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Oskarshamn site investigation

Characterization of soil samples from three valleys in the Laxemar area

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

Data in SKB's database can be changed for different reasons. Minor changes in SKB's database will not necessarily result in a revised report. Data revisions may also be presented as supplements, available at www.skb.se.

A pdf version of this document can be downloaded from www.skb.se.

Abstract

The Swedish Nuclear and Waste Management Company (SKB) carries out site investigations in the Oskarshamn area. One important part in this is to clarify the connections between bedrock, soils and ground surface ecosystems to understand flow conditions from bedrock to the ground surface.

Soils from three small valleys in the Laxemar area were sampled in October/November 2006, and from 17 samples, eight composite samples were pooled. Sample preparation was performed by Department of Forest Soils, Swedish University of Agricultural Sciences. The samples were then characterized for a number of parameters important for geochemical sorption. Chemical soil analysis, element analysis, mineralogical analysis and BET-surface analysis were carried out. Water from four groundwater monitoring wells were also sampled and analysed for a large number of parameters.

The soil material differed considerably from peat and gyttja to till, sand, clay and clay gyttja. Soil chemical analysis was performed by Department of Forest Soils, Swedish University of Agricultural Sciences after drying the samples in 35°C. Analysis included pH_{H20} and pH_{CaCl2} , C, N, exchangeable Ca, Mg, Na, K and Mn in 1 M ammonia-acetate at pH 7, titratable acidity, extractable K and P in ammonia-lactate (AL) and together with Cu in 2 M hydrochloric acid (HCl). Further, *Aqua Regia* extractions were made with determinations of Fe, Al, Mn, Na, K, Ca, and Mg. Also determinations of Fe, Al and Mn in dithionite citrate solution were carried out.

Chemical conditions revealed differences between the soils with mainly a poor sand and low contents of many elements in the till soils but anyhow rather high base saturation and relatively high pH value. The carbon and nitrogen contents were mainly relatively low except for the gyttja soil with over 2% N. The highest contents of most elements were found in the gyttja soil but despite this, pH was rather low. Also the clay soil furnished rather high contents, especially in *Aqua Regia* extractions. The peat/gyttja carbon content was low and probably influenced by mineral soil material and water adding iron, calcium and aluminium to the soil. Also copper was high in the peat/gyttja.

Seven soil samples were analysed by X-ray diffraction (XRD) by Geological survey of Sweden, in order to characterise their mineral contents; two till samples, one sand sample, one clay sample, two gyttja clay samples and one gyttja sample. In the tills, minerals in the matrix fraction (grain size fraction < 2 mm) and in the sand, mineral in bulk sample were determined qualitatively and quantitatively. Minerals of the clay fraction were determined separately but only qualitatively. In the clay sample, in the gyttja clay samples and in the gyttja sample bulk samples as well as clay fractions were analysed only qualitatively.

The matrix of the till samples was dominated by quartz, plagioclase and K-feldspar; furthermore, peaks from amphibole (hornblende), chlorite, muscovite and calcite were also present. The clay fractions of the till samples were dominated by illite and chlorite.

The bulk analysis of the sand sample showed that it was dominated by quartz, plagioclase and K-feldspar; furthermore, peaks from amphibole (hornblende), chlorite and muscovite were also present. The clay fraction of the sand sample was dominated by illite and chlorite.

The clay sample bulk analysis showed that it was dominated by quartz, plagioclase, K-feldspar, illite and chlorite. Amphibole (hornblende) peaks were also present. The clay fraction of the clay sample was dominated by illite, chlorite and kaolinite.

The bulk analyses of the gyttja clay samples showed them to be, excepting amorphous material, dominated by quartz, plagioclase, K-feldspar, illite and chlorite. The samples also exhibited peaks from kaolinite. The clay fractions were dominated by illite and chlorite, in one sample together with kaolinite.

The bulk analysis of the mineral part of the gyttja sample showed it to contain, in addition to amorphous material, quartz, plagioclase, K-feldspar, illite and chlorite as major components. The clay fraction was dominated by illite, chlorite and kaolinite.

The eight soil samples was also analysed for about 50 elements and 10 oxides by ALS Scandinavia AB. The analyses were performed by ICP-AES, ICP-SFMS and AFS. In all techniques except AFS plasma formed by argon gas was used. Furthermore, the eight soil samples leached in dithionite citrate was analysed for about 60 elements. The leachings had earlier been performed by Swedish University of Agricultural Sciences.

Four groundwater monitoring wells was sampled in March 2007 and analysed for a large number of parameters, including about 50 elements, anions, pH, conductivity, alkalinity, HS⁻, Fe (II), Fe (tot), nutrients, TOC and DOC. Laboratories performed analyses were ALS Scandinavia AB, Äspö Laboratory and Department of Systems Ecology, University of Stockholm. Water was also sampled and stored for planned geochemical sorption studies.

BET measurements were performed on eight site-specific materials from Oskarshamn according to the ISO 9277 standard method. BET is a method for measuring the specific surface area of a solid material by use of gas adsorption. The measurements were performed by the Technical Research Institute of Sweden (SP). The results showed to be as expected, in view of the characteristics of the different soil types. The correspondence between the replicates was relatively good (double samples). The BET values differed clear between fine soils and till, and also between till and sand.

Sammanfattning

Svensk Kärnbränslehantering AB (SKB) genomför platsundersökningar i Oskarshamnsområdet. En viktig del i dessa är att klarlägga kopplingar mellan berggrund, jordlager och ytekosystem för att förstå transportmekanismer från berggrunden till ytsystemen.

I oktober/november 2006 togs cirka 45 jordprover från tre dalgångar i Laxemar. Sjutton stycken av dessa jordprover valdes ut för att användas i ett karakteriseringsprogram, med parametrar viktiga för geokemisk sorption. Provberedningen utfördes av Sveriges Lantbruksuniversitet, institutionen för skoglig marklära. Några prover slogs ihop på grund av materialbrist och slutligen analyserades åtta stycken jordprover. Karakteriseringen har utförts av flera olika laboratorier och bestod bland annat av jordkemiska analyser, elementanalyser, mineralogiska analyser samt BET-yta. Vattenprovtagning från fyra grundvattenrör belägna i områdena utfördes också och ett stort antal kemiska parametrar analyserades.

Jordmaterialet var av klart olika sammansättning och omfattade material från torv, gyttja, lergyttja, lera, sand till morän. Skillnader i kemisk sammansättning och adsorberade joner var således att vänta. Jordkemiska analyser utfördes av Sveriges Lantbruksuniversitet efter att de åtta proverna torkats i 35 °C. Kemiska analyser omfattade pH_{H20} och pH_{CaCl2}, C, N, utbytbart Ca, Mg, Na, K och Mn i 1 M ammoniumacetat vid pH 7, aciditet, extraherbart K och P i ammoniumlaktat och även med Cu i 2 M saltsyra (HCl). Dessutom utfördes extraktioner i kungsvatten *(Aqua Regia)* med bestämningar av Fe, Al, Mn, Na, K, Ca, och Mg. Även bestämningar av Fe, Al och Mn i ditionitcitrat utfördes. Det gjordes också vattenhaltsbestämningar och analys för kompakt densitet.

De kemiska förhållandena återspeglade till stor del markens innehåll av organiskt material och lera. Av detta följer att sand och moränjordarna uppvisade mindre innehåll av ämnen än övriga jordar. Moränerna hade dock relativt högt pH och basmättnaden var hög trots begränsat ämnesinnehåll. Kol- och kväveinnehållen var mestadels relativt låga förutom avseende gyttjajorden. Denna uppvisade också störst innehåll av de flesta ämnen men trots detta ett relativt lågt pH. Lerjorden visade också ganska stort innehåll av ämnen särskilt avseende extraktionen med kungsvatten (*Aqua Regia*). Torv/gyttjaprovets kolinnehåll var lågt och sannolikt var materialet påverkat av minerogent material och inflödande minerogent grundvatten. Detta gav tämligen höga värden på järn, aluminium och kalcium. Dessutom var kopparinnehållet i torv/gyttjaprovet det största bland ingående jordar.

Sju jordprov analyserades med hjälp av röntgendiffraktometri (XRD) för karakterisering av mineralogi vid Sveriges Geologiska Undersökning (SGU); två moränprov, ett sandprov, ett lerprov, två prov av gyttjelera och ett gyttjeprov. I moränproven analyserades matrixfraktionen (kornstorlek < 2 mm) och i sandprovet totalprov, med kvalitativ och kvantitativ analys. Mineralogin i lerfraktionen analyserades kvalitativt i separata provberedningar. Lerprovet, gyttjelereprovet samt gyttjeprovet analyserades kvalitativt i både totalprov och lerfraktion.

Matrix i moränproven dominerades av kvarts, plagioklas och kalifältspat. Därutöver uppträdde också toppar från amfibol, klorit, muskovit och kalcit. Lerfraktionen i proven dominerades av illit och klorit.

Totalprovsanalys av sandprovet visade att detta dominerades av kvarts, plagioklas och kalifältspat; därutöver uppträdde också toppar från amfibol, klorit och muskovit i diffraktogrammet. Lerfraktionen dominerades av illit och klorit.

Totalprovsanalys av lerprovet visade att det domineras av kvarts, plagioklas, kalifältspat, illit och klorit. Amfiboltoppar uppträdde också. Lerfraktionen dominerades av illit, klorit och kaolinit.

Totalprovsanalyser av gyttjeleraproven visade att de, utöver amorft material, domineras av kvarts, plagioklas, kalifältspat, illit och klorit. Proven uppvisade även kaolinittoppar, samt i ett fall, svaga pyrittoppar. Lerfraktionerna dominerades av illit och klorit, samt i ett prov, kaolinit.

Totalprovsanalys av mineralkomponenten i gyttjeprovet visade att den (utöver amorft material) innehåller kvarts, plagioklas, kalifältspat, illit och klorit som huvudkomponenter. Lerfraktionen dominerades av illit, klorit och kaolinit.

De åtta jordproverna analyserades också med avseende på cirka 50 element och 10 oxider. Analyserna utfördes av ALS Scandinavia AB med ICP-AES, ICP-SFMS och AFS. Dessutom analyserades även lakningar i ditionitcitrat, utförda på de åtta jordproverna, med avseende på cirka 60 element. Lakningarna hade tidigare utförts av Sveriges Lantbruksuniversitet.

Fyra grundvattenrör provtogs i mars 2007 och analyserades på ett stort antal parametrar, bland annat cirka 50 element, anjoner, pH, konduktivitet, alkalinitet, sulfid, Fe (II) och Fe (tot), näringsämnen och kol (DOC och TOC). Laboratorierna som utförde analyserna var ALS Scandinavia AB, Äspölaboratoriet och Systemekologen, Stockholms Universitet. Vatten sparades också för kommande undersökningar beträffande geokemisk sorption.

BET-mätningar utfördes av SP Sveriges Tekniska Forskningsinstitut på åtta platsspecifika jordprover från Oskarshamn enligt standardmetoden ISO 9277. BET är en metod för att mäta den specifika ytarean på ett fast material med hjälp av gasadsorption. Resultaten var i stort som förväntat med hänsyn taget till materialens olikheter, och repeterbarheten var relativt god (dubbelprover). Resultaten visar bland annat tydliga skillnader mellan finjordar och morän och mellan morän och sand.

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1 Introduction

This document reports the data gained by the soil- and groundwater investigations in three valleys in the Oskarshamn/Laxemar area, which is some of the activities performed within the site investigation at Oskarshamn. The work was carried out in accordance with activity plans listed in Table 1-1. Activity plans are SKB's internal controlling documents. All data from the investigations have been stored in the database SICADA and are traceable by the activity plan numbers.

The soil samples were used to characterize the conditions in three deep valleys in the Oskarshamn area (Figure 1-1). The characterization relates to soil conditions with importance to the transport of radio nuclides and to geochemical sorption.

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

Activity Plan	Number	Version
Karakterisering av jordprover från tre dalgångar i Laxemar	AP PS 400-07-012	1.0
Batchsorptionsmätningar på jord	AP PS 400-07-019	1.0
Hydrokemisk jordrörsmonitering 2007	AP PS 400-07-020	1.0



Figure 1-1. Overview from the three valleys where soil- and groundwater samples were taken for characterization. 1: Valley Mederhultsån, 2: Valley Ekerumsbäcken and 3: Valley Laxemarån.

2 Objective and scope

The soils of the Oskarshamn area are fairly young. The soil material is of till origin, which was influenced by the sea during the transgressions of the Baltic Sea. By this, redistribution of soil material occurred and left coarse water washed tills in higher locations, also with thin soils and bare bedrock. Elsewhere, in depressions the redistributed fine material has been deposited as sorted sediment soils. During the overall transgression, sea bays have been cut off and now forms wet soils and peatlands.

The soil conditions of the regolith are of great significance in the transfer of water and elements from the bedrock to the surface ecosystems. Information on the spatial variations with horizon-tal distances as well as with soil depth contributes in clarification of pathways and transfer in the regolith. The identified valleys are of special interest as it would be expected to be primary site for carrying nuclides to the surface soils.

During October–November 2006, drilling, sampling of soil, and installation of ground water wells was performed in the Oskarshamn area /1/. The soil samples were used to characterize the conditions in three deep valleys in the Oskarshamn area (Figure 1-1). The characterization relates to soil conditions with importance to the transport of radio nuclides and to geochemical sorption. Several laboratories were included to find out the special geochemical prerequisites for element turnover. Eight soil samples were prepared and analysed, and some samples were formed as composite samples. In addition, water samples were taken at one occasion in four groundwater monitoring wells. The water was analysed for a large number of parameters. All sites sampled can be viewed in Figure 2-1, 2-2 and 2-3. In Table 2-1 the different parts of the characterization is listed.



Figure 2-1. Sites in the valley Mederhultsån, where soil- and groundwater samples were taken for characterization.



Figure 2-2. Sites in the valley Ekerumsbäcken, where soil- and groundwater samples were taken for characterization.



Figure 2-3. Sites in the valley Laxemarån, where soil- and groundwater samples were taken for characterization.

Activity	Laboratory/performer	Sample type	No of samples	Comment
Particle size distribution, organic content, carbonate content	SWECO Geolab	Soil (B-samples)	45	Reported in SKB P-07-91 /1/
Water sampling	SKB internal	Groundwater	4	Groundwater monitoring wells
Water analysis	Äspö laboratory, ALS Scandinavia AB, Luleå, Department of Systems Ecology, University of Stockholm	Groundwater	4	Groundwater monitoring wells
Compact density and water content	SLU, Department of Forest Soils	Soil (A-samples)	17	Original single samples
Soil preparations	SLU, Department of Forest Soils	Soil (A-samples)	12	All original single samples used to form the eight samples
Compact density and water content	SLU, Department of Forest Soils	Soil (A-samples)	8	Composite samples included
Soil chemical analyses	SLU, Department of Forest Soils	Soil (A-samples)	8	
Analysis of elements	ALS Scandinavia AB, Luleå	Soil (A-samples)	8	
Analysis of elements	ALS Scandinavia AB, Luleå	Leachings from SLU	8	Dithionite citrate
Mineralogical characterisation	Geological Survey of Sweden	Soil (A-samples)	7	Peat excluded
BET measurements	SP Technical Research Institute of Sweden	Soil (A-samples)	8	

Table 2-1. The different parts of the characterisation performed.

3 Execution

3.1 Soil material, preparation and soil chemical analysis

Soil was in autumn 2006 sampled in connection to groundwater installations and investigations /1/ (Figure 1-1). Seventeen samples were prepared for analysis /2/ (Table 3-1). In this context samples for some analysis should be field fresh without drying and therefore the first preparations with 2 mm sieving was made on field moist samples. The original samples ranged a quite wide content of substance and were partly very wet which explains the great loss of weight for some samples, e.g. the sand samples (Table 3-1). The till samples contained stones and material that did not pass when sieving, and the sample weight decreased a lot (Table 3-1).

The number of samples totally included were 17 but by compilation pooled into 8 composite samples for the analysis. The original samples were thought to be mixed according to the parent material composition /2/ (Table 3-2). Three composite samples were made while the other five samples were the primary samples selected for analyses. These latter samples were not pooled because the amount of field sample material was sufficient for the analysis. The other three had to be pooled to reach sufficient amount of material. The three pooled samples were then named with ASM-codes, in order to separate them from the single samples, which were named with PSM-codes. In Table 3-3 the eight soil samples used for the characterization/chemical analysis are listed.

Sample ID ¹	Name	Parent material	Secup-Seclow (m)	Field sample weight (g)	After sieving weight (g)	Dry sample weight (g)
PSM001477:1	Torv I	Gyttja	0.0–0.9	577	556	555
PSM001477:2	Gyttja I	Gyttja	0.9–2.6	1,088	1,008	917
PSM001477:3	Lergyttja I	Clay gyttja	2.6–3.0	468	447	385
PSM001477:4	Sand I	Sand	3.0–5.3	1,817	1,762	478
PSM001477:5	Lera I	Clay	5.3–6.5	681	647	406
PSM001477:6	Morän I	Till	8.0–9.0	221	16	4
PSM001477:7	Morän I	Till	9.0–10.0	420	81	44
PSM001472:3	Lergyttja II	Clay gyttja	6.0-7.2	986	964	276
PSM001472:5	Lera II	Clay	8.5–10.9	609	569	341
PSM001472:7	Morän II	Till	12.0–12.5	1,707	474	444
PSM001473:2	Morän II	Till	6.5–7.65	2,001	417	409
PSM001479:1	Torv I	Peat	0.0-0.7	433	413	377
PSM001479:2	Gyttja I	Gyttja	0.7–3.6	862	840	183
PSM001479:4	Sand I	Sand	5.1–9.3	2,007	1,977	711
PSM001479:6	Morän I	Till	12.0–13.0	1,284	543	490
PSM001479:7	Morän I	Till	13.6–14.6	434	-	-
PSM001480:6	Lera II	Clay	5.7–7.8	1,010	938	649

Table 3-1. Field samples, content from	field, after sieving and dry weight in g
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¹Sample name according to field protocol at sampling. The first six digits identify the profile and the number after colon relates to the order in the profile.

Table 3-2.	Original s	oil samples	and the planned	structure of bulking.
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Soil type	ID-code/sample	Addition for bulk ¹
Torv I, gyttja	PSM001477:1	PSM001479:1 (peat)
Gyttja I, gyttja	PSM001477:2	PSM001479:2
Lergyttja/gyttjelera I, clay gyttja/gyttja clay	PSM001477:3	PSM001472:3 (priority)
Sand I, sand	PSM001477:4	PSM001479:4
Lera I, clay	PSM001477:5	PSM001480:6 (priority)
Morän I, till	PSM1477:6 + PSM1477:71	PSM1479:6 + PSM1479:71
Morän II, till	PSM001472:7	PSM001473:2
Lergyttja/gyttjelera II, clay gyttja/ gyttja clay	PSM001472:3 (if necessary together with PSM001477:3)	_2
Lera II, clay	PSM001480:6 (if necessary together with PSM001477:5)	PSM001472:5

¹ Addition described separatly /2/.

² Clay II replaces Clay gyttja II if sufficient sample of clay gyttja II not available.

Sample ID code	Sample name	Pooled ratio by wet weight (%)	Ratios by dry weight (%)	Dry matter (q)
			0 ()	(0)
ASM000124	2T	PSM001477:1 (57%) + PSM001479:1 (43%)	80% + 20%	300
ASM000125	2LGI	PSM001477:3 (60%) + PSM001472:3 (40%)	52% + 48%	233
ASM000126	3MI	PSM001477:6 (2.5%) + PSM001477:7 (12.5%) + PSM001479:6 (85%)	1% + 8% + 91%	537
PSM001472:7	MII	PSM001472:7	100%	441
PSM001472:3	LGII	PSM001472:3	100%	192
PSM001477:2	GI	PSM001477:2	100%	209
PSM001477:4	SI	PSM001477:4	100%	478
PSM001477:5	LI	PSM001477:5	100%	406

 Table 3-3. The eight soil samples for characterization/chemical analysis and the actual composition of the pooling of sub samples.

The pooled sample ASM000124 is a mix of PSM001477:1 and PSM001479:1, of which PSM1477:1 was originally classified as peat but subsequently reclassified as gyttja. The pooled sample ASM000124 is therefore classified as peat/gyttja.

Water contents were determined on the 17 samples from field. After selection and pooling of samples, portions of these were sent to the different laboratories.

Soil chemical analysis was performed by Department of Forest Soils, Swedish University of Agricultural Sciences after drying the samples in 35°C. Analysis included pH_{H2O} and pH_{CaCl2} , C, N, exchangeable Ca, Mg, Na, K and Mn in 1 M NH₄Ac at pH 7, titratable acidity, extractable K and P in ammonia-lactate (AL) and together with Cu in 2M hydrochloric acid (HCl). Further, *Aqua Regia* extractions were made with determinations of Fe, Al, Mn, Na, K, Ca, and Mg. Also determinations of Fe, Al and Mn among several other elements in dithionite citrate solution were carried out, but by another laboratory, i.e. ALS Scandinavia AB, Luleå. Analysis was performed according to the ICP Forest Manual (2006) /3/ and for NH₄Ac extractions Karltun et al. (1996) /4/.

3.2 Mineralogical characterization

Seven samples were analysed in order to characterise their mineral contents; two till samples, one sand sample, one clay sample, two gyttja clay samples and one gyttja sample. In the tills, minerals in the matrix fraction (grain size fraction < 2 mm) and in the sand, mineral in bulk sample were determined qualitatively and quantitatively. Minerals of the clay fraction were determined separately but only qualitatively. In the clay sample, in the gyttja clay samples and in the gyttja sample bulk samples as well as clay fractions were analysed only qualitatively. The analyses were performed at the Geological Survey of Sweden (SGU) by the use of X-ray diffraction.

Samples with high water/moisture content were supplied, ca 30 g of each sample. From the till samples and the sand sample 15 g, and from the clay, gyttja and gyttja clay samples 10 g were taken from each for separation of fractions $< 2 \mu m$ (clay fraction). The remaining material from the till and sand samples was dried in laboratory oven at 110°C. Also the clay, gyttja clay and gyttja samples, 5 g, 5 g and 10 g, respectively, were dried at this temperature.

The dried till and sand samples were crushed to a grain size < 0.5 mm and then split down to 1.7–1.8 g in a laboratory micro-splitter. An internal standard, the synthetic equivalent of zincite (ZnO) was added to the samples, making up 10% by weight,. The sample + zincite mixtures were then ground for 10 minutes in alcohol in a micronising mill utilising agate grinding elements. The powders thus obtained were dried and prepared for analysis by sidewards packing under vibration in order to maximise the randomness of orientation of the crystallites. The dried clay, gyttja and gyttja clay samples were ground to a fine powder in an agate mortar and the prepared for analysis in the same way.

The portions taken out for separation of fractions $< 2 \ \mu m$ were suspended in distilled water in beakers and treated in ultrasonic for about half an hour. The suspensions were stirred and set for sedimentation. After a set time the upper part of the suspensions containing clay particles was siphoned from the suspensions and filtered for oriented specimen's preparation /5/. Separation of clay particles in samples with high content of organic matter, viz. the gyttja and gyttja clay samples was somewhat problematic due to flocculation of the particles even then a dispersion agent (sodium hexametaphosphate) is added. To remove the organic matter from the samples an oxidizing agent, sodium hypochlorite (NaClO₄) was used /6, 7/. Treatment of samples in a solution sodium hypochlorite (> 10%): water (1:1) applied during ca 70 hours. After that the samples free from organic matter were washed in distilled water and clay particles separated in the same way as in the other samples.

The X-ray diffraction analyses were carried out at the Geological Survey of Sweden in Uppsala using a Siemens D5000 (theta-theta) diffractometer (CuK α -radiation). The X-ray generator was operated at 50 kV and 40 mA for qualitative and quantitative analysis of the random oriented crystallites. Scans were run from 5° to 65° (2-Theta) counting 2 s per 0.02°. These analyses were performed with a 2.0 divergence slit, a 0.6 mm antiscatter slit and 0.1 mm receiving slit in the ray path. For analysis of clay mineral analyses generator was operated at lower voltage, 40 kV and 40 mA, respectively. When the clay separations were analysed, scans were run from 2° to 35° (2-Theta) counting 1 s per 0.02°, featuring a 1° divergence slit, a 2 mm antiscatter slit and 0.1 mm receiving slit in the ray path.

The X-ray diffraction raw files were taken up in the Bruker/Siemens software DIFFRAC^{PLUS} (version 2.2), including the PDF /8/ database for mineral identification. The best-fit lines for the identified minerals in the samples are shown with different colours in the X-ray diffractograms shown for the randomly analysed specimen.

Qualitative analyses of the clay minerals were carried out with preferred orientation of clay mineral crystallites in four steps; sample in natural, dried condition, sample saturated with ethylene glycol (EG), sample heated to 400°C and sample leached with hydrochloric acid (1 HCl: $4 H_2O$). Data from Brindley and Brown /9/ was applied for identification of the clay minerals.

The quantitative X-ray diffraction analyses were carried out by means of Rietveld technique in TOPAS R software /10/.

3.3 Analysis of elements and oxides in soil samples

The analyses were performed by ICP-AES, ICP-SFMS and AFS (ICP stands for Inductively Coupled Plasma). In all techniques except AFS a plasma formed by argon gas was used.

ICP-AES stands for optical emission spectrometry with inductively coupled plasma. The plasma flows through a radiofrequency field where it is kept in a state of partial ionisation, i.e. the gas consists partly of electrically charged particles. This allows it to reach very high temperatures of up to 10,000°C. At high temperature, most elements emit light of characteristic wavelengths, which can be measured and used to determine their concentrations.

In ICP-SFMS (sector field mass spectrometry), the plasma is of the same type as in ICP-AES, but it is used to convert elements to ions which are then separated by mass-to-charge ratio in a mass spectrometer. This allows the different elements in a sample (and their natural isotopes) to be separated and their concentrations determined.

Atomic fluorescence (AFS) has been used for the determination of Se. This technique uses photon emission from atoms as in ICP-AES, although excitation is not achieved thermally, but by light of a wavelength characteristic of the element. This light is absorbed by the atom and subsequently re-emitted to generate the analytical response. Determination of Hg in leach water samples was performed with AFS, all other sample types were analysed by ICP-SMFS for Hg-analysis.

The collected samples that were analysed consisted of soil samples. Parameters analysed can be viewed in Table 3-4 and Table 3-5. Extractions for determination of leaching were performed by the Department of Forest Soils, Swedish University of Agricultural Sciences, whereas the analyses of elemental composition in dithionite citrate solutions were made at ALS Scandinavia AB (Table 3-5).

The soil samples were delivered by Swedish University of Agricultural Sciences and the sample preparations and elemental analyses were performed by ALS Scandinavia AB. Macroelements was determined by a subcontractor, GBA (Gesellschaft für Bioanalytik, Hamburg).

Appropriate digestion methods suitable for different types of samples have been used. Table 3-6 shows an overview of the analysis packages.

Oxide	Unit	Oxide	Unit
Al ₂ O ₃	%dw	Na₂O	%dw
CaO	%dw	P_2O_5	%dw
Fe_2O_3	%dw	SiO ₂	%dw
K ₂ O	%dw	TiO ₂	%dw
MgO	%dw	Sum oxides	%dw
MnO	%dw	LOI (Loss on ignition)	%dw

Table 3-4. Oxides determined in soil samples in this study.

Element	Unit	Analyse package	Element	Unit	Analys package
Ag	mg/kg dw	M7	Nb	mg/kg dw	MG1
As	mg/kg dw	MG1	Nd	mg/kg dw	MG1
В	mg/kg dw	M7	Ni	mg/kg dw	MG1
Ва	mg/kg dw	MG1	Pb	mg/kg dw	M7
Be	mg/kg dw	M7	Pr	mg/kg dw	MG1
Br	mg/kg dw	MG1 ²	Rb	mg/kg dw	MG1
Cd	mg/kg dw	MG1	S	mg/kg dw	MG1
Се	mg/kg dw	MG1	Sb	mg/kg dw	M7
CI	mg/kg dw	MG1 ²	Sc	mg/kg dw	MG1
Co	mg/kg dw	M7	Se	mg/kg dw	M7
Cr	mg/kg dw	MG1	Sm	mg/kg dw	MG1
Cs	mg/kg dw	M7	Sn	mg/kg dw	MG1
Cu	mg/kg dw	MG1	Sr	mg/kg dw	MG1
Dy	mg/kg dw	MG1	Та	mg/kg dw	MG1
Er	mg/kg dw	MG1	Tb	mg/kg dw	MG1
Eu	mg/kg dw	MG1	Th	mg/kg dw	MG1
Ga	mg/kg dw	MG1	TI	mg/kg dw	M7
Gd	mg/kg dw	MG1	Tm	mg/kg dw	MG1
Hf	mg/kg dw	MG1	U	mg/kg dw	MG1
Hg	mg/kg dw	MG1	V	mg/kg dw	MG1
Но	mg/kg dw	MG1	W	mg/kg dw	MG1
I	mg/kg dw	MG1 ²	Y	mg/kg dw	MG1
La	mg/kg dw	MG1	Yb	mg/kg dw	MG1
Li	mg/kg dw	M7	Zn	mg/kg dw	M7
Lu	mg/kg dw	MG1	Zr	mg/kg dw	MG1
Мо	mg/kg dw	MG1			
Dry substance (105°C)	%				
Macro elements:					
Total carbon	mg/kg dw				
Total organic carbon	mg/kg dw				
Total nitrogen	mg/kg dw				
Total organic nitrogen	mg/kg dw				

Table 3-5.	Elements d	etermined i	n soil	samples	and in	dithionite	citrate	solutions ¹
in this stu	ıdy.							

¹ In dithionite citrate AI, Ca, Fe, K, Mg, Mn, Na, P, Si, and Ti was also analysed. Macro elements and Br, CI and I, was not analysed in dithionite citrate.

²Br, Cl and I, the sample was leached in highly purified water.

Table 3-6. Overview of analysis packages.

Type of sample	Analysis package	Macroelements ¹
Soil	MG1, M7	TOC, C-tot, N-tot, N-org.
Leach liquid	E2A	-

¹ Subcontractor, GBA, has been used for these analyses.

Description of the analysis packages:

MG1

• The sample was dried at 50°C. For the elements As, Cd, Hg, Cu, Ni and S, the sample was leached with 7 M nitric acid (HNO₃) in a closed Teflon vessel in a microwave oven. Concentrations have been reported on a dry weight (105°C) basis. For Br, Cl and I, the sample was leached in highly purified water. The other elements were determined after fusion with lithium metaborate followed by dissolution in diluted nitric acid. For the elements included in MG1, see Table 3-5.

M7

• Samples were digested using hydrofluoric acid (HF)/perchloric acid (HClO₄)/nitric acid (HNO₃) on a hot plate. The elements determined by method M7 are Ag, B, Be, Co, Cs, Pb, Sb, Se, Tl, Li and Zn.

E2A

• The sample was diluted with nitric acid (HNO₃) and then analysed.

Macro elements

- Total carbon and total organic carbon (TOC) measurements, were carried out according to standard method DIN ISO 10694, Soil quality Determination of organic and total carbon after dry combustion (elementary analysis).
- Total nitrogen and organic nitrogen measurements, were carried out according to standard method DIN ISO 11261, Soil quality Determination of total nitrogen Modified Kjeldahl method.

The instruments were optimised and calibrated at the start of each working day. Calibration consisted of running a sequence of synthetic blanks, sample preparation blanks, quality control samples (certified reference materials) prepared in parallel with the unknowns, and standard solutions. The calibration sequence was repeated after every 10–15 sample measurements. For measurements by ICP-AES and ICP-SFMS, the internal standard technique was employed to allow correction for instrumental drift and non-spectral interference effects during the analyses.

SICADA orders were registered under three different order numbers in the LIMS (Laboratory Information Management System). Data from LIMS were extracted to Excel-files with the laboratory standard program LMM (LabMasterMail). Using a special macro for SICADA, information was extracted from the Excel-files to the SICADA template, and then the templates were saved with names corresponding to the order numbers. The macro-file constituted a database that translated the element code to SICADA element code. After the SICADA templates were delivered to SKB the activity leader included possible information concerning the samples.

3.4 BET- measurements

BET (Brunauer, Emmet, Teller, see /11/) is a method for measuring the specific surface area of a solid material by use of gas adsorption. BET measurements have been performed on site-specific materials from Laxemar according to the ISO 9277 standard method. BET measurements are performed at the SP Technical Research Institute of Sweden (SP).

The determination of specific surface area does not produce sorption coefficients (*Kd* or *Ka*) i.e. parameters that are used in the safety assessment calculation to determine the retardation of radionuclides due to adsorption on to mineral surfaces. However, the BET surface areas, as well as the CEC, are good diagnostic parameters in order to give rough qualitative estimations of the sorption capacity of different geologic materials.

BET surface areas in this investigation are measured on eight soil samples (Table 3-3). All samples were dried at 80°C for 48 hours. Clay and gyttja were slightly grinded in a mortar and was then further dried at 80°C for 24 hours.

3.5 Sampling and analysis of groundwater monitoring wells

Four groundwater monitoring wells (Figure 2-1, 2-2 and 2-3) were sampled in Mars 2007 and the water was analysed for large number of parameters (Table 3-7 and Table 3-8). From each groundwater well a vessel holding five litres was stored in refrigerator. The water was planned to be used in future sorption studies.

Outdoor and indoor treatment of water samples are listed in Appendix 1.

Table 3-7.	The four sampled	groundwater	monitoring wells.
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ID code	Valley/stream	Sampling date
SSM000260	Mederhultsån	2007-03-20
SSM000261	Mederhultsån	2007-03-20
SSM000262	Ekerumsbäcken	2007-03-22
SSM000263	Laxemarån	2007-03-22

Table 3-8. Parameters analysed from groundwater monitoring wells.

Parameter	Laboratory
pH, conductivity, alkalinity	Äspö Laboratory
Negative ions (F, Br, Cl, SO ₄)	Äspö Laboratory
Fe II + Fe-tot	Äspö Laboratory
HS⁻	Äspö Laboratory
Main components (cat ions), B-10, As, Ti, environmental metals, lantanoides, trace elements	ALS Sandinavia AB, Luleå
Hg	ALS Sandinavia AB, Luleå
lodine	ALS Sandinavia AB, Luleå
Nutrients (NH ₄ , NO ₂ , NO ₃ , PO ₄ , Si)	Systemekologen, Stockholm
Total N and P	Systemekologen, Stockholm
DOC	Systemekologen, Stockholm
TOC	Systemekologen, Stockholm
Archive	-

3.6 Nonconformities

Extractions for determination of leaching were performed by the Department of Forest Soils, Swedish University of Agricultural Sciences, whereas the analyses of elemental composition in dithionite citrate solutions instead were made at ALS Scandinavia AB.

For the leaching samples extracted with dithionite citrate, sulphur was not reported, due to leaching with sodium thiosulfate, $Na_2S_2O_3$.

The pooled sample ASM000124 is a mix of PSM001477:1 and PSM001479:1, of which PSM1477:1 was originally classified as peat but subsequently reclassified as gyttja. The pooled sample ASM000124 is therefore classified as peat/gyttja.

4 Results

4.1 Water content in soil samples

Water contents were determined on the 17 soil samples. This resulted in ratios of dry matter ranging from 0.21 to 0.93 and consequently water contents of 7–79% (Table 4-1).

4.2 Composite samples dry matter and compact density

After selection and pooling of samples, these were dried in 35°C whereupon chemical analysis was performed. To determine the content of elements by actual dry weight, it was necessary to determine the ration of dry weight from these "air dried samples". The values varied between 0.93 and 1.00 (Table 4-2).

It would also have been interesting to know the dry bulk density for estimations of the element content on area base but because the samples was not taken by known volumetric value, only the compact density of the material could be determined. In ordinary salic and granitic soils this would be 2.65 g/cm³, but dependent on content of heavy minerals or organic matter, the values could differ. In the case of the samples included, the organic contents partly were considerable, especially for peat/gyttja mainly being only organic matter. The range of the compact densities in the samples was 1.64–2.67 g/cm³ (Table 4-2).

Sample ID	Sample name	Parent material	Dry matter ratio	H₂O by weight (%)
PSM001472:3	Lergyttja/gyttjelera I	Clay gyttja	0.29	71
PSM001472:5	Lera II	Clay	0.60	40
PSM001472:7	Morän II	Till	0.93	7
PSM001473:2	Morän II	Till	0.93	7
PSM001477:1	Torv I	Gyttja	0.54	46
PSM001477:2	Gyttja I	Gyttja	0.21	79
PSM001477:3	Lergyttja/gyttjelera I	Clay gyttja	0.33	67
PSM001477:4	Sand I	Sand	0.27	72
PSM001477:5	Lera I	Clay	0.63	37
PSM001477:6	Morän I	Till	0.22	78
PSM001477:7	Morän I	Till	0.54	46
PSM001479:1	Torv I	Peat	0.22	78
PSM001479:2	Gyttja I	Gyttja	0.22	78
PSM001479:4	Sand I	Sand	0.36	64
PSM001479:6	Morän I	Till	0.90	10
PSM001479:7	Morän I	Till	0.86	14
PSM001480:6	Lera I	Clay	0.69	31

Table 4-1. The seventeen field samples with dry matter ratio and water content.

Sample ID	Sample name	Dry matter ratio	Compact density g/cm ³
ASM000124	2T	0.94	1.65
ASM000125	2LGI	0.96	2.11
ASM000126	3MI	1	2.65
PSM001472:7	MII	0.96	2.66
PSM001472:3	LGII	0.99	2.1
PSM001477:2	GI	0.93	1.64
PSM001477:4	SI	1	2.67
PSM001477:5	LI	1	2.65

 Table 4-2. Dry matter of the already air dried samples and compact densities of the eight samples.

4.3 Sample pH, carbon and nitrogen

The samples included differed considerably regarding the parent material and could be expected to vary also in range over pH, carbon and nitrogen. The pH in H₂O, giving actual values for the field showed fairly low values in the sand (3.89) and also in one clay gyttja soil (4.26) while the peat/gyttja (4.81) was slightly higher compared to raised bog *sphagnum* peat but was probably a fen peat influenced by mineral soil water. Considerably higher pH were found in the till soils with values around pH 7 (Table 4-3). The pH in the CaCl₂ solution showed a lower potential proton content with the lowest value on 3.82 in the sand and the highest value 6.67 in one till soil (Table 4-3).

Carbon and also nitrogen content in the till soils were very low while peat/gyttja and gyttja reached higher values but for carbon far from pure organic material and with the gyttja soil being on the lower limit for gyttja. Nitrogen content could mainly be considered low, but with the peat/gyttja content being ordinary, while the gyttja soil had a fairly high value (Table 4-3).

4.4 Extractable base cations in NH₄Ac

The fairly lenient extraction of adsorbed elements on the soil particles with ammonia acetate revealed variations between the soils (Table 4-4). High base cation contents were found in the gyttja, peat/gyttja and clay gyttja soils while the base saturation was high in the till and clay soils. Cation exchange capacity reached of course the highest values in the gyttja, peat/gyttja and clay gyttja soils, while the sand and tills were poor (Table 4-4).

Sample ID	Sample name	pH _{н20}	pH _{CaCl2}	C (%)	N (%)
ASM000124	2T	4.81	4.37	15.0	1.14
ASM000125	2LGI	4.26	4.16	5.38	0.71
ASM000126	3MI	6.94	6.42	0.09	0.02
PSM001472:7	MII	7.25	6.67	0.06	0.01
PSM001472:3	LGII	5.75	5.58	6.20	0.81
PSM001477:2	GI	4.26	4.21	19.9	2.25
PSM001477:4	SI	3.89	3.82	0.05	0.03
PSM001477:5	LI	6.33	5.69	0.43	0.09

Table 4-3. Chemical characteristics of the eight samples with pH, carbon (C) and nitrogen (N) content.

Sample ID	Sample name	Mn	Mg	Са	Na	к	Tot acidity	CEC
ASM000124	2T	0.01	1.90	17.0	0.18	0.23	23.2	42.5
ASM000125	2LGI	0.09	7.59	12.3	1.74	0.64	9.69	32.1
ASM000126	3MI	0.02	0.20	4.14	0.08	0.06	0.00	4.51
PSM001472:7	MII	0.02	0.13	4.37	0.10	0.05	0.00	4.69
PSM001472:3	LGII	0.07	9.27	8.27	3.20	0.96	3.98	25.7
PSM001477:2	GI	0.12	14.9	42.5	0.73	0.31	26.7	85.2
PSM001477:4	SI	0.01	0.15	0.59	0.04	0.04	1.19	2.01
PSM001477:5	LI	0.05	3.78	7.06	0.29	0.79	1.30	13.3

Table 4-4. Exchangeable cations (NH₄Ac), acidity and cation exchange capacity (mmol_c/100g dw) in the eight soils of the Laxemar area.

4.5 Extractable cations and metals in Aqua regia

For the eight samples of the three valleys, contents of elements fairly strongly bound to the soil material were extracted by *Aqua Regia* that would reveal a potential content of elements (Table 4-5).

The sand soil was the poorest with low contents of both metals and base cations, while the clay gyttja and gyttja soils furnished fairly high content with the deviation regarding sodium and potassium in the gyttja soil. Also the clay soil had a high content and especially manganese and potassium deviated from the other soils, these two elements rather often show similar patterns. The peat/gyttja soil showed values in between the other soils but for manganese the value was lowest together with the poor sandy soil. The till soils were relatively rich in iron, calcium and magnesium, but other elements were low in comparison (Table 4-5).

4.6 Potassium, phosphorus and copper contents

Important elements with further extractions were potassium and phosphorus together with copper. The contents of these were revealed by the weak extraction by ammonia lactate and the stronger HCl giving a potential available content. The three valley soils showed high contents of both potassium and phosphorus in the clay and gyttja soils. Potassium reached also high values in the clay gyttja soils but phosphorus was only comparably low values. Instead, peat/gyttja and till soils furnished high contents of phosphorus. Low contents were found in the sand (Table 4-6).

Sample ID	Sample name	Fe g/kg	Mn g/kg	Mg g/kg	Ca g/kg	Al g/kg	Na g/kg	K g/kg
ASM000124	2T	15.7	0.08	2.94	5.81	24.1	0.19	2.16
ASM000125	2LGI	24.2	0.22	7.05	3.97	19.4	0.67	4.11
ASM000126	3MI	17.4	0.23	4.41	5.33	6.1	0.12	1.18
PSM001472:7	MII	9.8	0.16	3.03	4.74	4.6	0.08	0.89
PSM001472:3	LGII	28.5	0.27	8.50	3.69	22.4	1.11	5.30
PSM001477:2	GI	14.6	0.13	5.22	12.77	11.4	0.24	2.23
PSM001477:4	SI	6.8	0.09	1.64	2.13	3.0	0.06	0.48
PSM001477:5	LI	32.8	8.50	9.60	4.81	26.1	0.38	6.14

Table 4-5. Base cation and metal contents in the eight soil samples of the three Laxemar valleys extracted by *Aqua Regia* (g/kg dw).

Table 4-6. Extractable potassium (K), phosphorus (P) and copper (Cu) (mg/100g dw) in
ammonia lactate (AL) and hydrochloric acid (HCI) for the eight samples from the Laxemar
valleys.

Sample ID	Sample name	K (AL) mg/100g	K (HCI) mg/100g	P (AL) mg/100g	P (HCI) mg/100g	Cu (HCl) mg/100g
ASM000124	2T	8.9	59.8	4.2	21.6	80.5
ASM000125	2LGI	24.3	148	5.8	12.1	37.4
ASM000126	3MI	3.1	38.9	6.9	26.8	7.2
PSM001472:7	MII	2.8	37.2	3.6	19.9	3.9
PSM001472:3	LGII	36.0	161	10.6	13.4	36.8
PSM001477:2	GI	12.1	76.5	3.5	23.0	36.9
PSM001477:4	SI	1.8	17.3	2.0	11.5	2.7
PSM001477:5	LI	30.7	209	15.1	25.4	21.0

Copper contents reached the highest values in the peat/gyttja followed by gyttja and clay gyttja soils with the pure clay soil being somewhat lower but the very lowest were found in the tills and especially the sandy soil (Table 4-6).

4.7 Dithionite extraction

Complex bound elements, as in oxides and amorphous compounds, in the soil exert important influences on the adsorption of elements on the surfaces of the complexes in the soil. One method to find out the amount of complexes is to extract the soil with dithionite citrate solution and this was made on the eight samples from the three valleys. The extraction revealed comparably high contents of extractable Fe in the peat/gyttja, gyttja and clay soils and somewhat higher values also in the clay gyttja soils as compared with the till and sandy soils (Table 4-7).

Aluminium contents were very high in the peat/gyttja soil and fairly high in the gyttja and clay soils but with low values in the till and sandy soils. The content of Mn is more evenly distributed between the samples without very high values but comparably higher in clay and gyttja soils compared to the others with the sandy soil with a low content (Table 4-7).

Sample ID	Sample name	Fe g/kg dw	Al mg/kg dw	Mn mg/kg dw
ASM000124	2T	6.25	3,659.8	30.9
ASM000125	2LGI	2.61	367.7	30.8
ASM000126	3MI	0.99	49.0	22.9
PSM001472:7	MII	0.58	30.6	12.9
PSM001472:3	LGII	1.15	173.7	32.2
PSM001477:2	GI	5.05	761.1	50.0
PSM001477:4	SI	0.69	55.1	4.4
PSM001477:5	LI	5.75	779.7	64.3

Table 4-7. Dithionite citrate extractable iron (Fe), Aluminium (Al) and manganese (Mn) for the eight samples from the Laxemar valleys.

4.8 X-ray diffraction analysis

4.8.1 Till sample ASM000126

Matrix (grain size fraction < 2 mm)

Quartz, plagioclase ("calcian albite" = oligoclase) and potassium feldspar (microcline) are major minerals in the till matrix as indicated by intense peaks in the X-ray diffractogram which fit to lines for these minerals from the /8/ database. Peaks from hornblende, muscovite (in $< 2 \mu m$ grain size fraction classified as illite), chlorite and calcite are also present in the diffractogram (Figure 4-1). The yellow lines show the positions of peaks of the internal standard (ZnO). Results of the quantitative determinations of minerals in the sample are given in Table 4-8 and Table 4-9.

Mineral		Till sample ASM000126	Till sample PSM001472:7	Sand sample PSM001477:4
	%	10.2	9.8	10.0
Quartz	%	25.2	24.9	32.2
Potassium feldspar	%	21.1	23.7	22.9
Plagioclase	%	37.2	34.3	31.3
Amphibole	%	1.4	1.4	1.1
Muscovite	%	1.9	2.9	0.6
Chlorite	%	2.8	2.8	1.9
Calcite	%	0.08	0.07	

Table 4-8. Mineral composition of matrix (fraction < 2 mm) of two till samples and bulk material of a sand sample (with added internal synthetic ZnO standard, 10% by weight) according to quantitative X-ray diffraction analyses carried out by means of Rietveld technique in TOPAS R software /10/.

Table 4-9. Mineral composition of matrix (fraction < 2 mm) of two till samples and bulk material of a sand sample without the standard according to quantitative X-ray diffraction analyses carried out by means of Rietveld technique in TOPAS R software /10/. Percentages have been normalised to 100 without standard.

Mineral		Till sample ASM000126	Till sample PSM001472:7	Sand sample PSM001477:4
Quartz	%	28.1	27.6	35.8
Potassium feldspar	%	23.5	26.3	25.4
Plagioclase	%	41.5	38.1	34.8
Amphibole	%	1.6	1.6	1.2
Muscovite	%	2.1	3.2	0.7
Chlorite	%	3.1	3.1	2.1
Calcite	%	0.09	0.08	

ASM000126. Fraction < 2 mm. Random orientation.



Figure 4-1. X-ray diffractogram of matrix fraction of sample ASM000126. The analysis was performed with random orientation of crystals.

Clay fraction (grain size fraction < $2 \mu m$)

To identify clay minerals preferred orientation of specimens have to be applied for the analysis. Peak intensities from the sheet silicates (clay minerals) are thereby increased (Figure 4-2).

Illite and chlorite are the predominant clay minerals in the clay fraction (cf. blue diffractogram in Figure 4-2). Very small amounts of kaolinite are also present (cf. turquoise diffractogram). The clay fraction also contains an expanding clay mineral which is interpreted as an interstratified illite/vermiculite (blue diffractogram). Compare changes of X-ray patterns for the black and blue diffractograms at low angles $5^{\circ}-9^{\circ}$ 2-Theta. When the sample is heated (red diffractogram) the swelling layers contract to the same spacing as for the major illite peak (10 Å = 8.8° 2-Theta) which thereby increases in intensity. In addition to clay minerals, quartz, feldspars (potassium feldspar and plagioclase) and small amounts of amphibole are present in the clay fraction (cf. black diffractogram).

4.8.2 Till sample PSM001472:7

Matrix (grain size fraction < 2 mm)

Similar to the sample ASM000126 quartz, plagioclase ("calcian albite" = oligoclase) and potassium feldspar (microcline) are major minerals in the till matrix, as indicated by intense peaks in the X-ray diffractogram which fit to lines for these minerals from the /8/ database. Peaks from hornblende, muscovite (in < 2 μ m grain size fraction classified as illite), chlorite and calcite are also present in the diffractogram (Figure 4-3). The yellow lines show the positions of peaks of the internal standard (ZnO). Results of the quantitative determinations of minerals in the sample are given in Table 4-8 and Table 4-9.



Figure 4-2. X-ray diffractograms of $< 2 \mu m$ fraction of sample ASM000126. The analyses were performed with preferred orientation of crystallites.



Figure 4-3. X-ray diffractogram of matrix fraction of sample PSM001472:7. The analysis was performed with random orientation of crystals.

Illite and chlorite are the predominant clay minerals in the clay fraction (cf. blue diffractogram in Figure 4-4). The clay fraction also contains an expanding clay mineral which is interpreted as an interstratified illite/vermiculite (blue diffractogram). Compare changes of X-ray patterns for the black and blue diffractograms at low angles $5^{\circ}-9^{\circ}$ 2-Theta. Kaolinite has not been idenfied in this sample. When the sample is heated (red diffractogram) the swelling layers contract/ collapse to produce a reflection at the same position as for the major illite peak (10 Å = 8.8° 2-Theta), which thereby increases in intensity. In addition to clay minerals, quartz, feldspars (potassium feldspar and plagioclase) and small amounts of amphibole are present in the clay fraction (cf. black diffractogram).

4.8.3 Sand sample PSM001477:4

Bulk sample

Similar to the till samples (ASM000126 and PSM001472:7) quartz, plagioclase ("calcian albite" = oligoclase) and potassium feldspar (microcline) are major minerals, as indicated by strong peaks in the X-ray diffractogram which fit to lines for these minerals from the /8/ database. Peaks from hornblende, muscovite (in < 2 μ m grain size fraction classified as illite) and chlorite are also present in the diffractogram (Figure 4-5). The yellow lines show the positions of peaks of the internal standard (ZnO). Results of the quantitative determinations of minerals in the sample are given in Table 4-8 and Table 4-9.





Figure 4-4. X-ray diffractograms of $< 2 \mu m$ fraction of sample PSM001472:7. The analyses were performed with preferred orientation of crystallites.



Figure 4-5. X-ray diffractogram of sand sample PSM001477:4. The analysis was performed with random orientation of crystals.

Illite and chlorite are the predominant clay minerals in the clay fraction (cf. blue diffractogram in Figure 4-6). Very small amount of kaolinite is also present (cf. turquoise diffractogram). The clay fraction also contains an expanding clay mineral which is interpreted as an interstratified illite/vermiculite (blue diffractogram). Compare the changes of the X-ray patterns for the black and blue diffractograms at low angles 5°–9° 2-Theta. The swelling layers could also be smectite layers instead of vermiculite layers. This cannot be resolved without more comprehensive preparation and analyses. When the sample is heated (red diffractogram), the swelling layers contract to the same spacing as for the major illite peak (10 Å = 8.8° 2-Theta) which thereby increases in intensity. In addition to clay minerals, quartz, feldspars (potassium feldspar and plagioclase) and small amounts of amphibole are present in the clay fraction (cf. black diffractogram).

4.8.4 Clay sample PSM001477:5

Bulk sample

Quartz, plagioclase ("calcian albite" = oligoclase), potassium feldspar (microcline), illite and chlorite are major minerals as indicated by strong peaks in the X-ray diffractogram, which fit to lines for these minerals from the /8/ database. Peaks from hornblende are also present in the diffractogram (Figure 4-7).



Figure 4-6. X-ray diffractograms of $< 2 \mu m$ *fraction of sample PSM001477:4. The analyses were performed with preferred orientation of crystallites.*



PSM001477:5. Bulk sample. Random orientation.

Figure 4-7. X-ray diffractogram of clay sample PSM001477:5. The analysis was performed with random orientation of crystals.

Illite, chlorite and kaolinite are the predominant clay minerals in the clay fraction (cf. blue diffractogram in Figure 4-8). The clay fraction also contains an expanding clay mineral which is interpreted as an interstratified illite/vermiculite (blue diffractogram). Compare changes of X-ray patterns for the black and blue diffractograms at low angles $5^{\circ}-9^{\circ}$ 2-Theta. When the sample is heated (red diffractogram) the swelling layers contract/collapse to give a peak at the same position as the major illite peak (10 Å = 8.8° 2-Theta) which thereby increases in intensity. In addition to clay minerals, quartz, feldspars (potassium feldspar and plagioclase) and small amounts of amphibole are present in the clay fraction (cf. black diffractogram).

4.8.5 Gyttja clay sample ASM000125

Bulk sample

Quartz, plagioclase ("calcian albite" = oligoclase), potassium feldspar (microcline), illite and chlorite peaks in the X-ray diffractogram (Figure 4-9) fit to lines for these minerals from the /8/ database. Kaolinite is also present. The organic matter (which is amorphous) in the sample, generates a distinctive hump in the X-ray pattern in the 2-Theta interval 19°–32° and even a more diffuse general pattern than what is normal for material without an amorphous component.



Figure 4-8. X-ray diffractograms of $< 2 \mu m$ *fraction of sample PSM001477:5. The analyses were performed with preferred orientation of crystallites.*



Figure 4-9. X-ray diffractogram of clay sample ASM000125. The analysis was performed with random orientation of crystals.

Illite and chlorite are the predominant clay minerals in the clay fraction (cf. blue diffractogram in Figure 4-10). Small amounts of kaolinite are also present (cf. turquoise diffractogram). The clay fraction furthermore contains an expanding clay mineral which is interpreted as an interstratified illite/vermiculite (blue diffractogram). Compare changes of X-ray patterns for the black and blue diffractograms at low angles $5^{\circ}-9^{\circ}$ 2-Theta. The swelling layers could possibly be smectite layers instead of vermiculite layers. This cannot be established without further and more in-depth preparation and analytical work. When the sample is heated (red diffractogram), the swelling layers contract/collapse to the same spacing as for the major illite peak (10 Å = 8.8° 2-Theta) which thereby increases in intensity. In addition to clay minerals, quartz, feldspars (potassium feldspar and plagioclase) and small amounts of amphibole are present in the clay fraction (cf. black diffractogram).

4.8.6 Gyttja clay sample PSM001472:3

Bulk sample

Quartz, plagioclase ("calcian albite" = oligoclase), potassium feldspar (microcline), illite, chlorite and kaolinite peaks in the X-ray diffractogram (Figure 4-11) fit to lines for these minerals from the /8/ database. Some pyrite peaks are also present. The organic matter in the sample, which is amorphous, makes a hump in the X-ray pattern in the 2-Theta interval $19^{\circ}-32^{\circ}$ and even a more diffuse pattern than is normal for material without an amorphous component.



Figure 4-10. X-ray diffractograms of $< 2 \mu m$ fraction of sample ASM000125. The analyses were performed with preferred orientation of crystallites.



Figure 4-11. X-ray diffractogram of clay sample PSM001472:3. The analysis was performed with random orientation of crystals.

Illite, chlorite and kaolinite are the predominant clay minerals in clay fraction (cf. blue diffractogram in Figure 4-12). The clay fraction also contain an expanding clay mineral which is interpreted as an interstratified illite/vermiculite (blue diffractogram). Compare changes of X-ray patterns for the black and blue diffractograms at low angles $5^{\circ}-9^{\circ}$ 2-Theta. The swelling layers could also be smectite layers instead of vermiculite layers. This cannot be established without more elaborate and in-depth study. When the sample is heated (red diffractogram) the swelling layers contract to the same spacing as for the major illite peak (10 Å = 8.8° 2-Theta) which thereby increases in intensity. In addition to clay minerals, quartz, feldspars (potassium feldspar and plagioclase) and small amounts of amphibole are present in the clay fraction (cf. black diffractogram).

4.8.7 Gyttja sample PSM001477:2

Bulk sample

Quartz, plagioclase ("calcian albite" = oligoclase), potassium feldspar (microcline), illite and chlorite peaks in the X-ray diffractogram (Figure 4-13) fit to lines for these minerals from the /8/ database. The organic matter in the sample, which is amorphous, makes a hump in the X-ray pattern in the 2-Theta interval 19° - 32° and contributes to give a more diffuse pattern than what is normal for material without an amorphous component.



PSM001472:3. Clay fraction, oriented (black = Na-hypochlorite treat., blue = ditto EG-sat., red = heated, turquoise = HCI leached).

Figure 4-12. X-ray diffractograms of $< 2 \mu m$ fraction of sample PSM001472:3. The analyses were performed with preferred orientation of crystallites.



Figure 4-13. X-ray diffractogram of clay sample PSM001477:2. The analysis was performed with random orientation of crystals.

Illite, chlorite and kaolinite are the predominant clay minerals in clay fraction (cf. blue diffractogram in Figure 4-14). The clay fraction also contain an expanding clay mineral which is interpreted as an interstratified illite/vermiculite (blue diffractogram). Compare changes of X-ray patterns for the black and blue diffractograms at low angles $5^{\circ}-9^{\circ}$ 2-Theta. The swelling layers could also be smectite layers instead of vermiculite layers. It cannot be established without more comprehensive examinations. When the sample is heated (red diffractogram) the swelling layers contracts to the same spacing as for the major illite peak (10 Å = 8.8° 2-Theta) which thereby increases in intensity. In addition to clay minerals quartz, feldspars (potassium feldspar and plagioclase) are present in the clay fraction (cf. black diffractogram).

4.8.8 Overview of clay minerals

Qualitative XRD analyses of the clay minerals were carried out with preferred orientation of clay mineral crystallites in four steps; sample in natural dried condition, sample saturated with ethylene glycol, sample heated to 400°C and sample leached with hydrochloric acid. A summary of the results from the qualitative analyses of clay minerals in the seven samples can be viewed in Table 4-10.



PSM001477:2. Clay fraction, oriented (black = Na-hypochlorite treat., blue = ditto EG-sat., red = heated, turquoise = HCl leached).

Figure 4-14. X-ray diffractograms of $< 2 \mu m$ *fraction of sample PSM001477:2. The analyses were performed with preferred orientation of crystallites.*

Sample/ ID-code	Chlorite	Illite	Illite fine fraction	Kaolinite	Mixed layer clay	Swelling clay
Clay Gyttja sample ASM000125	x	х	x	x	х	x
Till sample ASM000126	х		х	х	х	х
Till sample PSM001472:7	х		х		х	х
Clay Gyttja sample PSM001472:3	х	х	х	х	х	х
Gyttja sample PSM001477:2	х	х	х	х	х	х
Sand sample PSM001477:4	х		х	х	х	х
Clay sample PSM001477:5	х	х	х	х	х	x

Table 4-10. Results of qualitative analyses of clay minerals in the seven samples (x indicates occurrence).

4.9 Analysis of elements and oxides in soil samples

In Table 4-11 the results from analysis of element and oxides in the eight soil samples are listed. Results from element analysis from soil samples leached in dithionite citrate are listed in Table 4-12 and 4-13. In Table 4-13 data is transformed to mg/kg dw.

Element/ Oxide	Unit	Det. limit	ASM 124 Peat/ gyttja	ASM 125 Clay Gyttja	ASM 126 Till	PSM 1472:7 Till	PSM 1472:3 Clay Gyttja	PSM 1477:2 Gyttja	PSM 1477:4 Sand	PSM 1477:5 Clay
TS	%	_	44.3	31.8	90	93.1	31.1	20.4	81.5	64.3
SiO ₂	% dw	0.08	39.7	56.3	68.6	68.8	57.2	26.9	72.8	59.5
AI_2O_3	% dw	0.03	7.16	9.9	14.2	13.6	10.9	4.96	12.4	15
CaO	% dw	0.08	1.12	0.97	2.49	2.11	0.981	2.02	1.38	1.44
Fe_2O_3	% dw	0.005	5.97	11.3	6.76	7.65	8.29	4.8	5.06	12.5
K ₂ O	% dw	0.05	1.36	2.6	3.9	4.14	2.83	1.56	3.89	4.04
MgO	% dw	0.02	0.626	1.58	1.04	0.775	1.86	1.05	0.397	2.14
MnO	% dw	0.003	0.0475	0.113	0.092	0.0962	0.0896	0.0592	0.0667	0.136
Na ₂ O	% dw	0.04	0.567	1.31	3.74	3.6	1.43	0.606	3.44	2.04
P_2O_5	% dw	0.002	0.239	0.0983	0.167	0.127	0.112	0.212	0.0711	0.181
TiO ₂	% dw	0.002	0.291	0.384	0.526	0.356	0.44	0.229	0.256	0.64
Sum	% dw	-	57.1	84.6	101.5	101.3	84.1	42.4	99.8	97.6
LOI	% dw	_	37.4	11.2	0.2	-0.3	14.1	39.9	0.2	2
Ag	mg/kg dw	0.005	0.781	0.698	0.749	0.662	0.748	1.36	0.644	0.765
As	mg/kg dw	0.1	4.12	4.29	1.01	1.35	4.14	8.22	1.13	2.39
В	mg/kg dw	1	< 1	< 1	1.03	< 1	1.07	< 2	< 1	1.44
Ва	mg/kg dw	2	282	397	975	891	441	206	808	678
Be	mg/kg dw	0.005	2.39	1.97	2.47	2.61	2.13	1.43	3.24	2.83
Br	mg/kg dw	-	9.81	17.4	< 1	< 1	7.47	156	< 1	< 1
Cd	mg/kg dw	0.01	0.757	0.206	0.0345	0.0288	0.225	0.603	0.0218	0.0715
Ce	mg/kg dw	0.04	193	80.3	102	82	93.5	71.3	133	116
CI	mg/kg dw	_	59.1	92	79.6	66.6	143	74.4	90.3	48.7
Co	mg/kg dw	0.001	8.22	19	8.47	8.14	13.2	7.42	4.79	18.5
Cr	mg/kg dw	10	95	153	75.2	88.8	111	70.1	69.5	156
Cs	mg/kg dw	0.01	3.84	4.97	2.26	2.01	5.44	2.6	1.6	6.58
Cu	mg/kg dw	0.1	113	51.6	18	20	61.4	53.3	15.9	29.8
Dy	mg/kg dw	0.04	9.58	4.24	3.89	3.08	4.45	3.89	2.67	5.82
Er	mg/kg dw	0.04	5.38	2.49	2.29	1.81	2.54	2.52	1.47	3.37
Eu	mg/kg dw	0.04	2.65	0.898	1.27	0.911	0.972	0.861	0.808	1.22
Ga	mg/kg dw	0.8	9.56	14.3	16.4	15	13.4	7.16	13.3	20
Gd	mg/kg dw	0.04	12.7	5.26	4.47	3.38	5.06	4.64	3.01	6.31
Hf	mg/kg dw	0.04	2.66	3.74	7.71	6.87	3.31	2.1	4.32	7.01
Hg	mg/kg dw	0.04	0.113	< 0.04	< 0.05	< 0.04	< 0.04	0.0668	< 0.05	< 0.04
Но	mg/kg dw	0.04	1.91	0.872	0.769	0.627	0.88	0.823	0.541	1.14
I	mg/kg dw	_	3.5	1.46	< 0.5	< 0.5	1.19	7.23	< 0.5	< 0.5
La	mg/kg dw	0.04	99.2	39.1	45.7	37	38.7	34.4	32	50.5
Li	mg/kg dw	0.4	13.6	25.3	14.7	12.8	28.3	13.6	10.1	35.1
Lu	mg/kg dw	0.04	0.689	0.328	0.368	0.275	0.362	0.4	0.255	0.493
Мо	mg/kg dw	0.4	13.3	7.93	4.81	6.52	5.37	20.9	5.27	6.29
Nb	mg/kg dw	0.04	4.82	9.18	13.4	9.91	9.52	2.02	11.1	17.2
Nd	mg/kg dw	0.04	87.5	30.9	34.9	25.5	31.4	28.1	22.2	39.5
Ni	mg/kg dw	80.0	31.6	54.7	43.2	22	42.5	35.2	13	43.3
Pb	mg/kg dw	0.001	14.6	13.4	16.2	15.9	17.7	9.31	13.8	22.3
Pr	mg/kg dw	0.04	23.5	8.25	9.73	7.15	8.46	7.29	6.25	10.7

Table 4-11. Element- and oxide analysis of the eight soil samples, performed by ALS Scandinavia AB.

Element/ Oxide	Unit	Det. limit	ASM 124 Peat/ gyttja	ASM 125 Clay Gyttja	ASM 126 Till	PSM 1472:7 Till	PSM 1472:3 Clay Gyttja	PSM 1477:2 Gyttja	PSM 1477:4 Sand	PSM 1477:5 Clay
Rb	mg/kg dw	10	57.9	94.7	126	140	94.4	59.8	143	136
S	mg/kg dw	8	5370	11,900	222	173	13,200	23,200	1,980	283
Sb	mg/kg dw	0.005	0.394	0.481	0.281	0.384	0.397	0.416	0.346	0.367
Sc	mg/kg dw	1	9.37	9.02	6.89	5.4	10.4	5.89	3.71	13.2
Se	mg/kg dw	0.02	1.03	< 0.02	< 0.02	< 0.02	< 0.02	1.07	< 0.02	< 0.02
Sm	mg/kg dw	0.04	15.2	5.59	5.76	4.47	5.82	5.01	3.77	7.39
Sn	mg/kg dw	0.8	1.64	3.74	3.83	6.98	2.23	< 1	3.26	5.12
Sr	mg/kg dw	2	84.5	109	536	392	123	116	317	181
Та	mg/kg dw	0.4	0.591	0.827	1.2	0.847	0.843	0.348	0.838	1.57
Tb	mg/kg dw	0.04	1.67	0.724	0.633	0.503	0.74	0.648	0.45	0.95
Th	mg/kg dw	0.4	10.9	9.75	10.1	8.71	10.5	5.45	6.66	14.8
ТΙ	mg/kg dw	0.005	0.44	0.438	0.524	0.592	0.578	0.355	0.635	0.585
Tm	mg/kg dw	0.04	0.736	0.334	0.337	0.272	0.363	0.361	0.223	0.524
U	mg/kg dw	0.4	18.1	5.34	4.06	3	4.09	16.2	2.04	4.31
V	mg/kg dw	2	69.4	89.6	63.6	52.4	87.8	47.1	33.9	109
W	mg/kg dw	0.8	1.68	4.62	1.79	2.91	1.98	1.75	1.78	2.15
Y	mg/kg dw	0.04	56.2	24.7	21.3	16.6	24.3	25	14.4	30.6
Yb	mg/kg dw	0.04	4.54	2.25	2.26	1.79	2.32	2.33	1.45	3.33
Zn	mg/kg dw	1	43.3	73.7	45.1	33.8	74.4	60.4	20.5	84.3
Zr	mg/kg dw	2	73.9	83.4	247	205	96.2	72.7	95.4	205
C-tot	mg/kg dw	_	170,000	60,000	810	880	58,000	170,000	960	4,200
TOC	mg/kg dw	_	170,000	51,000	< 500	< 500	55,000	160,000	820	3,800
N-org	mg/kg dw	_	10,000	4,000	< 100	< 100	5,200	17,000	< 100	150
N-tot	mg/kg dw	-	11,650	5,320	< 100	< 100	6,710	19,480	< 100	356

Table 4-12. Element analysis of dithionite citrate leaching of the eight soil samples, performed by ALS Scandinavia AB.

Element	Unit	Det. limit	Blank	ASM 124 Peat/ gyttja	ASM 125 Clay Gyttja	ASM 126 Till	PSM 1472:7 Till	PSM 1472:3 Clay Gyttja	PSM 1477:2 Gyttja	PSM 1477:4 Sand	PSM 1477:5 Clay
Ag	µg/l	3	< 3	< 3	< 3	< 3	< 3	< 3	< 3	< 3	< 3
Al	µg/l	10	24.9	138,000	14,200	2,000	1,210	7,030	28,300	2,240	30,900
As	µg/l	3	< 3	102	34	2.6	< 3	26.3	66.5	4.93	21.8
В	µg/l	0.05	16.2	57.9	307	23.8	23.1	493	1,160	15.7	94.8
Ва	µg/l	0.5	815	3,730	1,580	1,040	998	1,780	1,380	927	2,550
Be	µg/l	0.05	0.258	36.8	1.54	0.612	0.727	1.1	4.25	0.91	2.2
Са	mg/l	5	< 5	196	99.1	110	46.1	74.4	410	7.14	63.8
Cd	µg/l	0.1	< 0.1	14.9	0.184	0.157	0.149	< 0.1	0.7	0.105	0.199
Ce	µg/l	0.05	< 0.05	6,500	832	119	105	785	865	238	641
Co	µg/l	0.3	< 0.3	69.7	46.9	4.69	3.3	50.9	40.2	4.63	29
Cr	µg/l	0.5	14.7	420	77.4	58.3	23.2	71.6	94.1	49.4	82.1
Cs	µg/l	0.05	0.303	0.722	0.182	4.07	1.74	0.171	0.23	1.26	0.0544
Cu	µg/l	5	< 5	1,780	36.4	6.61	7.15	39.7	133	5.51	41.4
Dy	µg/l	0.05	< 0.05	354	83.5	6.62	6.94	83.1	83.8	8.24	44.6
Er	µg/l	0.05	< 0.05	184	42.1	3.73	3.81	42	50	4.12	25.3
Eu	µg/l	0.05	< 0.05	95.2	17	1.5	1.38	16.8	17.3	2.17	7.32
Fe	mg/l	1	0.248	236	101	40.1	22.6	46.6	188	28	228
Ga	µg/l	0.05	0.233	11.9	9.35	1.62	0.682	9.36	6.19	1.58	10.3
Gd	µg/l	0.05	< 0.05	444	102	7.56	7.06	103	91.9	11.2	45.9
Hf	µg/l	0.05	< 0.05	18	5.49	1.84	1.72	6.34	1.68	0.774	12.8
Hg	µg/l	0.2	< 0.2	0.907	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2
Ho	µg/l	0.05	0.0827	65.2	15.6	1.46	1.43	15.7	16.6	1.56	8.73
К	mg/l	20	< 20	< 20	< 20	< 20	< 20	< 20	< 20	< 20	< 20
La	µg/l	0.05	0.0849	3,580	532	61.2	49.9	483	583	129	283
Li	µg/l	0.05	16.6	12.9	28	17.2	17	27.4	22.5	27.6	25.7
Lu	µg/l	0.05	< 0.05	23.2	4.98	0.534	0.565	5.19	7.74	0.579	3.5
Mg	mg/l	5	< 5	11.1	37.2	< 5	< 5	44.4	73.3	< 5	24.8
Mn	µg/l	1.5	13.6	1,180	1,200	936	514	1,310	1,870	190	2,560
Мо	µg/l	0.5	2.57	166	21.5	7.86	4.42	12.9	56.1	8.03	16.4
Na	mg/l	5	43,200	41,500	41,500	43,700	44,500	41,500	42,000	43,000	43,700
Nb	µg/l	0.05	0.125	49.2	5.43	12.4	9.23	6.4	3.9	7.74	19
Nd	µg/l	0.05	< 0.05	3,470	554	55.8	48.2	536	590	97.8	259
Ni	µg/l	2.5	10.9	490	238	21.7	15.5	227	327	19.7	55.6
Р	µg/l	50	113	14,000	4,130	400	406	4,700	5,480	360	3,530
Pb	µg/l	0.5	4.64	213	7.68	23.3	21.1	8.54	16.4	7.52	79.8
Pr	µg/l	0.05	< 0.05	859	139	14.6	13.1	131	146	28.1	68.3
Rb	µg/l	0.05	2	17.2	12.4	46.8	27.6	11.8	16.1	12.2	7.13
Sb	µg/l	0.5	< 0.5	3.64	1.03	0.731	0.632	1.05	0.817	0.547	2.16
Sc	µg/l	0.05	0.0681	194	43.7	2.8	3.02	40.2	47.1	3.1	29.1
Se	µg/l	0.3	4.71	29.1	5.63	4.24	3.68	5.48	14.3	4.7	4.05
Si	mg/l	2	< 2	24	25.4	6.78	5.12	17.9	19.3	4.87	76.7
Sm	µg/l	0.05	0.066	589	111	8.92	8.84	111	114	16.1	50
Sn	µg/l	3	< 3	8.92	< 3	3.89	3.03	9.52	< 3	7.61	14.4
Sr	µg/l	0.5	120	1,390	880	239	199	964	2,140	149	502
Та	ug/l	0.05	< 0.05	1.27	< 0.05	0.405	0.366	0.0589	0.104	0.319	0.843
Tb	µg/l	0.05	< 0.05	62	14.6	1.19	1.19	14.7	14.2	1.62	7.5
Th	µg/l	1	< 1	303	160	26	23.7	166	76.3	28.3	152
Ti	µg/l	0.05	4.51	6,110	759	887	642	889	240	618	2,250
TI	µg/l	0.05	0.46	1.36	0.285	0.763	0.642	0.368	0.357	0.688	0.361
Tm	µg/l	0.05	< 0.05	25	5.86	0.536	0.539	5.78	7.38	0.569	3.76
U	µg/l	0.03	0.398	534	96.7	18.9	12.1	62.9	377	8.73	23.4
V	µg/l	0.3	0.418	867	278	67.2	40	293	227	58.8	313
W	µg/l	3	< 3	8.94	5.71	4.31	3.34	4.29	10.8	< 3	12.4
Y	µg/l	0.05	0.123	2,080	498	43.8	42.4	493	566	48.8	252
Yb	µg/l	0.05	< 0.05	149	34.9	3.41	3.48	34.7	48.2	3.6	23.2
Zn	µg/l	10	28.2	223	284	69.1	38.9	265	348	39.7	126
Zr	µg/l	0.05	0.942	696	294	58.1	52.3	355	83	22	530

Table 4-13. Element analysis of dithionite citrate leaching of the eight soil samples, performed by ALS Scandinavia AB. Data is transformed to mg/kg dw.

Element	Unit	ASM 124 Peat/ gyttja	ASM 125 Clay Gyttja	ASM 126 Till	PSM 1472:7 Till	PSM 1472:3 Clay Gyttja	PSM 1477:2 Gyttja	PSM 1477:4 Sand	PSM 1477:5 Clay
Ag	mg/kg dw	< 0,08	< 0,08	< 0,07	< 0,08	< 0,07	< 0,08	< 0,08	< 0,08
Al	mg/kg dw	3,659.8	367.7	49.0	30.6	173.7	761.1	55.1	779.7
As	mg/kg dw	2.706	0.882	0.064	< 0,08	0.652	1.790	0.123	0.551
В	mg/kg dw	1.106	7.543	0.188	0.178	11.825	30.789	0.000	1.985
Ва	mg/kg dw	77.321	19.844	5.580	4.721	23.934	15.209	2.787	43.813
Be	mg/kg dw	0.969	0.033	0.009	0.012	0.021	0.107	0.016	0.049
Са	mg/kg dw	5,198.9	2,570.7	2,728.2	1,189.4	1,845.2	11036.3	177.7	1611.1
Cd	mg/kg dw	0.395	0.005	0.004	0.004	< 0,0024	0.019	0.003	0.005
Ce	mg/kg dw	172.414	21.582	2.951	2.709	19.469	23.284	5.923	16.187
Co	mg/kg dw	1.849	1.217	0.116	0.085	1.262	1.082	0.115	0.732
Cr	mg/kg dw	10.751	1.626	1.081	0.219	1.411	2.137	0.864	1.702
Cs	mg/kg dw	0.011	0.000	0.093	0.037	0.000	0.000	0.024	0.000
Cu	mg/kg dw	47.215	0.944	0.164	0.184	0.985	3.580	0.137	1.045
Dy	mg/kg dw	9.390	2.166	0.164	0.179	2.061	2.256	0.205	1.126
Er	mg/kg dw	4.881	1.092	0.093	0.098	1.042	1.346	0.103	0.639
Eu	mg/kg dw	2.525	0.441	0.037	0.036	0.417	0.466	0.054	0.185
Fe	mg/kg dw	6,253.4	2,613.5	988.4	576.7	1,149.6	5,053.9	690.7	5,751.3
Ga	mg/kg dw	0.309	0.236	0.034	0.012	0.226	0.160	0.034	0.254
Gd	mg/kg dw	11.777	2.646	0.188	0.182	2.555	2.474	0.279	1.159
Hf	mg/kg dw	0.024	< 0,005	< 0,005	< 0,005	< 0,005	< 0,005	< 0,005	< 0,005
Hg	mg/kg dw	0.477	0.142	0.046	0.044	0.157	0.045	0.019	0.323
Ho	mg/kg dw	1.727	0.403	0.034	0.035	0.387	0.445	0.037	0.218
K	mg/kg dw	< 531	< 519	< 496	< 516	< 496	< 538	< 498	< 505
La	mg/kg dw	94.958	13.798	1.516	1.285	11.977	15.691	3.208	7.144
Li	mg/kg dw	0.000	0.296	0.015	0.010	0.268	0.159	0.274	0.230
Lu	mg/kg dw	0.615	0.129	0.013	0.015	0.129	0.208	0.014	0.088
Mg	mg/kg dw	294.4	965.0	< 124	< 129	1,101.2	1,973.1	124.4	626.3
Mn	mg/kg dw	30.939	30.776	22.877	12.910	32.153	49.970	4.390	64.303
Mo	mg/kg dw	4.335	0.491	0.131	0.048	0.256	1.441	0.136	0.349
Nb	mg/kg dw	1.302	0.138	0.304	0.235	0.156	0.102	0.190	0.477
Nd	mg/kg dw	92.042	14.371	1.384	1.244	13.294	15.882	2.434	6.540
NI	mg/kg dw	12.708	5.891	0.268	0.119	5.360	8.509	0.219	1.129
P	mg/kg dw	368.355	104.202	7.118	7.559	113.765	144.468	6.147	86.288
Pb	mg/kg dw	5.527	0.079	0.463	0.425	0.097	0.317	0.072	1.898
Pr	mg/kg dw	22.785	3.606	0.362	0.338	3.249	3.930	0.699	1.725
RD	mg/kg dw	0.403	0.270	1.111	0.660	0.243	0.380	0.254	0.130
Sb	mg/kg dw	0.097	0.027	0.018	0.016	0.026	0.022	0.014	0.055
SC	mg/kg dw	5.144	1.132	0.068	0.076	0.995	1.266	0.075	0.733
Se	mg/kg dw	0.647	0.024	0.000	0.000	0.019	0.258	0.000	0.000
Si	mg/kg dw	636.6	658.9	168.2	132.1	443.9	519.5	121.2	1,936.9
Sm	mg/kg dw	15.622	2.878	0.220	0.226	2.751	3.067	0.399	1.261
Sn	mg/kg dw	0.237	< 0,08	0.096	0.078	0.236	< 0,08	0.189	0.364
Sr Te	mg/kg dw	33.087	19.715	2.951	2.038	20.933	54.374	0.722	9.646
ты	mg/kg dw	0.034	< 0,0013	0.010	0.009	0.001	0.003	0.008	0.021
	mg/kg dw	1.645	0.379	0.030	0.031	0.305	0.382	0.040	0.189
т:	mg/kg dw	0.037	4.150	0.040	10.011	4.117	2.004	15 260	3.030
	mg/kg dw	161.949	19.572	21.887	16.447	21.937	0.339	15.269	56.704
11 Tm	mg/kg dw	0.024	0.000	0.000		0.000	0.000	0.000	0.000
	mg/kg dW	U.003	0.152	0.013	0.014	0.143	0.199	0.014	0.095
U V	mg/kg dw	14.154	2.498 7.004	0.459	0.302	1.000	10.137	0.207	0.001
V	mg/kg dW	22.900	1.201	0.107	1.021	1.200	0.099	1.400	1.093
VV	mg/kg dw	0.231	0.148	0.107	0.080	0.100	0.291	< 0,075	0.313
Ύ Vh	mg/kg dw	55.169	12.915	1.083	1.091	12.224	15.232	1.211	0.301
Y D Zn	mg/kg dw	3.952	0.905	0.085	0.090	U.861	1.297	0.090	0.586
∠n Zr	mg/kg dW	0.10/	0.030	1.014	0.270	5.8/J	8.008	0.280	2.470
ΔI	mg/kg dw	10.437	1.002	1.410	1.325	0./01	2.209	0.524	13.300

4.10 Water analysis

In Table 4-14 the results from analysis of groundwater monitoring wells are listed. Sampling was performed in March 2007. In Appendix 1 information of sampling in the field and sample preparations are listed.

Parameter	Unit	Det. limit	SSM000260	SSM000261	SSM000262	SSM000263
(ALS Scandinavia AB)						
AI	µg/l	0.2	201	3,290	76	530
As	µg/l	0.05	0.169	2.75	0.527	0.946
B10/B11 Atomic		_	0.2403	0.2406	0.2408	0.2375
Ва	µg/l	0.01	31.9	70.8	27.6	65.4
Са	mg/l	0.1	68.9	63.3	43	96
Cd	µg/l	0.002	0.0024	0.0977	0.0073	0.0122
Ce	µg/l	0.005	3.29	34.2	1.21	5.26
Со	µg/l	0.005	0.216	2.37	0.195	0.576
Cr	µg/l	0.01	0.379	5.68	1.69	1.02
Cs	µg/l	0.03	0.234	0.47	0.199	0.145
Cu	µg/l	0.1	0.511	7.47	2.22	9
Dy	µg/l	0.005	0.158	1.55	0.115	0.282
Er	µg/l	0.005	0.0943	0.789	0.0921	0.156
Eu	µg/l	0.005	0.0356	0.326	0.0197	0.0555
Fe	mg/l	0.4	1.34	8.18	3.63	0.903
Gd	µg/l	0.005	0.221	1.93	0.136	0.404
Hf	µg/l	0.005	0.0327	0.191	0.0328	0.078
Hg	µg/l	0.002	< 0.002	< 0.002	< 0.002	< 0.002
Но	µg/l	0.005	0.0313	0.29	0.024	0.0517
1	µg/l	-	12.4	82.1	17.5	22.8
К	mg/l	0.4	3.55	5.66	3.81	19.8
La	µg/l	0.005	1.76	14.3	0.659	2.72
Li	µg/l	4	9.79	16.7	8.65	15.8
Lu	µg/l	0.005	0.0139	0.0993	0.0183	0.0217
Mg	mg/l	0.09	11.1	13.7	7.96	14.3
Mn	µg/l	0.03	375	640	475	506
Мо	µg/l	0.05	0.576	0.48	0.803	2.71
Na	mg/l	0.1	20.5	27.5	34.6	138
Nd	µg/l	0.005	1.57	13	0.652	2.51
Ni	µg/l	0.05	0.729	5.84	3.17	2.43
Р	µg/l	1	166	1,210	126	238
Pb	µg/l	0.01	0.929	7.63	0.338	1.09
Pr	µg/l	0.005	0.379	3.42	0.166	0.616
Rb	µg/l	0.03	3.31	8.9	2.29	11.3
S	mg/l	0.16	18.6	11.9	13	20.8
Sb	µg/l	0.01	0.0747	0.163	2.21	0.114
Sc	µg/l	0.05	0.0694	0.618	0.117	0.176
Si	mg/l	0.03	10.8	16.3	11	9.49
Sm	µg/l	0.005	0.229	2.33	0.126	0.434
Sr	µg/l	2	253	268	224	480
Tb	µg/l	0.05	0.0274	0.278	0.0178	0.0483

Table 4-14. Results from analysis of water from the four groundwater monitoring wells.

Parameter	Unit	Det. limit	SSM000260	SSM000261	SSM000262	SSM000263
Th	µg/l	0.02	0.329	1.6	0.167	0.62
Ti	µg/l	0.001	24.6	179	8.82	37.5
TI	µg/l	0.005	< 0.005	0.0463	0.0085	0.0112
Tm	µg/l	0.005	0.0126	0.111	0.0118	0.0205
U	µg/l	0.0005	0.227	4.8	1.37	1.59
V	µg/l	0.005	2.47	12.3	5.53	2.63
Y	µg/l	0.005	1.16	8.93	1.04	1.72
Yb	µg/l	0.005	0.0838	0.719	0.0997	0.142
Zn	µg/l	0.2	3.12	24.7	12.3	3.92
Zr	µg/l	0.03	1.43	6.58	1.67	2.32
(Äspö Laboratory)						
HCO ₃	mg/l	0.3	239	249	152	135
CI	mg/l	0.2	11.9	12.6	40.5	331
SO ₄	mg/l	0.2	51.96	44.42	36.35	58.39
Br	mg/l	0.2	0.050	0.190	0.220	1.420
F	mg/l	0.2	1.79	2.50	1.69	1.15
FE (tot)	mg/l	0.006	1.304	3.851	2.846	0.523
FE II	mg/l	0.006	1.127	3.785	1.177	0.407
рН	pН	-	7.25	6.96	7.05	7.17
Conductivity	mS/m	0.4	52.6	52.9	47.5	143.0
Sulfide	mg/l	0.006	0.061	< 0.006	0.02	0.039
(Dep. of Systems Ecology, Stockholm)						
PO₄-P	mg/l	0.00012	0.061	0.472	0.059	0.168
PO₄-P acid hydrolysis	mg/l	0.00012	0.071	0.868	0.063	0.152
Tot-P	mg/l	0.00011	0.203	0.99	0.168	0.255
NH ₄ -N	mg/l	0.00016	0.873	12.6*	1.18	0.174
(NO ₂ +NO ₃)-N	mg/l	0.00005	0.42	0.005	0.642	2.33
NO ₂ -N	mg/l	0.00005	0.028	0.001	0.371	0.007
NO ₃ -N	mg/l	-	0.392	0.004	0.271	2.32
Tot-N	mg/l	0.00019	1.9	5.4	2.18	3.01
SiO ₄ -Si	mg/l	0.00041	9.68	12.42	10.16	8.26
TOC	mg/l	0.1	8.66	13.14	12.6	8.65
DOC	mg/l	0.1	9.78	11.55	12.63	8.78

* Note that the concentration of NH_4 > Tot-N. Something was wrong with the two samples. The concentration of NH_4 in the Tot-N sample was 4.16 mg/l.

4.11 BET measurements

In Table 4-15 the results from BET measurements are listed. The results seem to be as expected in view of the characteristics of the different soil types. The correspondence between the replicates was relatively good. The BET values differed clear between fine soils and till, and also between sand and till. Both organic and "inorganic" fine soils seemed to have BET values of the same approximate size.

ID-code	SLU- code	Sample	Weight A (g)	Weight B (g)	BET (A) (m²/g)	BET (B) (m²/g)	BET (average) (m²/g)
ASM000124	2T	Peat/gyttja	2.3917	1.9742	11.17	13.66	12.42
ASM000125	2LGI	Lergyttja/gyttjelera I	1.4886	1.3408	19.60	19.61	19.61
ASM000126	3MI	Till I	4.8027	3.993	1.13	1.22	1.18
PSM001472:7	MII	Till II	5.9381	3.2937	1.19	0.82	1.01
PSM001472:3	LGII	Lergyttja/gyttjelera II	1.623	1.5384	19.32	18.99	19.16
PSM001477:2	GI	Gyttja I	1.1632	0.8287	10.28	10.07	10.18
PSM001477:4	SI	Sand I	4.1121	3.2787	0.136	0.163	0.150
PSM001477:5	LI	Clay I	3.3934	2.893	27.03	27.21	27.12

Table 4-15.	Results	of BET	measurements.
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5 References

- /1/ Morosini Mansueto et al. 2007. Oskarshamn site investigation. Hydrogeological characterization of deepest valley soil aquifers and soil-rock transition zone at Laxemar, 2006. Subarea Laxemar. SKB P-07-91, Svensk Kärnbränslehantering AB.
- /2/ Malmström M, Berglund S, 2007. Experimentell bestämning av platsspecifika K_d-värden för jord och sediment: Försöksplan för steg 1, utförande. Version 3.1, 2007-04-08.
- /3/ **ICP Forests, 2006.** Manual on sampling and analysis of soil. UN ECE CLRTAP, ICP on Assessment and monitoring of air pollution effects on forests.
- /4/ **Karltun et al. 1996.** Markkemiska analyser inom Ståndortskarteringen. Metodbeskrivning. http://www-sml.slu.se/sk/sk.htm1#LITT.
- /5/ **Drever S I, 1973.** The preparation of oriented clay mineral specimens for X-ray diffraction analysis by a filter-membrane peel technique. American Mineralogist 58, 553–554.
- /6/ Snäll S, 1988. Mineralogy and maturity of the alum shales of south-central Jämtland, Sweden. SGU Serie C 818.
- /7/ Cassidy M M, Mankin C J, 1960. Chlorox used in preparation of black shale for clay mineral analysis. Oklahoma Geology Notes. Oklahoma Geological Survey 20, 275–281.
- /8/ PDF 1994. Powder diffraction file computer data base. Set 1-43. International Centre for Diffraction Data, Park Lane, Swartmore, PA, USA.
- /9/ Brindley G W, Brown G, 1984. Crystal structures of clay minerals and their X-ray identification. Mineralogical Society, Monograph no. 5, Mineralogical Society, 41 Queen's Gate, London SW7 5HR.
- /10/ Bruker A X S, 2003. TOPAS V2.1: General profile and structure analysis software for powder diffraction data. User's Manual, Bruker AXS, Karlsruhe, Germany.
- /11/ Brunauer C A, Emmet, Teller E, 1938. Adsorption of gases in multi-molecular layers. J. Am. Chem. Soc. 60:309–319.

Appendix 1

Sampling of groundwater monitoring wells

Bottle	Number	Components	Preparation of sample in the field	Filling instructions	Indoor treatment	Analysing laboratory
250 ml	2	Archive	_	Fill up	Filter, with "Pallfilter" 0,45 µm	Stored in freezer
5,000 ml	1	Archive	_	Fill up	_	Stored in refrigerator
250 ml	1	Alkalinity, pH, Conductivity	_	Fill up	_	Äspö Laboratory
250 ml	1	Anions (F⁻, Cl⁻, Br⁻, SO42⁻)	_	Fill up	_	Äspö Laboratory
500 ml acid rinsed	1	Fe II + Fe (tot)	-	Fill up	Filter, with membrane filter, and add 5 ml concentrated HCl	Äspö Laboratory
Winkler bottles	2	HS⁻	0,5 ml 1M ZnAc and 1M NaOH	Flow over	Äspö Laboratory	Äspö Laboratory
500 ml acid rinsed	1	Standard elements,	_	Fill up	Filter. with membrane filter,	ALS, Luleå
		B-10, As, In, Ti, I,			add 1 ml concentrated HNO3	
		Environmental metals,				
		Lantanoides,				
		Trace elements.				
		Archive (acid rinsed)				(Stored in freezer)
1,000 ml	1	POP, PON, POC	_	Fill up	_	Systemekologen
Test tubes	4	NO ₃ , NO ₂ , (NO ₂ +NO ₃), PO ₄ , NH ₄	0.45 µm filter	Fill up	60°C for 1 hour in oven	Systemekologen
100 ml	1	Tot-NP	_	Fill up ¹	_	Systemekologen
20 ml	1	DOC	0.45 µm filter	Fill up	One drop of 1M HCI	Systemekologen
20 ml	1	ТОС	_	Fill up	One drop of 1M HCl	Systemekologen
100 ml	1	Deuterium, O-18	_	Fill up	_	IFE, Norway
500 ml (dried)	1	Tritium	_	Flow over	_	EIL, Canada

Sampling of groundwater in monitoring wells. Outdoor and indoor treatment of samples.

¹ Fill up from 1,000 ml bottle (POP, PON, POC).