11 10:47: BHNIV       1      130
89-09-11 10:47: BHOMR       1      Äspö
89-09-11 10:47: ANSV        1      kgn
89-09-11 10:47:
start av testmätning

89-09-11 10:47:
stoppa testmätning

```



### 1.5. Descriptions of concatenated files

#### Description of file type .MIC

The .MIB files are transferred to floppy disks which are sent to IVL, where they are concatenated with other .MIB to a .MIC file. The file type .MIC usually consists of merged .MIB files.

#### Description of file type .MRC

The .MRB files are transferred to floppy disks which are sent to IVL, where they are concatenated with other .MRB to a .MRC file. The file type .MRC usually consists of merged .MRB files.

#### Description of file type .CRC

The .CRB files are transferred to floppy disks which are sent to IVL, where they are concatenated with other .CRB to a .CRC file. The file type .CRC usually consists of merged .CRB files.

#### Description of file type .CIC

The .CIB files are transferred to floppy disks which are sent to IVL, where they are concatenated with other .CIB to a .CIC file. The file type .CIC usually consists of merged .CIB files.

## 1.6. Description of .CRD file type

The file contains calibration measurements (DTR file type).

The file .CRD is created from the file .CRC through the program CMREAD.EXE.

Description of file format:

pcode	format	comment
BH	CHAR(4)	borehole identification code
BHL	NUM(4)	length to length to sampled section (m)
MANSCH	CHAR(1)	manschett type, E = single packer, D = double packer, O = open borehole
DATE	CHAR(6)	date of measurement (yymmdd)
TIME	CHAR(4)	time of measurement (hhmm)
EAUB	NUM(9,4)	gold electrode reading, borehole probe, calibration solution (mV)
EAUY	NUM(9,4)	gold electrode reading in flow through cell at the surface, calibration solution (mV)
ECB	NUM(9,4)	glassy carbon electrode reading, borehole probe, calibration solution (mV)
ECY	NUM(9,4)	glassy carbon electrode reading in flow through cell at the surface, calibration soln. (mV)
ECIY	NUM(9,4)	reading, extra glassy carbon electrode, calib. soln., surface cell (mV)
EPTB	NUM(9,4)	platinum electrode reading, borehole probe, calibration solution (mV)
EPTY	NUM(9,4)	platinum electrode reading in flow through cell at the surface, calibration soln. (mV)
EPTIB	NUM(9,4)	reading, extra platinum electrode, calib. soln., borehole probe (mV)
EPTIY	NUM(9,4)	reading, extra platinum electrode, calib. soln., surface cell (mV)
EREFB	NUM(9,4)	reference electrode reading in borehole probe, calibration solution (mV)
EREF1Y	NUM(9,4)	reference electrode #1 reading in flow through cell at the surface, calibration soln. (mV)
EREF2Y	NUM(9,4)	reference electrode #2, reading in flow through cell at the surface, calib. soln. (mV)
EREF1Y	NUM(9,4)	reference electrode #1, reading in flow through cell at the surface, calib. soln. (mV)
EPHB	NUM(9,4)	glass electrode reading, borehole probe, calibration solution (mV)
EPHIB	NUM(9,4)	glass electrode #1, reading, borehole probe, calibration solution (mV)
EPHY	NUM(9,4)	glass electrode reading in flow through cell at the surface, calibration soln. (mV)
EPHIY	NUM(9,4)	glass electrode #1, reading in flow through cell at the surface, calib. soln. (mV)
EKONDY	NUM(9,4)	electrical conductivity, reading of calibration solution, measured in surface cell
KONDK	NUM(9,4)	lit. value of electrical conductivity, calib. soln. (mS/m)
KONDSKAL	NUM(9,4)	scale interval

EO2Y	NUM(9,4)	oxygen probe reading in calib. soln. measured in the flow through cell at the surface
Q	NUM(9,4)	water flow rate (ml/min)
ETB	NUM(9,4)	temperature reading in calib. soln, borehole probe
ET1Y	NUM(9,4)	temp. reading #1 in calib. soln., flow through cell at the surface
ET2Y	NUM(9,4)	water temp. reading #2 in calib. soln., flow through cell at the surface
EPSB	NUM(9,4)	sulphide electrode reading in borehole probe, calib. soln. (mV)
EPSY	NUM(9,4)	sulphide electrode reading), flow through cell at the surface, calib. soln. (mV)
EPSIY	NUM(9,4)	reading, extra sulphide electrode, surface cell, calib. soln. (mV)
XXT	NUM(9,4)	not used (extra parameter)

## 1.7. Calculations made in CRD file ( DTR )

KTB	NUM(9,4)	$KTB=TB + 273.16$
EOPHB4	NUM(9,4)	$EOPHB4=EPHB + 0.7916*KTB.$
EOPHB7	NUM(9,4)	$EOPHB7=EPHB + 0.1984*KTB*(7.06 - 0.0025*TB),$
EOPHB10	NUM(9,4)	$EOPHB10=EPHB + 0.1984*KTB*(10.3 - 0.0125*TB),$
EOPHIB4	NUM(9,4)	$EOPHIB4=EPHIB + 0.7916*KTB.$
EOPHIB7	NUM(9,4)	$EOPHIB7=EPHIB + 0.1984*KTB*(7.06 - 0.0025*TB),$
EOPHIB10	NUM(9,4)	$EOPHIB10=EPHIB + 0.1984*KTB*(10.3 - 0.0125*TB),$
EOCB4	NUM(9,4)	$EOCB4=501.28-1.518*TB-ECB$
EOCB7	NUM(9,4)	$EOCB7=335.5-1.953*TB-ECB$
EOPTB4	NUM(9,4)	$EOPTB4=501.28-1.518*TB-EPTB$
EOPTB7	NUM(9,4)	$EOPTB7=335.5-1.953*TB-EPTB$
EOPTIB4	NUM(9,4)	$EOPTIB4=501.28-1.518*TB-EPTIB$
EOPTIB7	NUM(9,4)	$EOPTIB7=335.5-1.953*TB-EPTIB$
E0AUB4	NUM(9,4)	$E0AUB4=501.28-1.518*TB-EAUB$
E0AUB7	NUM(9,4)	$E0AUB7=335.5-1.953*TB-EAUB$
KS01B	NUM(9,4)	$KS01B=0.0992*(5.53+0.01*TB)$
KS05B	NUM(9,4)	$KS05B=0.0992*(1.73+0.036*TB)$
EOPSB01	NUM(9,4)	$EOPSB01=EPSB - (KS01B * KTB )$
EOPSB05	NUM(9,4)	$EOPSB05=EPSB - (KS05B * KTB )$
KT1Y	NUM(9,4)	$KT1Y=T. Y + 273.16$
KT2Y	NUM(9,4)	$KT2Y=T2Y + 273.16$
EOPHY4	NUM(9,4)	$EOPHY4=EPHY + 0.7916*KT1Y$
EOPHY7	NUM(9,4)	$EOPHY7=EPHY + 0.1984*KT1Y*(7.06 - 0.0025*T1Y)$
EOPHY10	NUM(9,4)	$EOPHY10=EPHY + 0.1984*KT1Y*(10.3 - 0.0125*T1Y)$
EOPHIY4	NUM(9,4)	$EOPHIY4=EPHIY + 0.7916*KT2Y$
EOPHIY7	NUM(9,4)	$EOPHIY7=EPHIY + 0.1984*KT2Y*(7.06 - 0.0025*T2Y)$
EPHIY10	NUM(9,4)	$EPHIY10=EPHIY + 0.1984*KT2Y*(10.3 - 0.0125*T2Y)$
E0CY4	NUM(9,4)	$E0CY4=501.28 - 1.518*T1Y - ECY$
E0CY7	NUM(9,4)	$E0CY7=335.5 - 1.953*T1Y - ECY$
E0CIY4	NUM(9,4)	$E0CIY4=501.28 - 1.518*T2Y - ECIY$
E0CIY7	NUM(9,4)	$E0CIY7=335.5 - 1.953*T2Y - ECIY$
E0PTY4	NUM(9,4)	$E0PTY4=501.28 - 1.518*T1Y - EPTY$
E0PTY7	NUM(9,4)	$E0PTY7=335.5 - 1.953*T1Y - EPTY$
E0PTIY4	NUM(9,4)	$E0PTIY4=501.28 - 1.518*T1Y - EPTIY$
E0PTIY7	NUM(9,4)	$E0PTIY7=335.5 - 1.953*T1Y - EPTIY$
E0AUY4	NUM(9,4)	$E0AUY4=501.28 - 1.518*T1Y - EAUY$
E0AUY7	NUM(9,4)	$E0AUY7=335.5 - 1.953*T1Y - EAUY$
KS01Y1	NUM(9,4)	$KS01Y1=0.0992*(5.53 + 0.01*T1Y)$
KS05Y1	NUM(9,4)	$KS05Y1=0.0992 * (1.73 + 0.036*T1Y)$
KS01Y2	NUM(9,4)	$KS01Y2=0.0992*(5.53 + 0.01*T2Y)$
KS05Y2	NUM(9,4)	$KS05Y2=0.0992*(1.73 + 0.036*T2Y)$
E0PSY01	NUM(9,4)	$E0PSY01=EPSY - (KS01Y1 * KT1Y)$
E0PSY05	NUM(9,4)	$E0PSY05=EPSY - (KS05Y1 * KT1Y)$
E0PSIY01	NUM(9,4)	$E0PSIY01=EPSIY - (KS01Y2 * KT2Y)$
E0PSIY05	NUM(9,4)	$E0PSIY05=EPSIY - (KS05Y2 * KT2Y)$

O2Y	NUM(9,4)	$Q2Y=EO2Y/100*20$
KONDY	NUM(9,4)	$KONDY=EKONDY/10*KONDSKAL$
FKONDY	NUM(9,4)	$FKONDY=(KONDK - KONDY)/KONDY$
KONDYJ	NUM(9,4)	$KONDYJ=(1+FKONDY)*KONDY$
ECB-EPTB	NUM(9,4)	$ECB-EPTB=(ECB - EPTB), ECB-EPTB (diff<10)$
ECB-EAUB	NUM(9,4)	$ECB-EAUB=(ECB - EAUB), ECB-EAUB (diff<10)$
EBTB-EAUB	NUM(9,4)	$EBTB-EAUB=(EBTB - EAUB)$
ECY-EPTY	NUM(9,4)	$ECY-EPTY=(ECY - EPTY), ECY-EPTY (diff<10)$
ECY-EAUY	NUM(9,4)	$ECY-EAUY=(ECY - EAUY), ECY-EAUY (diff<10)$
EPTY-EAUY	NUM(9,4)	$EPTY-EAUY=(EPTY - EAUY), EPTY-EAUY (diff<10)$
ECIY-EPTIY	NUM(9,4)	$ECIY-EPTIY=(ECIY - EPTY), ECIY-EPTIY (diff < 10)$
ECIY-EAUIY	NUM(9,4)	$ECIY-EAUIY=(ECIY - EPTY), ECIY-EAUIY (diff < 10)$
EPTIY-EAUIY	NUM(9,4)	$EPTIY-EAUIY=(ECIY - EAUY), EPTIY-EAUIY (diff < 10)$

## 1.8. Description of .MRD file type

Measurement registrations (DTR file type).

The file .MRD is created from the file .MRC through the program CMREAD.EXE.

Description of file format:

pname	format	comment
BH	CHAR(4)	borehole identification code
BHL	NUM(4)	length to length to sampled section (m)
MANSCH	CHAR(1)	manschett type, E = single packer, D = double packer, O = open borehole
DATE	CHAR(6)	date of measurement (y,m,ddd)
TIME	CHAR(4)	time of measurement (hhmm)
E0AUB	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of gold electrode in the borehole probe (mV).
E0AUY	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of gold electrode, the meas. cell at the surface (mV)
EAUB	NUM(9,4)	gold electrode reading in borehole section (mV)
EAUY	NUM(9,4)	gold electrode reading in flow through cell at the surface (mV)
E0CB	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of glassy carbon electrode in borehole probe (mV)
E0CY	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of glassy carbon electrode in the surface cell (mV)
E0CIY	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of extra glassy carbon electrode in the surface cell (mV)
ECB	NUM(9,4)	glassy carbon electrode reading in the borehole section (mV)
ECY	NUM(9,4)	glassy carbon electrode reading in flow through cell at the surface (mV)
ECIY	NUM(9,4)	glassy carbon extra electrode reading in the flow through cell at the surface (mV)
E0PTB	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of platinum electrode in the borehole probe (mV)
E0PTIB	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of extra platinum electrode in the borehole probe (mV)
E0PTY	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of platinum electrode in meas. cell at the surface (mV)
E0PTIY	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of extra platinum electrode in the surface cell (mV)
EPTY	NUM(9,4)	platinum electrode reading in flow through cell at the surface (mV)
EPTIY	NUM(9,4)	reading, extra platinum electrode, flow through cell at the surface (mV)
EPTB	NUM(9,4)	platinum electrode reading, borehole probe (mV)
EPTIB	NUM(9,4)	reading, extra platinum electrode (mV)
E0PHB	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of glass electrode in the borehole probe (mV)
E0PHY	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of glass electrode in the meas. cell at the surface (mV)

EOPHIB	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of extra glass electrode in the borehole probe (mV)
EOPHIY	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of extra glass electrode, the meas. cell at the surface (mV)
EPHB	NUM(9,4)	glass electrode reading in the borehole section (mV)
EPHY	NUM(9,4)	glass electrode reading in flow through cell at the surface (mV)
EPHIB	NUM(9,4)	reading, extra glass electrode in the borehole section (mV)
EPHIY	NUM(9,4)	reading, extra glass electrode in flow through cell at the surface (mV)
EOPSB	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of sulphide electrode in the borehole probe (mV)
EOPSY	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of sulphide electrode, meas. cell at the surface (mV)
EOPSIY	NUM(9,4)	E <sup>0</sup> -value calculated from calibration of extra sulphide electrode, meas. cell at the surface (mV)
EPSB	NUM(9,4)	sulphide electrode reading in the borehole section (mV)
EPSY	NUM(9,4)	sulphide electrode reading in meas. cell at the surface (mV)
EPSIY	NUM(9,4)	reading, extra sulphide electrode in meas. cell at the surface (mV)
EREFB	NUM(9,4)	reference electrode reading in the borehole section (mV)
EREF1Y	NUM(9,4)	reference electrode #1 reading in meas. cell at the surface (mV)
EREF2Y	NUM(9,4)	reference electrode #2 reading in meas. cell at the surface (mV)
EREF1Y	NUM(9,4)	reading, extra reference electrode #1 in meas. cell at the surface (mV)
ETB	NUM(9,4)	temperature reading in the borehole section
ET1Y	NUM(9,4)	temperature reading #1 in meas. cell at the surface
ET2Y	NUM(9,4)	temperature reading #2 in meas. cell at the surface
EO2Y	NUM(9,4)	oxygen probe reading in meas. cell at the surface
EKONDY	NUM(9,4)	electrical conductivity reading in meas. cell at the surface
FKONDY	NUM(9,4)	conductivity correction factor from calibration
KONDK	NUM(9,4)	not used
KONDSKALA	NUM(9,4)	scale interval
Q	NUM(9,4)	water flow rate (ml/min)
XXT	NUM(9,4)	not used (extra parameter)
XXY	NUM(9,4)	not used (extra parameter)

## 1.9. Calculated virtual parameters in .MRD file using inserted calibration constants

EHCB	NUM(9,4)	$E_{HCB} = (E_{OCB} + ECB)$ redox potential $E_h$ obtained from glassy carbon electrode in borehole section (mV)
EHCY	NUM(9,4)	$E_{HCY} = (E_{OCY} + ECY)$ redox potential $E_h$ obtained from glassy carbon electrode in surface cell (mV)
EHCIY	NUM(9,4)	$E_{HCIY} = (E_{OCIY} + ECIY)$ redox potential $E_h$ obtained from extra glassy carbon electrode in surface cell (mV)
EHPTB	NUM(9,4)	$E_{HPTB} = (E_{OPTB} + EPTB)$ redox potential $E_h$ obtained from platinum electrode in the borehole section (mV)
EHPTIB	NUM(9,4)	$E_{HPTIB} = (E_{OPTIB} + EPTIB)$ redox potential $E_h$ obtained from extra platinum electrode in the borehole section (mV)
EHPTY	NUM(9,4)	$E_{HPTY} = (E_{OPTY} + EPTY)$ redox potential $E_h$ obtained from platinum electrode in the surface cell (mV)
EHPTIY	NUM(9,4)	$E_{HPTIY} = (E_{OPTIY} + EPTIY)$ redox potential $E_h$ obtained from extra platinum electrode in the surface cell (mV)
EHAUB	NUM(9,4)	$E_{HAUB} = (E_{Oaub} + EAUB)$ redox potential $E_h$ obtained from gold electrode in the borehole section (mV)
EHAUY	NUM(9,4)	$E_{HAUY} = (E_{Oauy} + EAUY)$ redox potential $E_h$ obtained from gold electrode in the surface cell (mV)
PSB	NUM(9,4)	$PSB = (EPSB - E0PSB) - \log [S^{2-}]$ measured in borehole section
PSY	NUM(9,4)	$PSY = (EPSY - E0PSY) - \log [S^{2-}]$ measured in surface cell
PSIY	NUM(9,4)	$PSIY = (EPSIY - E0PSIY) - \log [S^{2-}]$ measured in surface cell, extra electrode
PHB	NUM(9,4)	$PHB = (E0PHB - EPHB) * 5.04/KTB$ pH measured in borehole section
PHIB	NUM(9,4)	$PHIB = (E0PHIB - EPHIB) * 5.04/KTB$ pH measured in borehole section, extra electrode
PHY	NUM(9,4)	$PHY = (E0PHY - EPHY) * 5.04/KT1Y$ pH measured in surface cell
PHIY	NUM(9,4)	$PHIY = (E0PHIY - EPHIY) * 5.04/KT2Y$ pH measured in surface cell extra electrode
O2Y	NUM(9,4)	$O2Y = (E02Y/100*5)$ oxygen measured in surface cell (mg/l)
KONDY	NUM(9,4)	$KONDY = (EKONDY/10) * KONDSKALA$ electrical conductivity from reading (mS/m)
KONDYJ	NUM(9,4)	$KONDYJ = (1 + FKONDY) * KONDY$ electrical conductivity (mS/m), corrected using calibration factor
KTB	NUM(9,4)	$KTB = TB + 273.16$
KT1Y	NUM(9,4)	$KT1Y = (T1Y + 273.16)$
KT2Y	NUM(9,4)	$KT2Y = (T2Y + 273.16)$



## 1.10. Description of .MRS file type

The .MRS file contains the calculated virtual parameters from a reduced .MRD file with the extension .MRE.

## Description of file format:

pname	format	comment
BH	CHAR(4)	borehole idcode
BHL	NUM(4)	length to length to sampled section (m)
MANSCH	CHAR(1)	manschett type, E = single packer, D = double packer, O = open borehole
DATE	CHAR(6)	date of measurement (yymmdd)
TIME	CHAR(4)	time of measurement (hhmm)
Q	NUM(9,4)	water flow rate (ml/min)
PHB	NUM(9,4)	$PHB = (EOPHB - EPHB) * 5.04/KTB$
EHCB	NUM(9,4)	$EHCB = (EOCB + ECB) (mV)$
EHPTB	NUM(9,4)	$EHPTB = (EOPTB + EPTB) (mV)$
EHAUB	NUM(9,4)	$EHAUB = (EOAUB + EAUB) (mV)$
PSB	NUM(9,4)	$PSB = (EPSB - E0PSB)$
EREFB	NUM(9,4)	reference electrode reading, borehole probe (mV)
PHY	NUM(9,4)	$PHY = (EOPHY - EPHY) * 5.04/KT1Y$
EHCY	NUM(9,4)	$EHCY = (EOCY + ECY) (mV)$
EHPTY	NUM(9,4)	$EHPTY = (EOPTY + EPTY) (mV)$
EHAUY	NUM(9,4)	$EHAUY = (EOAUY + EAUY) (mV)$
PSY	NUM(9,4)	$PSY = (EPSY - E0PSY)$
EREF1Y	NUM(9,4)	reference electrode #1 reading in flow through cell at surface (mV)
EREF2Y	NUM(9,4)	reference electrode #2, reading in flow through cell at the surface (mV)
O2Y	NUM(9,4)	$O2Y = (EO2Y/100*5) (mg/l)$
KONDYJ	NUM(9,4)	$KONDYJ = (1 + FKONDY) * KONDY$
PHIY	NUM(9,4)	$PHIY = (EOPHIY - EPHIY) * 5.04/KT2Y$
EHC1Y	NUM(9,4)	$EHC1Y = (EOC1Y + EC1Y) (mV)$
PS1Y	NUM(9,4)	$PS1Y = (EPS1Y - E0PS1Y)$
EREF1Y	NUM(9,4)	reference electrode #1, reading in flow through cell at the surface (mV)
EHPT1Y	NUM(9,4)	$EHPT1Y = (EOPT1Y + EPT1Y) Eh-Pl, y ex. (mV)$
PHIB	NUM(9,4)	$PHIB = (EOPHIB - EPHIB) * 5.04/KTB$ pH, b ex.
EHPTIB	NUM(9,4)	$EHPTIB = (EOPTIB + EPTIB) Eh-Pl, b ex. (mV)$
XX4	NUM(9,4)	not used (extra parameter)
TB	NUM(9,4)	temperature reading in the borehole section
T1Y	NUM(9,4)	temp. reading #1, flow through cell at the surface
T2Y	NUM(9,4)	water temp. reading #2, flow through cell at the surface
XXT	NUM(9,4)	not used (extra parameter)

## 2. APPENDIX – DESCRIPTION OF FILE TYPES: ANALYTICAL DATA

### 2.1. Description of file type .AIB

The file type .AIB is an ASCII file from the field laboratory with registration of comments on analysis.

Description of file format:

.AIB is an ASCII file with 6 different columns with description as follows:

row 1

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss

row 2 – row 7

comment

row 8

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss

row 9 – row 16

comment

Example of file type .AIB

89-09-11 10:47:

Höga halter av sulfid stör kiselanalysen

89-09-11 10:47:

## 2.2. Description of file type .ARB

column	start pos	length	comment
DATE	0	8	formal date syntax yy-mm-dd
TIME	9	5	formal time syntax hh:ss
PCODE	16	10	parameter name
SEQNO	26	1	sequence number
HEADING	27	6	heading information
VALUE	33	10	analytical value, mobile field laboratory

## Possible parameters:

## Ion chromatography:

pcode	format	comment
NA	NUM(9,4)	sodium concentration in gw. sample (mg/l)
NAK	NUM(9,4)	measured conc. in calibration solution (mg/l)
NAL	NUM(9,4)	measured conc. in diluted sample (mg/l)
NAOMR	NUM(9,4)	conductivity range on ion chromatograph
NASF	NUM(9,4)	dilution factor
K	NUM(9,4)	potassium concentration in gw. sample (mg/l)
KK	NUM(9,4)	measured conc. in calibration solution (mg/l)
KL	NUM(9,4)	measured conc. in diluted sample (mg/l)
KOMR	NUM(9,4)	conductivity range on ion chromatograph
KSF	NUM(9,4)	dilution factor
NH4NJ	NUM(9,4)	ammonium nitrogen conc. (mg/l) measured using ion chromatography
NH4NJK	NUM(9,4)	measured conc. in calibration solution (mg/l)
NH4NJOMR.	NUM(9,4)	conductivity range on ion chromatograph
F	NUM(9,4)	fluoride concentration in gw. sample (mg/l)
FK	NUM(9,4)	measured conc. in calibration solution (mg/l)
FL	NUM(9,4)	measured conc. in diluted sample (mg/l)
FOMR	NUM(9,4)	conductivity range on ion chromatograph
FSF	NUM(9,4)	dilution factor
SO4	NUM(9,4)	sulphate concentration in gw. sample (mg/l)
SO4K	NUM(9,4)	measured conc. in calibration solution (mg/l)
SO4L	NUM(9,4)	measured conc. in diluted sample, (mg/l)
SO4OMR	NUM(9,4)	conductivity range on ion chromatograph
SO4SF	NUM(9,4)	dilution factor
BR	NUM(9,4)	bromide concentration in gw.sample (mg/l)
BRK	NUM(9,4)	measured conc. in calibration solution (mg/l)
BRL	NUM(9,4)	measured conc. in diluted sample (mg/l)
BROMR	NUM(9,4)	conductivity range on ion chromatograph
BRSF	NUM(9,4)	dilution factor
CLJ	NUM(9,4)	chloride conc. measured using ion chromatography (mg/l)
CLJK	NUM(9,4)	measured conc. in calibration solution (mg/l)
CLJL	NUM(9,4)	measured conc. in diluted sample (mg/l)
CLJOMR	NUM(9,4)	conductivity range on ion chromatograph
CLJSF	NUM(9,4)	dilution factor
NO3N	NUM(9,4)	nitrate-nitrogen concentration (mg/l)
NO3NK	NUM(9,4)	measured conc. in calibration solution (mg/l)

NO3NL	NUM(9,4)	measured conc. in diluted sample (mg/l)
NO3NOMR	NUM(9,4)	conductivity range on ion chromatograph
NO3NSF	NUM(9,4)	dilution factor

## Titrations:

CA	NUM(9,4)	calcium concentration in gw. sample (mg/l)
CAT	NUM(9,4)	titrant volume (ml)
CAV	NUM(9,4)	sample volume (ml)
MG	NUM(9,4)	magnesium concentration in gw. sample (mg/l)
MGT	NUM(9,4)	titrant volume Ca + Mg (ml)
CL	NUM(9,4)	chloride concentration in gw. sample (mg/l)
CLBR	NUM(9,4)	Br-conc. to subtract, as bromide is also titr.
CLS	NUM(9,4)	S <sup>2-</sup> -conc. to subtract, as sulfide is also titr.
CLT	NUM(9,4)	titrant volume, sample (ml)
CLTB	NUM(9,4)	titrant volume, blank solution (ml)
CLV	NUM(9,4)	sample volume (ml)

## Spectrophotometrical analysis:

FE	NUM(9,4)	total iron concentration in gw. sample (mg/l)
FE2	NUM(9,4)	concentration of ferrous iron in gw. sample (mg/l)
FEL	NUM(9,4)	Fe(tot) absorbance reading, sample (abs)
FE2L	NUM(9,4)	Fe <sup>2+</sup> , absorbance reading, sample (abs)
FEV	NUM(9,4)	Fe, sample volume (ml)
FE2V	NUM(9,4)	Fe <sup>2+</sup> , sample volume (ml)
FEF	NUM(9,4)	Fe, factor calculated from calibration curve (ug/abs)
FEKF	NUM(9,4)	Fe, factor calc. from control standard (ug/abs)
FEKL	NUM(9,4)	Fe, absorbance reading, control standard (abs)
FER	NUM(9,4)	Fe, absorbance reading, reference "blank solution" (abs)
FES	NUM(9,4)	Fe, amount of total iron in control standard (ug)
MN	NUM(9,4)	manganese concentration in gw. sample (mg/l)
MNF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
MNKF	NUM(9,4)	factor calc. from control standard (ug/abs)
MNKL	NUM(9,4)	absorbance reading, control standard (abs)
MNL	NUM(9,4)	absorbance reading, sample (abs)
MNR	NUM(9,4)	absorbance reading, reference "blank solution" (abs)
MNS	NUM(9,4)	amount of manganese in control standard (ug)
MNV	NUM(9,4)	sample volume (ml)
SIO2	NUM(9,4)	SiO <sub>2</sub> , silica concentration in gw. sample (mg/l)
SIO2F	NUM(9,4)	factor calculated from calibration curve, (ug/abs)
SIO2KF	NUM(9,4)	factor calc. from control standard (ug/abs)
SIO2KL	NUM(9,4)	absorbance reading, control standard (abs)
SIO2L	NUM(9,4)	absorbance reading, sample (abs)
SIO2R	NUM(9,4)	absorbance reading, reference "blank soln." (abs)
SIO2S	NUM(9,4)	amount of silica in control standard (ug)
SIO2V	NUM(9,4)	sample volume (ml)
PO4P	NUM(9,4)	PO <sub>4</sub> -P, phosphate-phosphorus conc. in gw. sample (mg P/l)
PO4PF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
PO4PKF	NUM(9,4)	factor calc. from control standard (ug/abs)
PO4PKL	NUM(9,4)	absorbance reading, control standard (abs)
PO4PL	NUM(9,4)	absorbance reading, sample (abs)

PO4PR	NUM(9,4)	absorbance reading, reference "blank solution" (abs)
PO4PS	NUM(9,4)	amount of phosphorus in control standard (ug)
PO4PV	NUM(9,4)	sample volume (ml)
NO2N	NUM(9,4)	NO <sub>2</sub> -N, nitrite-nitrogen conc. in gw. sample (mg N/l)
NO2NF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
NO2NKF	NUM(9,4)	factor calc. from control standard (ug/abs)
NO2NKL	NUM(9,4)	absorbance reading, control standard (abs)
NO2NL	NUM(9,4)	absorbance reading, sample (abs)
NO2NR	NUM(9,4)	absorbance reading, reference "blank solution" (abs)
NO2NS	NUM(9,4)	amount of nitrogen in control standard (ug)
NO2NV	NUM(9,4)	sample volume (ml).
NH4N	NUM(9,4)	NH <sub>4</sub> -N, ammonium-nitrogen conc. in gw. sample (mg N/l)
NH4NF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
NH4NKF	NUM(9,4)	factor calc. from control standard (ug/abs)
NH4NKL	NUM(9,4)	absorbance reading, control standard (abs)
NH4NL	NUM(9,4)	absorbance reading, sample (abs)
NH4NRP	NUM(9,4)	absorbance reading, reagent (abs)
NH4NRS	NUM(9,4)	absorbance reading, reagent + deion. water (abs)
NH4NS	NUM(9,4)	amount of ammonium-nitrogen in control standard (ug)
NH4NV	NUM(9,4)	sample volume (ml)
S	NUM(9,4)	sulphide concentration in gw. sample (mg/l)
SF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
SKF	NUM(9,4)	factor calc. from control standard (ug/abs)
SKL	NUM(9,4)	absorbance reading, control standard (abs)
SL	NUM(9,4)	absorbance reading, sample (abs)
SR	NUM(9,4)	absorbance reading, reference "blank solution" (abs)
SS	NUM(9,4)	amount of sulphide in control standard (ug)
SV	NUM(9,4)	sample volume (ml)

Remaining parameters:

URSPOLV	NUM(9,4)	Fluorescence for drilling water sample, (0.5 mg/l uranine = 25000)
URFIX	NUM(9,4)	Factor adjusting the fluorescence to 500 for 10 ug/l uranine standard
UR	NUM(9,4)	fluorescence reading, gw.sample
URPROC	NUM(9,4)	Percent remaining fluorescence $100 * UR / URSPOLV$
VAFL	NUM(9,4)	water flow rate (ml/min)
PHL	NUM(9,4)	pH measured in laboratory
KONDL	NUM(9,4)	electrical conductivity measured in laboratory

## 2.3. Description of file type .ARD

pcode	format	comment
BH	CHAR(4)	borehole identification code
BHL	NUM(4)	length to length to sampled section (m)
MANSCH	CHAR(1)	manschett type, E = single packer, D = double packer, O = open borehole
BHOMR	CHAR(12)	area code
DATE	CHAR(6)	date of measurement (yymmdd)
TIME	CHAR(4)	time of measurement (hhmm)
LAB	NUM(1)	laboratory,
VAFL	NUM(9,4)	water flow rate (ml/min)
PHB	NUM(9,4)	pH measured in borehole section
PHY	NUM(9,4)	pH measured in flow through cell at the surface
PHL	NUM(9,4)	pH measured in laboratory
KONDY	NUM(9,4)	electrical conductivity registered at surface (mS/m)
NA	NUM(9,4)	sodium concentration in gw. sample (mg/l)
NAK	NUM(9,4)	measured conc. in calibration solution (mg/l)
NAL	NUM(9,4)	measured conc. in diluted sample (mg/l)
NAOMR	NUM(9,4)	conductivity range on ion chromatograph
NASF	NUM(9,4)	dilution factor
K	NUM(9,4)	potassium concentration in gw. sample (mg/l)
KK	NUM(9,4)	measured conc. in calibration solution (mg/l)
KL	NUM(9,4)	measured conc. in diluted sample (mg/l)
KOMR	NUM(9,4)	conductivity range on ion chromatograph
KSF	NUM(9,4)	dilution factor
NH4NJ	NUM(9,4)	ammonium nitrogen conc. (mg/l) measured using ion chromatography
NH4NJK	NUM(9,4)	measured conc. in calibration solution (mg/l)
NH4NJOMR	NUM(9,4)	conductivity range on ion chromatograph
F	NUM(9,4)	fluoride concentration in gw. sample (mg/l)
FK	NUM(9,4)	measured conc. in calibration solution (mg/l)
FL	NUM(9,4)	measured conc. in diluted sample (mg/l)
FOMR	NUM(9,4)	conductivity range on ion chromatograph
FSF	NUM(9,4)	dilution factor
SO4	NUM(9,4)	sulphate concentration in gw. sample (mg/l)
SO4K	NUM(9,4)	measured conc. in calibration solution (mg/l)
SO4L	NUM(9,4)	measured conc. in diluted sample, (mg/l)
SO4OMR	NUM(9,4)	conductivity range on ion chromatograph
SO4SF	NUM(9,4)	dilution factor
BR	NUM(9,4)	bromide concentration in gw. sample (mg/l)
BRK	NUM(9,4)	measured conc. in calibration solution (mg/l)
BRL	NUM(9,4)	measured conc. in diluted sample (mg/l)
BROMR	NUM(9,4)	conductivity range on ion chromatograph
BRSF	NUM(9,4)	dilution factor
CLJ	NUM(9,4)	chloride conc. measured using ion chromatograph (mg/l)
CLJK	NUM(9,4)	measured conc. in calibration solution (mg/l)
CLJL	NUM(9,4)	measured conc. in diluted sample (mg/l)
CLJOMR	NUM(9,4)	conductivity range on ion chromatograph
CLJSF	NUM(9,4)	dilution factor
NO3N	NUM(9,4)	nitrate-nitrogen concentration (mg/l)
NO3NK	NUM(9,4)	measured conc. in calibration solution (mg/l)

NO3NL	NUM(9,4)	measured conc. in diluted sample (mg/l)
NO3NOMR	NUM(9,4)	conductivity range on ion chromatograph
NO3NSF	NUM(9,4)	dilution factor
CA	NUM(9,4)	calcium concentration in gw. sample (mg/l)
CAT	NUM(9,4)	titrant volume (ml)
CAV	NUM(9,4)	sample volume (ml)
MG	NUM(9,4)	magnesium concentration in gw. sample (mg/l)
MGT	NUM(9,4)	titrant volume Ca + Mg (ml)
CL	NUM(9,4)	chloride concentration in gw. sample (mg/l)
CLBR	NUM(9,4)	Br-conc. to subtract, as bromide is also titr.
CLS	NUM(9,4)	S <sup>2-</sup> -conc. to subtract, as sulfide is also titr.
CLT	NUM(9,4)	titrant volume, sample (ml)
CLTB	NUM(9,4)	titrant volume, blank solution (ml)
CLV	NUM(9,4)	sample volume (ml)
FE	NUM(9,4)	total iron concentration in gw. sample (mg/l)
FE2	NUM(9,4)	concentration of ferrous iron in gw. sample (mg/l)
FEL	NUM(9,4)	Fe(tot) absorbance reading, sample (abs)
FE2L	NUM(9,4)	Fe <sup>2+</sup> , absorbance reading, sample (abs)
FEV	NUM(9,4)	Fe, sample volume (ml)
FE2V	NUM(9,4)	Fe <sup>2+</sup> , sample volume (ml)
FEF	NUM(9,4)	Fe, factor calculated from calibration curve (ug/abs)
FEKF	NUM(9,4)	Fe, factor calc. from control standard (ug/abs)
FEKL	NUM(9,4)	Fe, absorbance reading, control standard (abs)
FER	NUM(9,4)	Fe, absorbance reading, reference "blank solution" (abs)
FES	NUM(9,4)	Fe, amount of total iron in control standard (ug)
MN	NUM(9,4)	manganese concentration in gw. sample (mg/l)
MNF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
MNKF	NUM(9,4)	factor calc. from control standard (ug/abs)
MNKL	NUM(9,4)	absorbance reading, control standard (abs)
MNL	NUM(9,4)	absorbance reading, sample (abs)
MNR	NUM(9,4)	absorbance reading, reference "blank solution" (abs)
MNS	NUM(9,4)	amount of manganese in standard solution (ug)
MNV	NUM(9,4)	sample volume (ml)
SI02	NUM(9,4)	SiO <sub>2</sub> , silica concentration in gw. sample (mg/l)
SI02F	NUM(9,4)	factor calculated from calibration curve, (ug/abs)
SI02KF	NUM(9,4)	factor calc. from control standard (ug/abs)
SI02KL	NUM(9,4)	absorbance reading, control standard (abs)
SI02L	NUM(9,4)	absorbance reading, sample (abs)
SI02R	NUM(9,4)	absorbance reading, reference "blank soln." (abs)
SI02S	NUM(9,4)	amount of silica in control standard (ug)
SI02V	NUM(9,4)	sample volume (ml)
PO4P	NUM(9,4)	PO <sub>4</sub> -P, phosphate-phosphorus conc. in gw. sample (mg P/l)
PO4PF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
PO4PKF	NUM(9,4)	factor calc. from control standard (ug/abs)
PO4PKL	NUM(9,4)	absorbance reading, control standard (abs)
PO4PL	NUM(9,4)	absorbance reading, sample (abs)
PO4PR	NUM(9,4)	absorbance reading, reference "blank solution" (abs)
PO4PS	NUM(9,4)	amount of phosphorus in control standard (ug)
PO4PV	NUM(9,4)	sample volume (ml)
NO2N	NUM(9,4)	NO <sub>2</sub> -N, nitrite-nitrogen conc. in gw. sample (mg N/l)

NO2NF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
NO2NKF	NUM(9,4)	factor calc. from control standard (ug/abs)
NO2NKL	NUM(9,4)	absorbance reading, control standard (abs)
NO2NL	NUM(9,4)	absorbance reading, sample (abs)
NO2NR	NUM(9,4)	absorbance reading, reference "blank solution" (abs)
NO2NS	NUM(9,4)	amount of nitrogen in control standard (ug)
NO2NV	NUM(9,4)	sample volume (ml).
NH4N	NUM(9,4)	NH <sub>4</sub> -N, ammonium-nitrogen conc. in gw. sample (mg N/l)
NH4NF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
NH4NKF	NUM(9,4)	factor calc. from control standard (ug/abs)
NH4NKL	NUM(9,4)	absorbance reading, control standard (abs)
NH4NL	NUM(9,4)	absorbance reading, sample (abs)
NH4NRP	NUM(9,4)	absorbance reading, reagent (abs)
NH4NRS	NUM(9,4)	absorbance reading, reagent + deion. water (abs)
NH4NS	NUM(9,4)	amount of ammonium-nitrogen in control standard (ug)
NH4NV	NUM(9,4)	sample volume (ml)
S	NUM(9,4)	sulphide concentration in gw. sample (mg/l)
HCO3	NUM(9,4)	HCO <sub>3</sub> , bicarbonate (mg/l)
SF	NUM(9,4)	factor calculated from calibration curve (ug/abs)
SKF	NUM(9,4)	factor calc. from control standard (ug/abs)
SKL	NUM(9,4)	absorbance reading, control standard (abs)
SL	NUM(9,4)	absorbance reading, sample (abs)
SR	NUM(9,4)	absorbance reading, reference "blank solution" (abs)
SS	NUM(9,4)	amount of sulphide in control standard (ug)
SV	NUM(9,4)	sample volume (ml)
URSPOLV	NUM(9,4)	fluorescence for drilling water sample, (0.5 mg/l uranine = 25000)
URFIX	NUM(9,4)	Factor adjusting the fluorescence to 500 for 10 ug/l uranine standard
UR	NUM(9,4)	fluorescence reading, gw.sample
URPROC	NUM(9,4)	Percent remaining fluorescence $100 * UR / URSPOLV$
O2Y	NUM(9,4)	oxygen conc. (mg/l)
X9		not used
X10		not used
X11		not used
X12		not used
X13		not used
DJUP	NUM(9,4)	depth (m)
DATIN	NUM(9,4)	date of input, mobile lab.
KONDL	NUM(9,4)	cond, lab. (mS/m)
AL	NUM(9,4)	Aluminum conc. (mg/l)
LI	NUM(9,4)	Lithium conc. (mg/l)
STRON	NUM(9,4)	Strontium conc. (mg/l)
SI	NUM(9,4)	Silicon conc. (mg/l)
TOC	NUM(9,4)	total organic carbon (mg/l)
I	NUM(9,4)	iodide conc. (mg/l)
TURB	NUM(9,4)	turbidity (FTU)
NO3NO2	NUM(9,4)	nitrate + nitrite conc. (mg N/l)
X1		not used



X2		not used
X3		not used
FEK	NUM(9,4)	Fe, kf (dif%), $FEK=(FEKF - FEF)*100/FEF$
SIO2K	NUM(9,4)	$SiO_2$ , kf (dif%), $SIO2K=(SIO2KF - SIO2F)*100/SIO2F$
SIO2SI	NUM(9,4)	$SIO2SI = SIO2*0.4674$ ,
MNK	NUM(9,4)	Mn, kf (dif%), $MNK=(MNKF-MNF)*100/MNF$ calibration factor
NO2NK	NUM(9,4)	$NO2NK=(NO2NKF - NO2NF)*100/NO2NF$ ,
NH4NK	NUM(9,4)	$NH_4N$ , kf $NH4NK=(NH4NKF - NH4NF)*100/NH4NF$ ,
PO4PK	NUM(9,4)	$PO4PK=(PO4PKF - PO4PF)*100/PO4PF$ , $PO_4P$ , kf (dif%)
NAEKV	NUM(9,4)	$NAEKV=Na/22.99$ ,
KEKV	NUM(9,4)	$KEKV=K/39.1$ ,
CAEKV	NUM(9,4)	$CAEKV=Ca/20.04$
MGEKV	NUM(9,4)	$MGEKV=MG/12.16$
CAMGEKV	NUM(9,4)	$CAMGEKV=CAMG/20.04 + MG/12.16$
MNEKV	NUM(9,4)	$MNEKV=MN/27.47$
FEEKV	NUM(9,4)	$FEEKV=FE/27.92$
HCO3EKV	NUM(9,4)	$HCO3EKV=HCO3/61.02$
CLJEKV	NUM(9,4)	$CLJEKV=CLJ/35.45$
CLEKV	NUM(9,4)	$CLEKV=CL/35.45$
FEKV	NUM(9,4)	$FEKV=F/19$
SO4EKV	NUM(9,4)	$SO4EKV=SO_4/48.03$
BREKV	NUM(9,4)	$BREKV=BR/79.91$
JONPOS	NUM(9,4)	$JONPOS=JONPOS/NAEKV+CAEKV+$ (IF K NOT missing THEN $KEKV$ ELSE 0) + (IF MG NOT missing THEN $MGEKV$ ELSE 0) + (IF FE NOT missing THEN $FEEKV$ ELSE 0) +
JONEG	NUM(9,4)	$JONEG=JONEG/HCO3EKV +$ (IF CLJ NOT missing THEN $CLJEKV$ ELSE 0) + (IF CL NOT missing THEN $CLEKV$ ELSE 0) + (IF F NOT missing THEN $FEKV$ ELSE 0) + (IF $SO_4$ NOT missing THEN $SO4EKV$ ELSE 0) + (IF BR NOT missing THEN $BREKV$ ELSE 0) +
JONBAL	NUM(9,4)	$JONBAL=JONPOS - JONEG$ (ion bal)
JONSUM	NUM(9,4)	$JONSUM=JONPOS + JONEG$
JONREL	NUM(9,4)	$JONREL=JONBAL*100/JONSUM$ ion bal (%)

## 2.4. Description of file type .ARS

Reduced .ARD file. DTR file type .ARS is in structure a copy of .ARD file format. .ARS file contains the calculated mean value (lab = 0 in .ARD file).

pcode	format	comment
BH	CHAR(4)	borehole identification code
BHL	NUM(4)	length to length to sampled section (m)
MANSCH	CHAR(1)	manschett type, E = single packer, D = double packer, O = open borehole
BHOMR	CHAR(12)	area code
DATE	CHAR(6)	date of measurement (yymmdd)
TIME	CHAR(4)	time of measurement (hhmm)
LAB	NUM(1)	laboratory,
VAFL	NUM(9,4)	water flow rate (ml/min)
PHB	NUM(9,4)	pH measured in borehole section
PHY	NUM(9,4)	pH measured in flow through cell at the surface
PHL	NUM(9,4)	pH measured in laboratory
KONDY	NUM(9,4)	electrical conductivity (mS/m)
NA	NUM(9,4)	sodium concentration
NH4NJ	NUM(9,4)	ammonium nitrogen (NH <sub>4</sub> -N) conc. measured using ion chromatography (mg/l)
K	NUM(9,4)	potassium concentration (mg/l)
F	NUM(9,4)	fluoride concentration (mg/l)
CLJ	NUM(9,4)	chloride conc. measured using ion chromatography (mg/l)
CL	NUM(9,4)	chloride concentration (mg/l)
NO3N	NUM(9,4)	nitrate-nitrogen (NO <sub>3</sub> -N) concentration (mg/l)
SO4	NUM(9,4)	sulphate (SO <sub>4</sub> ) concentration (mg/l)
BR	NUM(9,4)	bromide concentration (mg/l)
FE	NUM(9,4)	total iron concentration (mg/l)
FE2	NUM(9,4)	concentration of ferrous iron (mg/l)
SIO2	NUM(9,4)	SiO <sub>2</sub> , silica concentration (mg/l)
MN	NUM(9,4)	manganese concentration (mg/l)
NO2N	NUM(9,4)	NO <sub>2</sub> -N, nitrite-nitrogen conc. (mg N/l)
NH4N	NUM(9,4)	NH <sub>4</sub> -N, ammonium-nitrogen conc. (mg N/l)
PO4P	NUM(9,4)	PO <sub>4</sub> -P, phosphate-phosphorus conc. in gw. sample (mg P/l)
S	NUM(9,4)	sulphide concentration (mg/l)
HCO3	NUM(9,4)	HCO <sub>3</sub> , bicarbonate concentrations (mg/l)
CA	NUM(9,4)	calcium concentration (mg/l)
MG	NUM(9,4)	magnesium concentration (mg/l)
Cl	NUM(9,4)	chloride concentration (mg/l)
URPROC	NUM(9,4)	Percent remaining fluorescence
O2Y	NUM(9,4)	oxygen conc. (mg/l),
X9		not used
X10		not used
X11		not used
X12		not used
X13		not used
DJUP	NUM(9,4)	depth (m)
KONDL	NUM(9,4)	conductivity, lab measurement (mS/m)
AL	NUM(9,4)	Aluminum conc. (mg/l)

LI	NUM(9,4)	Lithium conc. (mg/l)
STRON	NUM(9,4)	Strontium conc. (mg/l)
SI	NUM(9,4)	Silicon conc. (mg/l)
TOC	NUM(9,4)	total organic carbon (mg/l)
I	NUM(9,4)	iodide conc. (mg/l)
TURB	NUM(9,4)	turbidity (FTU)
NO3NO2	NUM(9,4)	nitrate + nitrite conc. (mg N/l)
X1		not used
X2		not used
X3		not used

## 3. APPENDIX – DESCRIPTION OF TABLES IN GEOTAB

## 3.1. Description of Tables in GEOTAB containing on-line measurements

The following tables are stored under the creator (see GEOTAB User's Guide) GEO\_DB.

REDOX Table of redox potential (Eh) data

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to measured section (m)
DATE	*	CHAR(6)	DATE	date of measurement (yymmdd)
TIME	*	CHAR(6)	TIME	time for measurement (hhmmss)
EHCB		NUM(3)	EH	Eh measured in packed off borehole section, glassy carbon electrode (mV)
EHPTB		NUM(3)	EH	Eh measured in packed off borehole section, platinum electrode (mV)
EHAUB		NUM(3)	EH	Eh measured in packed off borehole section, gold electrode (mV)
EHCY		NUM(3)	EH	Eh measured at the surface in water from borehole section, glassy carbon electrode (mV)
EHCYI		NUM(3)	EH	Eh measured at the surface in water from borehole section, glassy carbon electrode (mV)
EHPTY		NUM(3)	EH	Eh measured at the surface in water from borehole section, platinum electrode (mV)
EHPTIY		NUM(3)	EH	Eh measured at the surface in water from borehole section, platinum electrode (mV)
EHAUY		NUM(3)	EH	Eh measured at the surface in water from borehole section, gold electrode (mV)
EHAUIY		NUM(3)	EH	Eh measured at the surface in water from borehole section, gold electrode (mV)
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

PHETC: Table containing pH, pS, temperature, conductivity and oxygen data

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to measured section (m)
DATE	*	CHAR(6)	DATE	date of measurement (yymmdd)
TIME	*	CHAR(6)	TIME	time for measurement (hhmmss)
TB		NUM(4,2)	TB	water temperature in packed off borehole section
PHB		NUM(4,2)	PH	pH measured in packed off borehole section
PHIB		NUM(4,2)	PH	pH measured in packed off borehole section
PHY		NUM(4,2)	PH	pH measured at the surface in water from borehole section
PHIY		NUM(4,2)	PH	pH measured at the surface in water from borehole section
CONDY		NUM(5,1)	ECOND	electrical conductivity, water from borehole section, measured at the surface (mS/m)
PSB		NUM(4,2)	PS	pS, (- log sulfide conc.) measured in borehole section

PSY	NUM(4,2) PS	pS, (- log sulfide conc.)in water from borehole section, measured at the surface
PSIY	NUM(4,2) PS	pS, (- log sulfide conc.) in water from borehole section, measured at the surface
O2Y	NUM(4,2) O2	conc. of dissolved oxygen (mg/l) in water from borehole section, measured at the surface
INDAT	CHAR(6) DATE	date of input to database (yymmdd)

## 3.2. Description of tables in GEOTAB containing analytical data

The tables are stored under the creator (see GEOTAB Operators Manual) GEO\_DB.

## MAIN Water Analysis – Major constituents and trace metals

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to sampled section (m)
DATE	*	CHAR(6)	DATE	sampling date (yymmdd)
SNO	*	NUM(4)	SNO	sampling number
NA		NUM(5,1)	NA	sodium (mg/l)
K		NUM(4,2)	K	potassium (mg/l)
CA		NUM(5,1)	CA	calcium (mg/l)
MG		NUM(4,1)	MG	magnesium (mg/l)
HCO3		NUM(4)	HCO3	bicarbonate (mg/l)
CL		NUM(7,1)	CL	chloride (mg/l)
F		NUM(3,2)	F	fluoride (mg/l)
SO4		NUM(5,2)	SO4	sulphate (mg/l)
BR		NUM(4,2)	BR	bromide (mg/l)
SI		NUM(3,1)	SI	silica (mg/l)
FE		NUM(5,3)	FE	iron (mg/l)
FEII		NUM(5,3)	FE	iron(II) (mg/l)
MN		NUM(3,2)	MN	manganese (mg/l)
AL		NUM(4,3)	AL	aluminum (mg/l)
LI		NUM(5,4)	LI	lithium (mg/l)
SR		NUM(5,3)	SR	strontium (mg/l)
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

## REM Water Analysis – Remaining Parameters

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to sampled section (m)
DATE	*	CHAR(6)	DATE	sampling date (yymmdd)
SNO	*	NUM(4)	SNO	sample number
PO4P		NUM(4,3)	PO4P	phosphate phosphorus (mg/l)
NO2N		NUM(4,3)	NO2N	nitrite nitrogen (mg/l)
NO3N		NUM(4,3)	NO3N	nitrate nitrogen (mg/l)
NH4N		NUM(4,3)	NH4N	ammonium nitrogen (mg/l)
S		NUM(3,2)	S	sulfide (mg/l)
I		NUM(4,3)	I	iodide (mg/l)
TOC		NUM(4,1)	TOC	total organic carbon (mg/l)
TURB		NUM(4,2)	TURB	turbidity (NTU)
PHL		NUM(3,1)	PHAV	pH measured in laboratory
PHYAV		NUM(3,1)	PHAV	pH measured on-line at the surface, a daily average
CONDL		NUM(5,1)	ECOND	electrical conductivity measured in laboratory (mS/m)
CONDYAV		NUM(5,1)	ECOND	el. cond. measured on-line at the surface, a daily average
O2YAV		NUM(4,2)	O2	oxygen, measured on-line at the surface, a daily average

WFLOW	NUM(6)	WFLOW	water flow rate (ml/min)
DRILLW	NUM(4,2)	DRILLW	drilling water residuc (%)
INDAT	CHAR(6)	DATE	date of input to database (yymmdd)

EQUIV      Water Analysis – Major constituents expressed in milliequivalents.

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to sampled section (m)
DATE	*	CHAR(6)	DATE	sampling date (yymmdd)
SNO	*	NUM(4)	SNO	sample number
NAEKV		NUM(5,2)	NAEKV	sodium (mequiv/l)
KEKV		NUM(3,2)	KEKV	potassium (mequiv/l)
CAEKV		NUM(5,2)	CAEKV	calcium (mequiv/l)
MGEKV		NUM(4,2)	MGEKV	magnesium (mequiv/l)
CAMGEKV		NUM(5,2)	CAMGEKV	calcium+magnesium (mequiv/l)
FEEKV		NUM(3,2)	FEEKV	iron divalent (mequiv/l)
HCO3EKV		NUM(4,2)	HCO3EKV	bicarbonate (mequiv/l)
CLEKV		NUM(5,2)	CLEKV	chloride (mequiv/l)
SO4EKV		NUM(4,2)	SO4EKV	sulphate (mequiv/l)
IONBAL		NUM(4,2)	IONBAL	ion balance (mequiv/l)
IONREL		NUM(4,2)	IONREL	relative ion balance error (%)
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

## 3.3. Description of tables in GEOTAB containing special analysis

## ISOTOPE Special analysis - Isotopes

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to sampled section (m)
DATE	*	CHAR(6)	DATE	sampling date (yymmdd)
SNO		NUM(4)	SNO	sample number
D		NUM(4,1)	D	deuterium (o/oo), deviation from Standard Mean Oceanic Water (SMOW)
TR		NUM(3)	TR	tritium (TU), TU is the number of tritium atoms per E+18 hydrogen atoms
O18		NUM(4,2)	O18	oxygen-18 (o/oo) deviations from SMOW
O18EX		NUM(4,2)	O18	oxygen-18 (o/oo) deviations from SMOW
S34		NUM(3,1)	S34	sulphur (o/oo), deviation from SMOW
C13		NUM(3,1)	C13	carbon-13 isotope (o/oo) of C-12
PMC		NUM(4,2)	C14	carbon-14 or PMC (% modern carbon)
AGEBP		NUM(5)	AGEBP	groundwater age (year)
AGEBPC		NUM(5)	AGEBP	groundwater age correction for C-13 content (year)
COM70		CHAR(70)	COM70	comment
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

## RRUT Special Analysis - Ra, Rn, U, Th

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to sampled section (m)
DATE	*	CHAR(6)	DATE	sampling date (yymmdd)
SNO		NUM(4)	SNO	sample number
RN222		NUM(3,*)	RN222	radon-222 (Bq/l) 1 Bq = 1.76E-10 ug Rn-222
RNDEV		NUM(3,*)	DMVAL	deviation for measured value of radon
RA226		NUM(3,*)	RA226	radium-226 (Bq/l) 1 Bq = 2.74E-5 ug Ra-226
RADEV		NUM(3,*)	DMVAL	deviation for measured value of radium
U		NUM(3,*)	U	uranium (Bq/l) 1 Bq = 39.4 ug U
UDEV		NUM(3,*)	DMVAL	deviation for measured value of uranium
TH		NUM(3,*)	TH	thorium (ug/l)
THDEV		NUM(3,*)	DMVAL	deviation for measured value of thorium
URATIO		NUM(3,*)	URATIO	activity ratio
COM70		CHAR(70)	COM70	comment
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

## GAS Special Analysis - Gases

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to sampled section (m)
DATE	*	CHAR(6)	DATE	sampling date (yymmdd)
SNO		NUM(4)	SNO	sample number
AQVOL		NUM(3)	VOLML	sample volume (l)



GASVOL	NUM(3)	VOLML	gas volume (ml)
N2	NUM(3,1)	N2	nitrogen (%)
O2G	NUM(4,3)	O2G	oxygen (%)
H2	NUM(4,3)	H2	hydrogen (%)
HE	NUM(4,3)	HE	helium (%)
AR	NUM(4,3)	AR	argon (%)
CH4	NUM(4,3)	CH4	methane (%)
CO2	NUM(4,3)	CO2	carbon dioxide (%)
COM70	CHAR(70)	COM70	comment
INDAT	CHAR(6)	DATE	date of input to database (yymmdd)

**PARTIC Special Analysis - Particulate Matter**

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to sampled section (m)
DATE	*	CHAR(6)	DATE	sampling date (yymmdd)
FNO	*	NUM(5)	FNO	filter number
SNO		NUM(4)	SNO	sample number
PORE		NUM(3,2)	PORE	pore size (um)
VOL		NUM(5)	SVOL	sample volume (ml)
ALP		NUM(5,1)	ALP	particulate aluminium (ug/l)
CAP		NUM(5,1)	CAP	particulate calcium (ug/l)
FEP		NUM(5,1)	FEP	particulate iron (ug/l)
MNP		NUM(4,1)	MNP	particulate manganese (ug/l)
SIP		NUM(4,1)	SIP	particulate silicon (ug/l)
SP		NUM(4,1)	SP	particulate sulfur (ug/l)
FE		NUM(4,3)	FEFILT	iron in filtrate (mg/l)
FEII		NUM(4,3)	FEFILT	ferrous iron in filtrate (mg/l)
COM70		CHAR(70)	COM70	comment
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

## 3.4. Description of tables in GEOTAB containing Flyleaf data

## WATERF1: Water Analysis - Flyleaf Page 1

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
START	*	CHAR(6)	DATE	measurement start date (yymmdd)
END	*	CHAR(6)	DATE	measurement end date (yymmdd)
COMP		CHAR(30)	COMP	company responsible for measurement
RESP		CHAR(79)	RESP79	laboratories responsible for chemical determinations
REPORT		CHAR(30)	REPORT	reference
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

## WATERF2 : Water Analysis - Flyleaf Page 2

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
LINENO	*	NUM()	LINENO	line number
COMMENT		CHAR(79)	COMMENT	comment
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

## WATERF3: Water Analysis - Flyleaf Page 3

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to sampled section (m)
START	*	CHAR(6)	DATE	measurement start date (yymmdd)
END	*	CHAR(6)	DATE	measurement end date (yymmdd)
PACKER		CHAR(79)	COMMENT	packer id: D= double, E = single, O = open borehole
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

## WATERF4: Water Analysis - Flyleaf Page 4

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
BHL	*	NUM(4)	BHL	borehole length to sampled section (m)
LINENO	*	NUM()	LINENO	line number
COMZONE		CHAR(79)	COMMENT	comment on measurement zone
INDAT		CHAR(6)	DATE	date of input to database (yymmdd)

## SPECANF- Special Analysis - Flyleaf

Column	Key	Type	Domain	Text
IDCODE	*	CHAR(5)	IDCODE	borehole identification code
START	*	CHAR(6)	DATE	sampling start date
END		CHAR(6)	DATE	sampling end date
RESP1		CHAR(40)	COM40	responsible for sampling data
RESP2		CHAR(40)	COM40	responsible for filter analysis
RESP3		CHAR(40)	COM40	responsible for gas analysis
RESP4		CHAR(40)	COM40	responsible for deuterium analysis
RESP5		CHAR(40)	COM40	responsible for tritium analysis
RESP6		CHAR(40)	COM40	responsible for C isotopes analysis
RESP7		CHAR(40)	COM40	responsible for O 18 analysis
RESP8		CHAR(40)	COM40	responsible for S 34 analysis

RESP9	CHAR(40)COM40	responsible for Ra, Rn, U, Th analysis
RESP10	CHAR(40)COM40	responsible for activity ratio
INDAT	CHAR(6) DATE	date of input to database (yymmdd)

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### **Annual Research and Development Report 1985**

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#### **GEOTAB. Overview**

Ebbe Eriksson<sup>1</sup>, Bertil Johansson<sup>2</sup>, Margareta Gerlach<sup>3</sup>, Stefan Magnusson<sup>2</sup>, Ann-Chatrin Nilsson<sup>4</sup>, Stefan Sehlstedt<sup>3</sup>, Tomas Stark<sup>1</sup>

<sup>1</sup>SGAB, <sup>2</sup>ERGODATA AB, <sup>3</sup>MRM Konsult AB

<sup>4</sup>KTH

January 1992

TR 92-02

**Sternö study site. Scope of activities and main results**

Kaj Ahlbom<sup>1</sup>, Jan-Erik Andersson<sup>2</sup>, Rune Nordqvist<sup>2</sup>,  
Christer Ljunggren<sup>3</sup>, Sven Tirén<sup>2</sup>, Clifford Voss<sup>4</sup>  
<sup>1</sup>Conterra AB, <sup>2</sup>Geosigma AB, <sup>3</sup>Renco AB,  
<sup>4</sup>U.S. Geological Survey  
January 1992

TR 92-03

**Numerical groundwater flow calculations at the Finnsjön study site – extended regional area**

Björn Lindbom, Anders Boghammar  
Kemakta Consultants Co, Stockholm  
March 1992

TR 92-04

**Low temperature creep of copper intended for nuclear waste containers**

P J Henderson, J-O Österberg, B Ivarsson  
Swedish Institute for Metals Research, Stockholm  
March 1992

TR 92-05

**Boyancy flow in fractured rock with a salt gradient in the groundwater – An initial study**

Johan Claesson  
Department of Building Physics, Lund University,  
Sweden  
February 1992

TR 92-06

**Characterization of nearfield rock – A basis for comparison of repository concepts**

Roland Pusch, Harald Hökmark  
Clay Technology AB and Lund University of  
Technology  
December 1991

TR 92-07

**Discrete fracture modelling of the Finnsjön rock mass: Phase 2**

J E Geier, C-L Axelsson, L Hässler,  
A Benabderrahmane  
Golden Geosystem AB, Uppsala, Sweden  
April 1992

TR 92-08

**Statistical inference and comparison of stochastic models for the hydraulic conductivity at the Finnsjön site**

Sven Norman  
Starprog AB  
April 1992

TR 92-09

**Description of the transport mechanisms and pathways in the far field of a KBS-3 type repository**

Mark Elert<sup>1</sup>, Ivars Neretnieks<sup>2</sup>, Nils Kjellbert<sup>3</sup>,  
Anders Ström<sup>3</sup>  
<sup>1</sup>Kemakta Konsult AB  
<sup>2</sup>Royal Institute of Technology  
<sup>3</sup>Swedish Nuclear Fuel and Waste Management Co  
April 1992