Investigation of G-BASE Regional Soil Geochemistry over Pleistocene Till Deposits in East Anglia Using Factor Analysis

Chemical and Biological Hazards Programme

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Investigation of G-BASE Regional Soil Geochemistry over Pleistocene Till Deposits in East Anglia Using Factor Analysis

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Acknowledgements

Contents

FIGURES

TABLES

Summary

This report presents the application of Factor Analysis (FA) using geochemical data of topsoil samples to investigate the geochemical composition and distribution of Pleistocene Tills in East Anglia.

The first part of the report introduces the background, aims and context of this particular study. The second part summarises the methodologies, covering Geochemical Baseline Survey of the Environment (G-BASE) sample collection, analytical procedures and the geological setting of the study area.

Section 3 presents the results of Factor Analysis, which is followed by a discussion and conclusions.

1 Introduction

The geochemistry of soils is related to factors such as bedrock geology, drift cover, land use, climate and topography (BGS, 2000). Although many elements contain vital information about their parent material, soil geochemistry has not been widely used for defining geological substrate (Mann, 2006). Hemmati and Chivas (2006) showed in southern Australia that the use of multivariate techniques such as factor analysis are a helpful means of manipulating, interpreting and representing soil geochemical data. Factor analysis was used at an introductory stage in the interpretation of geochemical data of the FOREGS Geochemical Baseline Mapping Programme (Pirc, *et al.* 2006; De Vos and Tavainen, 2006) to gain an insight into the structure of the multivariate spatial distribution of 60 or so determinants from European soils. Other recent publications have used multivariate analyses to interpret geochemical patterns and compositions of sediments, soils and waters (Batista *et al.*, 2006; Kumru and Bakac 2003; Reimann *et al.* 2001).

This study aims to investigate the potential of factor analysis to describe and interpret the geochemical composition and spatial distribution within a single geological unit using the vast geochemical data resources of the G-BASE dataset. Unlike many other areas of the UK, almost 90 % of East Anglia is covered by Pleistocene or Holocene superficial deposits, which have been transported and deposited in East Anglia by ice, wind and water. Pleistocene tills cover approximately 35 % of the British landmass, which makes Pleistocene till the largest land covering unit and in East Anglia the tills cover even more than half of the land surface.

This study selected soil sites located on tills in East Anglia to investigate the potential of Factor analysis in describing and exploiting geochemical soil data to benefit and develop better understanding of the heterogeneity of the deposits.

2 Material and Methods

2.1 SOIL SAMPLING

In East Anglia soil samples were collected from 5421 sites, covering an area of 10,842 square kilometres, during the summers of 1999 to 2004 by the British Geological Survey's (BGS) G-BASE project (Figure 1). The topsoil samples were collected in rural areas from every second kilometre square of the British National Grid at a depth of 5-20 cm (Johnson *et al.*, 2005). All G-BASE field sampling procedures are documented in a field procedures manual by Johnson (2005). Table 1 summarises sampling methods and sample types collected by the G-BASE project.

Figure 1: Extent and location of G-BASE soil sample sites (dots) in East Anglia (BNG displayed at 50 km intervals) (© Crown Copyright. All rights reserved. OS Licence No: 100017897/2007)

2.2 SAMPLING PREPARATION AND ANALYSES

The soil samples were dried and sieved to < 2 mm and pulverised in agate ball mills, then pelletised.Major and trace element determinations of soil samples were carried out by wavelength-dispersive X-ray fluorescence spectrometry (XRFS) (Ingham and Vrebos, 1994) and

energy dispersive XRF at the BGS laboratories in Keyworth, Nottingham. The XRFS analysis gives a range of 52 major and minor elements (listed in Table 1). Duplicate, replicate, primary and secondary reference materials are all included in every batch of samples submitted for analysis. These control samples are required to monitor and maintain precision and accuracy of all data. On receipt from the laboratories, the analytical data go though a series of data conditioning procedures (Lister and Johnson, 2005). The data conditioning procedure involves levelling data between sampling campaigns to ensure seamless geochemical maps. Finally, the conditioned analytical and field data is stored in the corporate BGS Geochemical Database based on ORACLE.

Table 1: Summary of G-BASE sample types and sampling methods (updated from Johnson *et al.*, 2005)

Sample	Sampling	Sample preparation and analyses
Stream sediment	Sediment is collected from the active drainage channel of 1st or 2nd order streams. The sediment is wet sieved firstly through a 2 mm nylon screen then a 150 µm nylon sieve. The fine stream sediment is collected in a Kraft™ paper bag. Sampling density varies according to land use and drainage pattern but averages at one sample every one to two square kilometre.	Sediments are dried initially by air drying then freeze drying before being pulverised in agate ball mills. Samples are pelletised ready for XRFS analyses at the BGS laboratories in Keyworth, UK. A combination of emission and dispersive techniques gives a range of 52 elements (Ag, Al, As, Ba, Bi, Br, Ca, Cd, Ce, Co, Cr, Cl, Cs, Cu, Fe, Ga, Ge, Hf, I, In, K, La, Mg, Mn, Mo, Na, Nb, Nd, Ni, P, Pb, Rb, S, Sb, Sc, Se, Si, Sm, Sn, Sr, Ta, Te, Th, Ti, Tl, U, V, W, Y, Yb, Zn and Zr)
Panned concentrate	The -2mm+150µm fraction from the sieving of the sediment is panned on site in a wooden Malaysian-style "dulang" pan. A full pan is panned down to give a constant volume in the centre of the pan. The heavy minerals are scanned for evidence of mineralisation or pollution.	Panned concentrates are not routinely analysed or examined in detail. They are stored for future reference and follow-up as required.
Stream water	Filtered (0.45 µm cellulose filter) and unfiltered waters are collected from the same site as the drainage sediment. Samples are stored in Nalgene™ bottles and acidified as required by the analytical method.	Alkalinity (by colorimetric titration), pH and conductivity determined on location. Samples analysed at BGS. **ICP-MS**: Ag, Al, As, Ba, Be, Bi, Cd, Ce, Co, Cr, Cs, Cu, Ho, La, Li, Mo, Mn, Nd, Ni, Pb, Rb, Sb, Se, Sn, Th, Tl, U, V, Y, Zn & Zr [31 elements]. **ICP-AES**: Al, B, Ba, Ca, Fe, K, Mg, Mn, Na, P, Si, S (reported as SO_4), Sr & Zn [14 elements]. **Ion Chromatography**: Br, Cl, F, NO_2, NO_3, SO_4, PO_4 [7 ions]. **TIC/TOC analyser** for Non-purgeable organic carbon (NPOC)
Surface and subsoil	Soils are collected using a one metre Dutch auger taking five sub-samples at the corners and centre of a 20 m square. A surface sample (5 to 20 cm) and a deeper sample (35 to 50 cm) are taken at each site. Samples are collected from alternate 1 km grid squares though in urban areas sampling density is increased to four samples every 1 km². Samples are collected in Kraft™ paper bags	The deeper soil samples are dried then sieved to -2 mm. The surface samples are dried and sieved to -2 mm and pulverised in agate ball mills then palletised for XRFS analyses as per stream sediment samples. Loss-on-ignition (450ºC) and pH is also routinely measured for soils.

2.3 GEOLOGICAL DESCRIPTION OF EAST ANGLIA

2.3.1 Solid and Superficial Geology of East Anglia – An Overview

This chapter will give an overview of the solid and superficial geology of East Anglia. Maps of the solid and superficial geology are presented below (Figure 2 and Figure 3).

The solid bedrock geology of East Anglia is younging from west to east. The oldest strata are Jurassic clays of the Kellaways, Oxford, Ampthill, West Walton and Kimmeridge Clay formations. These are localised in the west to northwest between Ely and King's Lynn. The bulk of East Anglia is covered by Cretaceous Chalk, stretching over the centre from north to south. Apart from a small area in the southeast of Eocene argillaceous rocks of the Thanet Sand, Lambeth Group, Harwich and London Clay formations, the youngest strata are Pliocene to Pleistocene unlithified sandstones (shelly sands with beds of clay and gravel) of the Red Crag and Norwich Crag formations. These cover the whole east of East Anglia reaching from Cromer in the north to Ipswich and Sudbury in the south. The northern limit of the Norwich Crag is around the Norwich area. The Crag to the north of this is younger and called the Wroxham Crag.
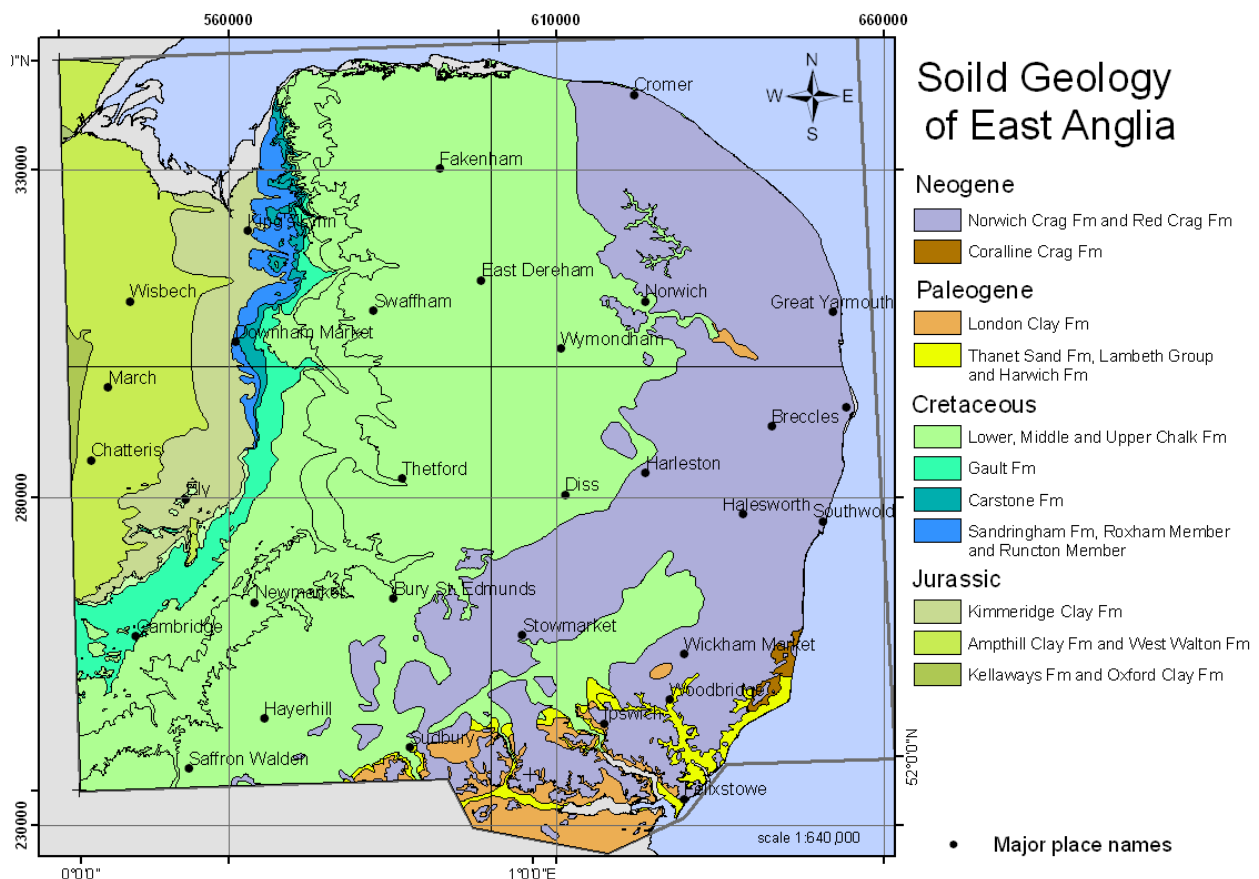
Figure 2: Solid geology map of East Anglia (1:250 000 BGS DigMap)

The Quaternary or superficial geology of East Anglia is very much influenced by the Anglian glaciation of the Pleistocene. Figure 3 shows the superficial cover on a scale of 1: 625 000 as a 1: 250 000 geological map for this area is not available.

Although the 1:625 000 map is very generalised, it is noticeable that East Anglia is nearly 85 % covered with unconsolidated superficial material. The most recent deposits of alluvium can be found in the Broads near Great Yarmouth, along the Norfolk Coast and around Wisbech with large areas of peat deposits just to the south. The major superficial deposits in East Anglia are glacial tills, comprising a mixture of gravel, sand, silt and clay. These deposits stretch from the north Norfolk coast through the centre and east coast down south. Mapped till deposits are

described as the Lowestoft Till Formation. Connected to those are glacial sand and gravel deposits located along the eastern coast and to the northeast. It should be mentioned that not all of the tills in East Anglia belong to the Lowestoft Formation. The youngest deposits, of Ipswichian (120000 yr) to Cromerian (500000 yr) age, occur north and east of the dotted line (Figure 3) linking Fakenham, East Dereham, Norwich and the North Sea coast mid-way between Cromer and Yarmouth.

Areas without superficial deposits are shown in grey (Figure 3). These lay between the peat and alluvial deposits in the west and the tills in the centre of East Anglia.
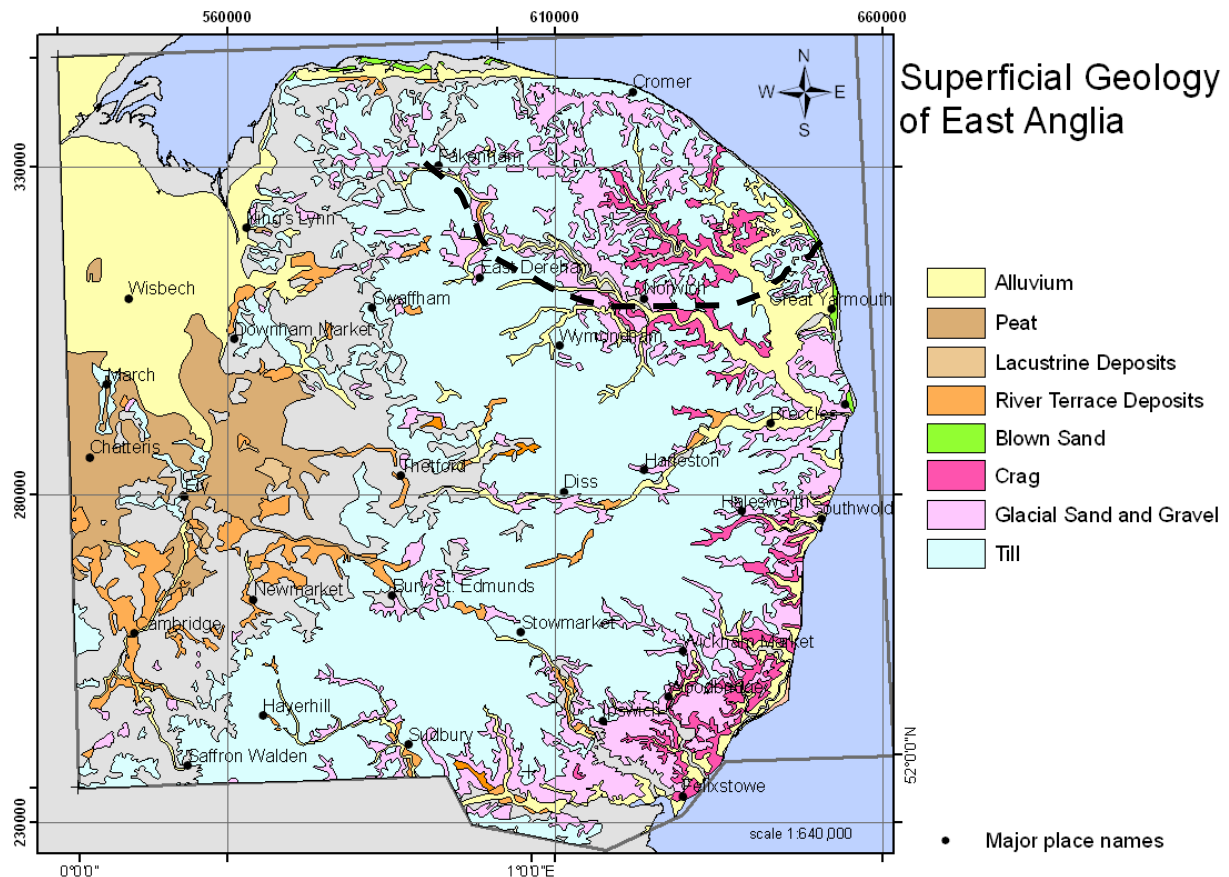
Figure 3: Superficial geology map for East Anglia (1: 625 000 BGS DigMap), areas of no superficial cover in grey.

2.3.2   Lowestoft Till Formation

The provenance of the Lowestoft Till material, coupled with measurements of the inclined pebble fabrics (West and Donner, 1965), and the regional trends observed within the composition of the matrix (Perrin *et al*., 1974), indicate that the Lowestoft Till was the sub-glacial product of a mass of ice probably originating in the North Sea.

There has however long been debate over the provenance and relative ages of the various chalky tills in the area (Rice, 1968; Horton, 1970; Perrin *et al*., 1973,1974); whether the Lowestoft Till and the Cromer Till of northeast Norfolk were products of contemporaneous ice sheets whose ice fronts were vying across Norfolk (Cox and Nickless, 1972); and whether the Lowestoft Till might be subdivided into an Upper Chalky Boulder Clay (the Gipping Till) and a Lower Chalky Boulder Clay whose accumulations were separated by the Hoxnian Interglacial (Baden-Powell, 1948; Bristow and Cox, 1973). The Lowestoft Till Formation is now regarded as a product of the British Eastern Ice sheet (Hart *et al*., 1990). One of the simpler explanations (Perrin *et al*., 1974) is that the 'Lowestoft' ice stream moved southwards across the western North Sea basin. En route, this sheet accumulated chalk and oolite and limestone-bearing Jurassic debris off the coast

of Yorkshire, overran the Cretaceous escarpments in Lincolnshire and Norfolk, and excavated the Jurassic clays of the Wash-Fenland basin. Subsequently, the sheet fanned out radially with lobes spreading eastwards and south-eastwards or, according to Hart (1987), eastwards then northwards, across the district.
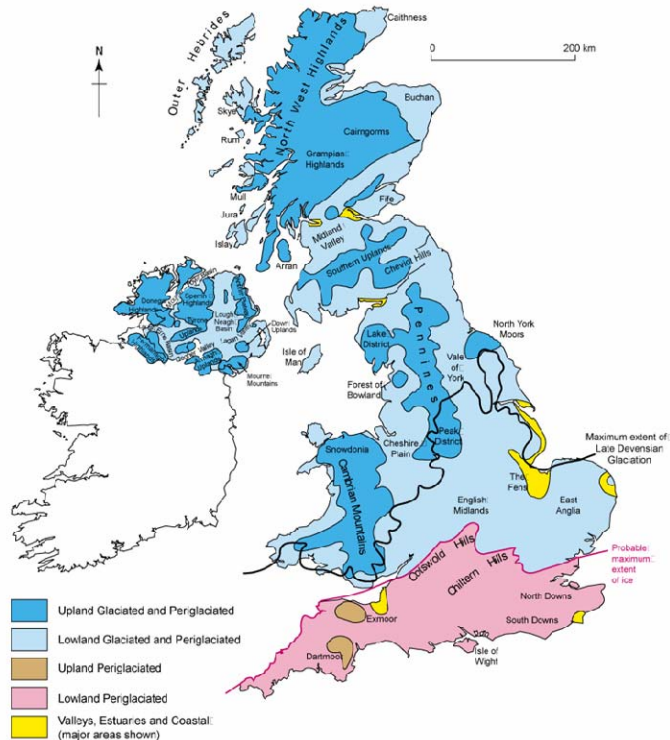
Figure 4: Glaciated and periglaciated areas across the UK during the Anglian and Devensian of the Pleistocene.

The typical lithology of unweathered Lowestoft Till is olive-grey (dark olive-grey when wet), sandy, silty clay with scattered lithic clasts. The matrix consists largely of reconstituted Kimmeridge Clay and other Mesozoic argillaceous rocks (Perrin *et al*., 1973, 1974). The lithic component is dominated by subangular to subrounded fragments of chalk (between 56 % and 84 %) (Perrin *et al*., 1973) but includes a wide range of other lithologies including older Mesozoic limestones and sandstones, flint and derived fossils; in addition, quartz and quartzite pebbles, and fragments of iron-pan may occur, derived from the Kesgrave Formation and the Crag (Arthurton *et al*., 1994). The clasts are ill-sorted and range from sand through to blocks more than 2 m across; the modal size is between 25 to 35 mm. Chalk comprises the bulk of the smaller clasts, whilst flint commonly form those which exceed 40 mm.

In its unweathered state, the Lowestoft Till is cohesive, with a low permeability. Where weathered, the till is rust-brown and is generally more friable and permeable than unweathered till. Depending on the degree of weathering, the till may be completely decalcified, the chalk having been removed by solution; where this is the case, the dominant clasts are flints or flint fragments. The depth of weathering is variable, with profiles extending to as much as 3 m below its top (Arthurton *et al*., 1994).

2.3.3 Superficial Thickness of Deposits in East Anglia

A superficial thickness model, produced under the BGS Information Products Programme was used to assess superficial thickness of the deposits in East Anglia (Figure 5). In order to determine the superficial thickness at each geochemical sample site, the location points were converted to a 3D shapefile in ArcMap 9.1, choosing the Advanced Superficial deposits Thickness Model (ASTM) v2 as the surface for the interpolation method. A new numeric column

was added to the 3D shape file and the thickness, Z, was calculated from the shape file geometry. Superficial thickness varied from 1.5 to 124.9 m with a median thickness of 28.7 m and a mean of 30.1 m.
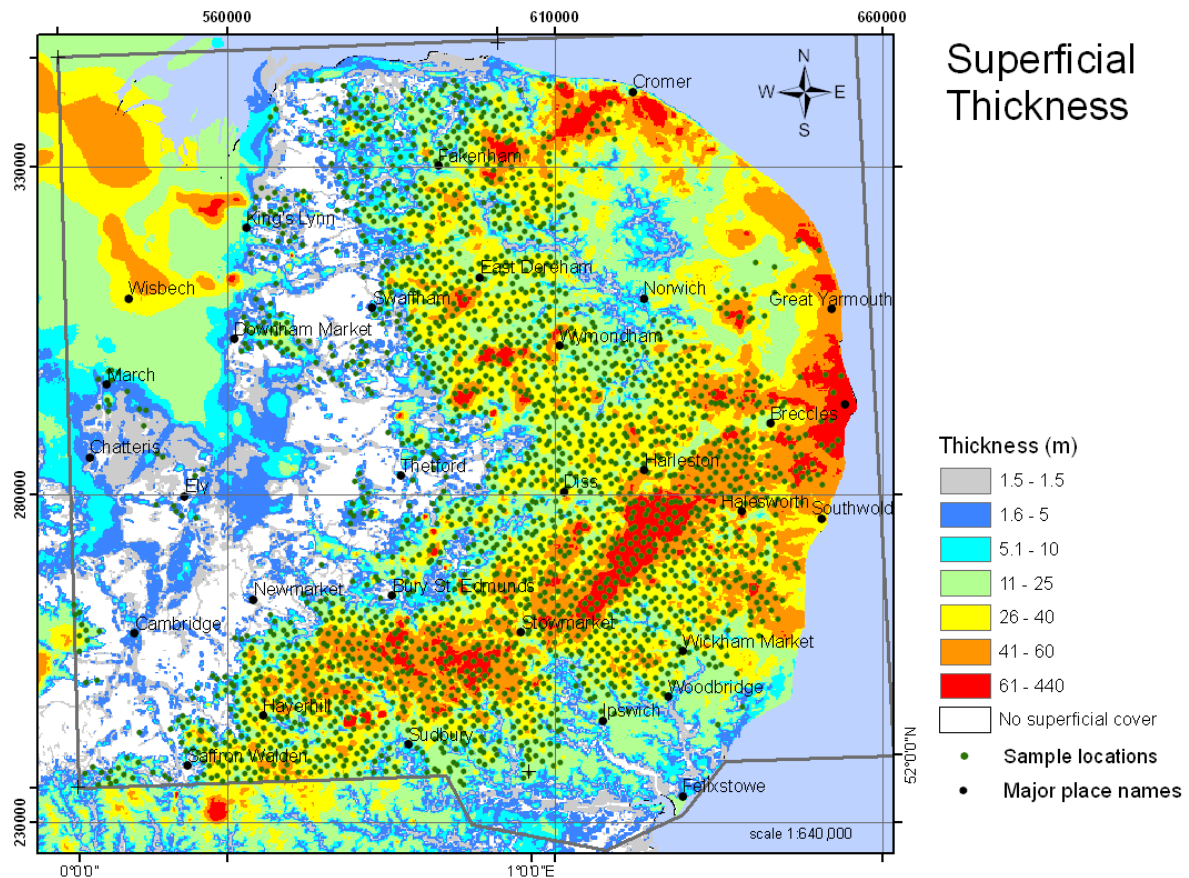
Figure 5: Superficial thickness map (ASTM v2) for East Anglia with dots indicating sample sites over Pleistocene till (Section 4.2.1).

Thicker deposits, shown in orange and red, are spatially coherent exhibiting an arced structure following the coast then trending southwest towards Cambridge. Areas without any superficial cover (see Figure 3) form a corridor from Cambridge in the south, to Thetford and further north beyond Swaffham and King's Lynn.

In central East Anglia between Thetford, Bury St Edmunds and Diss the superficial thickness map should be used with caution (verbal comment, Tony Morigi) as the thickness model is based on older, inaccurate geological maps. This area is currently undergoing mapping.

Additionally to information of the thickness map Appendix 6 shows the topographic elevation of East Anglia in relation to the sea level.

2.4   SOIL GEOCHEMICAL DATA

The geochemical soil data for East Anglia was downloaded from the corporate BGS Geochemistry Database. This data, as described in Section 2.1, is already conditioned and does not need to undergo any further quality control measures. For details how to download geochemical data see BGS internal report by Johnson *et al.* (2004).

2.4.1   Spatial Join

To investigate the geochemical data for sites collected on till deposits of the Lowestoft Formation, the dataset was spatially joined with the 1:50 000 digital superficial geology layer in

DigMAP in ArcMap v9.1 and exported into an Excel spreadsheet. Consequently the data was separated into the different lithostratigraphies. A total of 2316 sample sites are located on mapped till of which 2109 sites are classified by BGS lexicon codes (LEX-ROCK) as LOFT-DMTN (Lowestoft Formation - Diamicton), 5 as TILLD-DMTN (Till, Devensian - Diamicton) and 202 as TILMP-DMTN (Till, Middle Pleistocene - Diamicton). Figure 6 shows the spatial distribution of the selected 2316 sample sites in East Anglia.
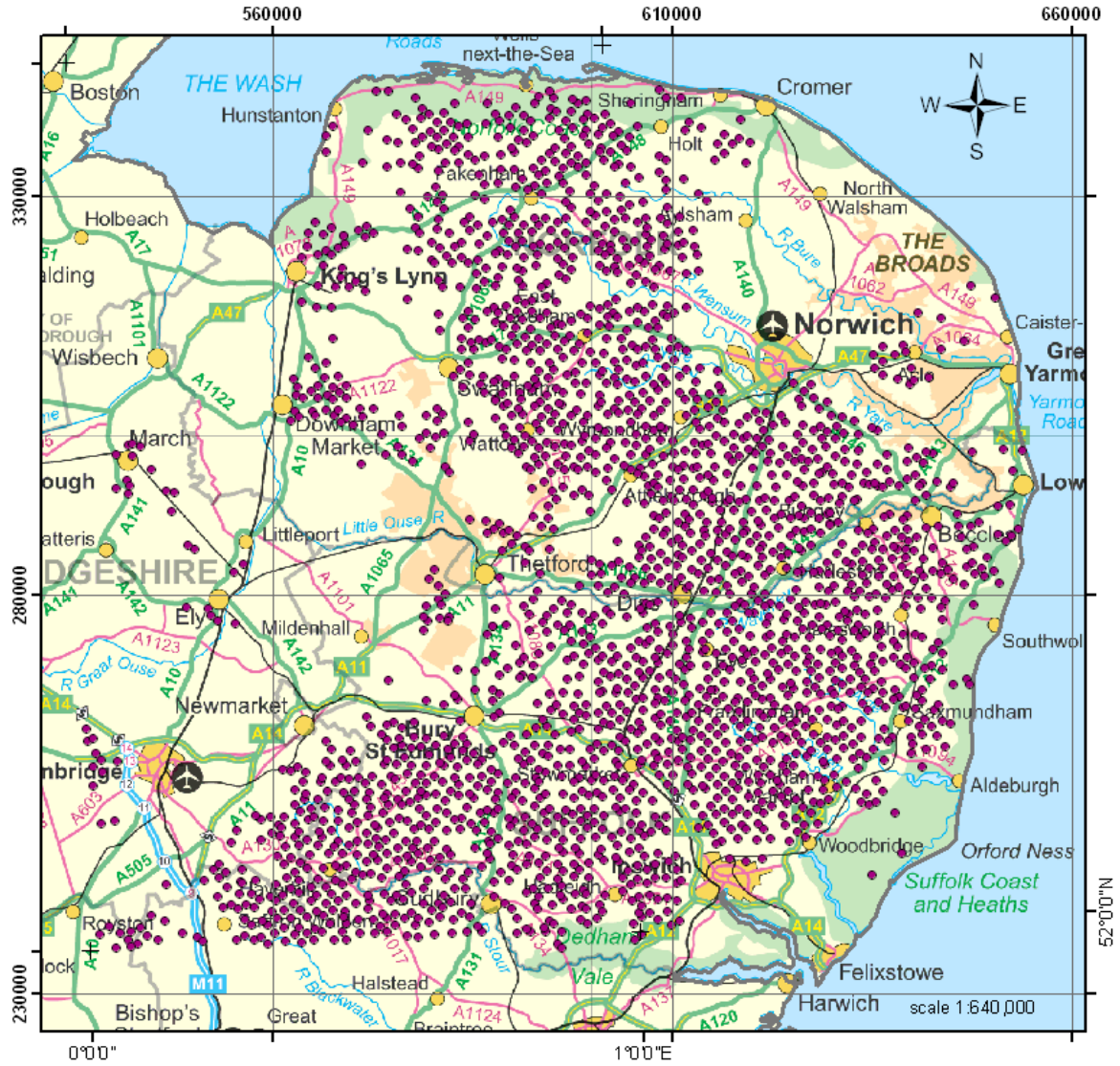
Figure 6: Map shows selected sample site locations (dots) over Pleistocene till deposits in East Anglia. (© Crown Copyright. All rights reserved. OS Licence No: 100017897/2007)

The sites are located from the North Norfolk coast, moving south through central East Anglia towards Sudbury and the M11, covering approximately half of the sampled area in East Anglia. There are several smaller clusters of sites near Downham Market, King's Lynn, Ely and March.

2.4.2 Descriptive Statistics and Distribution of Variables

This investigation comprises data for 40 major, minor and trace elements. Their minimum, maximum, mean and median values as well as the standard deviation are summarised in Table 2. Table 2 also lists the detection limit (DL) for each element reported by the XRF laboratories, Keyworth. Some minimum values were reported below the actual DL and were replaced by a less than DL symbol.

Reimann *et al.*, (2002) suggest removing variables from the datasets, where more than 25 % of analytical results are below the detection limit. Therefore, elements Ta, SO$_3$, Te, Tl, Yb, Sm, Ag, Cd, Cl, In and Mo have not been included in the multivariate analysis of the data set. Data for MgO is available, but was not used in this study.

Table 2: Summary of descriptive statistics (n = 2316)

Element	Unit	DL	Min	Max	Mean	Median	S.D.	Skewness
As	mg kg^{-1}	0.9	3.9	49	12	12	3	**1.89**
Ba	mg kg^{-1}	1	74	464	230	221	44	0.49
Bi	mg kg^{-1}	0.3	< DL	1.5	0.6	0.6	0.2	0.11
Br	mg kg^{-1}	0.8	2.1	63.9	8.3	8.1	3.5	**6.04**
Ce	mg kg^{-1}	1	8	138	44	42	12	0.48
Co	mg kg^{-1}	1.5	4.3	32.9	13.4	12.8	3.6	0.55
Cr	mg kg^{-1}	3	15.2	173.8	58.2	57.6	14.6	0.44
Cs	mg kg^{-1}	1	1	8	4	4	1	0.18
Cu	mg kg^{-1}	1.3	2.8	118.5	15.3	15.1	5.9	**3.61**
Ga	mg kg^{-1}	1	< DL	17.1	7.8	7.8	3.0	0.13
Ge	mg kg^{-1}	0.5	< DL	2.4	1.0	0.9	0.3	0.26
Hf	mg kg^{-1}	1	1.6	28.2	7.1	7	1.8	**1.84**
I	mg kg^{-1}	0.5	< DL	26.4	4.3	3.9	2.1	**2.47**
La	mg kg^{-1}	1	3	67	24	23	7	0.26
Nb	mg kg^{-1}	1	1.8	23.1	9.2	9	2.8	0.34
Nd	mg kg^{-1}	4	< DL	66.2	18.9	18.3	6.6	0.31
Ni	mg kg^{-1}	1.3	1.3	102.8	21	20	9	0.80
Pb	mg kg^{-1}	1.3	10.9	682.7	28.8	26.3	21.5	**18.15**
Rb	mg kg^{-1}	1	2.7	129.9	63.8	64.6	21.3	0.01
Sb	mg kg^{-1}	0.5	< DL	9	1.0	0.9	0.3	**11.69**
Sc	mg kg^{-1}	3	< DL	18.2	6.8	6.7	2.7	0.23
Se	mg kg^{-1}	0.2	< DL	1.9	0.3	0.3	0.2	**1.80**
Sn	mg kg^{-1}	0.5	0.8	159	2.9	2.5	3.8	**31.74**
Sr	mg kg^{-1}	1	16	239.1	62.8	54.2	29.3	**2.34**
Th	mg kg^{-1}	0.7	< DL	12.8	5.8	5.6	1.7	0.44
U	mg kg^{-1}	0.5	< DL	3.1	1.5	1.5	0.3	0.08
V	mg kg^{-1}	3	35	227	78.0	77.2	16.8	0.57
W	mg kg^{-1}	0.6	< DL	3.7	1.8	1.8	0.6	-0.03
Y	mg kg^{-1}	1	4.5	72.4	20.1	19.7	4.9	0.55
Zn	mg kg^{-1}	1.3	11.7	256.3	59.5	58.5	18.8	**1.24**
Zr	mg kg^{-1}	1	102.9	706.4	272.0	262.8	61.2	**1.66**
Al$_2$O$_3$	wt. %	0.2	0.3	16	7.9	8.1	2.8	-0.08
CaO	wt. %	0.3	< DL	25.63	2.38	1.09	3.36	**3.08**
Fe$_2$O$_3$	wt %	0.05	< DL	10.49	3.17	3.18	1.13	0.33
K$_2$O	wt. %	0.01	0.36	2.78	1.46	1.42	0.33	0.18
MnO	wt. %	0.005	< DL	0.252	0.052	0.049	0.023	0.92
Na$_2$O	wt. %	0.3	< DL	0.7	0.3	0.2	0.1	**1.18**
P$_2$O$_5$	wt. %	0.05	< DL	0.71	0.21	0.20	0.06	**1.75**
SiO$_2$	wt. %	0.1	22.8	95.6	67.3	67.9	10.6	-0.33
TiO$_2$	wt. %	0.02	< DL	0.873	0.388	0.388	0.140	0.02

Table 2 shows that there are elements within the set of data, where mean and median values differ quite significantly. This suggests that for some elements a minor amount of sites have very extreme values compared to bulk of regional background value. This might indicate outliers caused by anthropogenic contamination and which means the data is skewed.

It is recommended to use normal distributed geochemical data in Factor Analysis (Batista *et al.*, 2006); therefore data with skewness of greater 1 or below -1 were log transformed. Skewness is

listed in Table 2 and elements As, Br, CaO, Cu, Hf, I, P_2O_5, Pb, Sb, Se, Sn, Sr, Zn and Zr have been log transformed prior to statistical analysis.

To give an example of normally distributed data with a low skewness in comparison to data of high skewness, histograms for the elements Bi (0.11), Rb (0.01), Pb(18.15) and Sn (31.74) are shown below (Figure 7). Bin intervals for the histograms were chosen in a simple manner between one-quarter and one-half the standard deviation as recommended in Sinclair (1989).

Factor analysis, as a statistical method, requires randomness and independence of sampling, and a normal distribution of analytical observations (Pirc *et al*., 2006). This is satisfied by the sampling methods described in Section 2.2, investigating skewness of the data and log-transforming the data. Plotting cumulative probability plots of the determinants (Appendix 1) was used to detect outliers and unusual data structures in the geochemical data. In geochemistry, outliers are generally observations resulting from other secondary processes, such as anthropogenic contamination or mineralisation and not from extreme values of the background distribution (Filzmoser *et al*., 2005). Outliers should always be investigated, as they contain important information about data quality. Outliers can have a severe influence on the results of factor analysis (Pison *et al*., 2003) and should be dealt with prior to entering into this process.

In this study, data was studied visually for samples showing anomalies in their elemental concentrations and distribution. High values for heavy metals, above the normal regional geochemical variation, can indicate potential contamination. Four samples out of the 5748 sites were identified and removed from the dataset. Their sample IDs are 448925, 440708, 447313 and 442481. The samples showed elevated values for As, Ni, Zn, Fe and Pb, which suggested potential contamination. For two of the sample sites the G-BASE sample field cards had also recorded that the site could be contaminated.

With those samples removed, the dataset was imported into Minitab 15[©] for further investigation of their distribution and search for outliers.
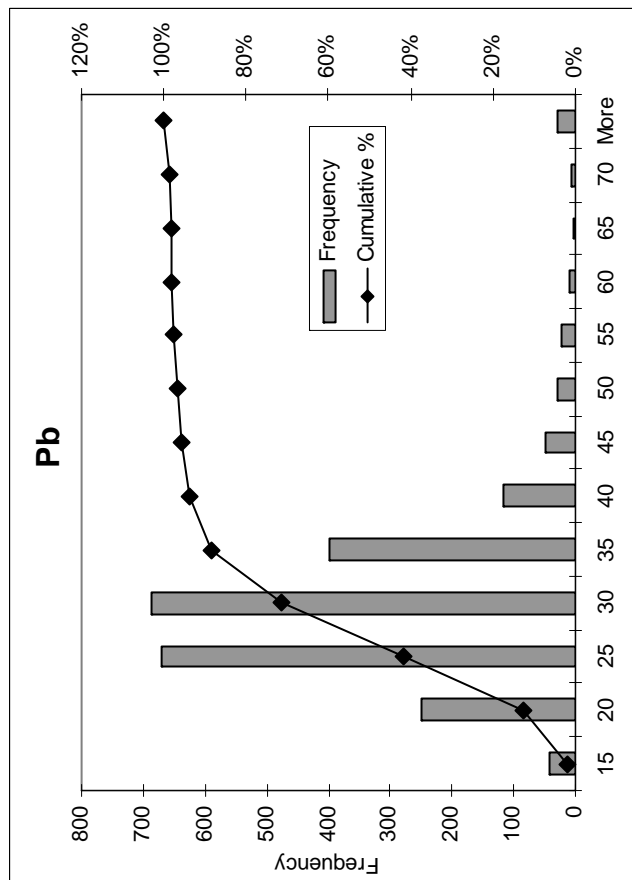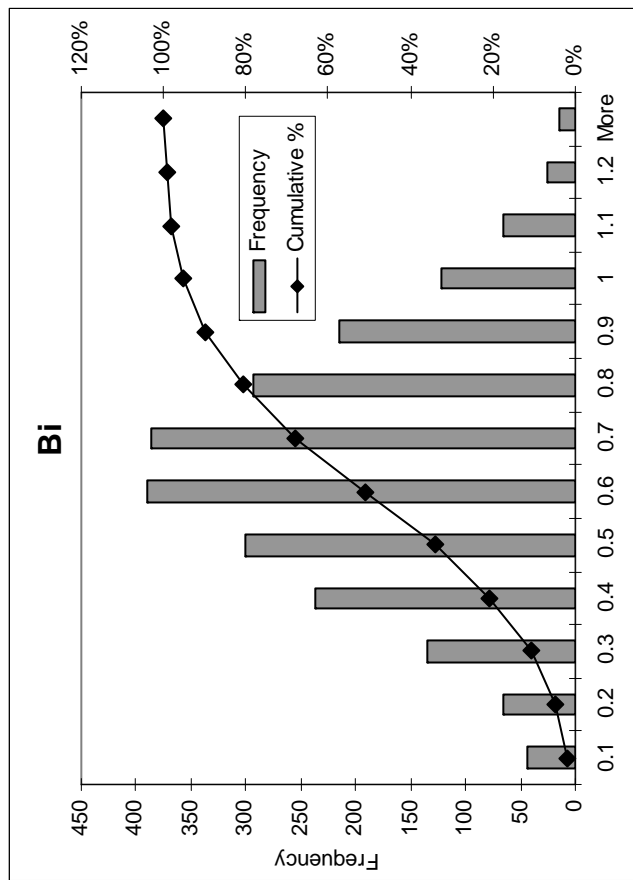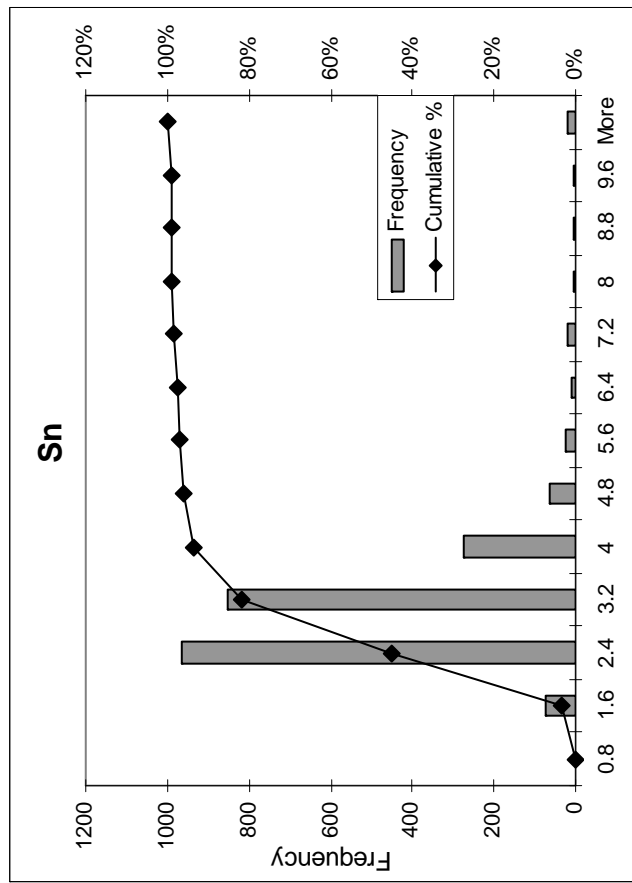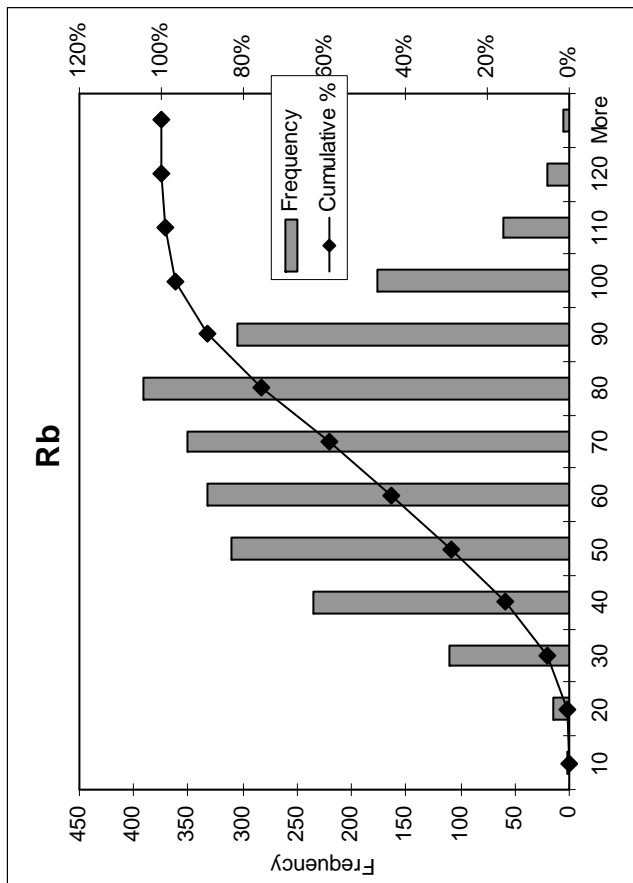
Figure 7: Histograms for Bi, Rb, Pb and Se (n = 2316) concentrations in mg kg^{-1}

2.5   FACTOR ANALYSIS

Factor analysis (FA) is one of the possible multivariate analysis techniques widely used for the interpretation of geochemical data of sediments, soils and waters (Batista *et al.*, 2006; Kumru and Bakac 2003; Reimann *et al.* 2001), hydrochemical data (Pirc *et al.*, 2006; Ruiz *et al.*, 1990) and radiometric data (Bakac, 2004). The basic aim of FA is to explain the correlations between the observed variables in terms of linear combination of a specific number of unobservable variables, called factors (Le Maitre, 1982). Factors allow a simple description of a multidimensional problem and variable relationships, which would not necessarily be exposed by a simple correlation analysis (Pirc *et al.*, 2006). Therefore, factor analysis seems to be an effective and simple tool to expose relationships amongst the geochemical soil data.

Factor analysis was carried out in Minitab™. The applied method was based on principal component analysis (PCA) using linear correlation coefficients and varimax rotation. PCA is by far the most common form of FA and seeks a linear combination of variables such that the maximum variance is extracted from the variables. It then removes this variance and seeks a second linear combination. This is called the principal axis method and results in orthogonal factors. PCA analyses total variance. Varimax rotation is an orthogonal rotation of the factor axes and was used in order to maximise the variance of the squared loadings of a factor on all the variables in a factor matrix. A varimax solution yields results which make it as easy as possible to identify each variable with a single factor (Garson, 2006)

To avoid problems during the process of Factor Analysis caused by missing values in the matrix, data of 58 sample sites were removed from the data set leaving a total of n = 2258 sample sites for Factor Analysis.

2.6   FACTOR SCORES

Factor scores, also called "component scores" in PCA, are the scores of each case (row) on each factor (column). To compute the factor score for a given site and for a given factor, factor score coefficients (see table in Appendix 3) are multiplied by the original data after they have been centred by subtracting means. This was carried out in Minitab during factor analysis. Six storage columns were added to the data sheet to accommodate the score results; one column for each factor.

The calculation of scores is very simple but it is helpful to plot and visualise the results of the actual Factor Analysis and the distribution of high and low factor loadings in a regional context.

These factor score data were saved and imported as a *.dbf file into ArcMap™ v9.1 and plotted as coloured graduated symbol maps. These score maps are presented for each calculated Factor in the following results section.

3 Results

In the following sections, the factors, loadings, elemental composition and score distribution will be presented separately. Each section will include maps of factor scores displayed as graduate symbols as well as tables listing element loadings according to their strength. The strength classification scale has been adapted from Pirc *et al*. (2006) and Batista *et al*. (2006). For interpretation, very strong loadings are > 0.70. Loadings between 0.70 and 0.50 are strong, between 0.50 and 0.30 are moderate and below 0.30 weak. After several test runs, an analysis with 6 factors was carried out. The loadings for all six factors represent 31.4 % of the total variance. The varimax rotated factor loadings for all elements can be found in Table 3.

Table 3: Varimax rotated Factor loadings for topsoil samples (n = 2258, and strongest loadings in bold)

Variable	Factor1	Factor2	Factor3	Factor4	Factor5	Factor6	Communality
As	0.568	0.465	0.176	-0.093	-0.081	0.122	0.6
Ba	**0.793**	0.073	0.178	0.033	-0.098	0.467	0.894
Bi	-0.052	0.06	0.043	0.025	-0.509	0.023	0.268
Br	0.417	0.268	0.053	-0.25	-0.586	-0.01	0.654
Ce	**0.924**	0.275	0.132	-0.039	-0.074	0.149	0.976
Co	**0.841**	0.338	0.155	-0.142	0.032	0.165	0.894
Cr	**0.912**	0.171	0.099	-0.093	-0.181	0.032	0.913
Cs	**0.861**	-0.038	0.131	-0.207	-0.142	-0.264	0.893
Cu	0.559	0.319	0.544	-0.051	-0.104	-0.166	0.751
Ga	**0.934**	0.038	0.148	-0.159	-0.178	-0.072	0.957
Ge	0.169	-0.028	0.302	-0.012	-0.419	0.061	0.3
Hf	-0.07	-0.068	-0.036	**0.916**	-0.003	0.076	0.855
I	0.645	0.459	0.025	-0.11	-0.349	0.125	0.777
La	**0.907**	0.308	0.117	-0.069	-0.089	0.116	0.958
Nb	**0.950**	0.026	0.141	-0.031	-0.12	0.106	0.95
Nd	**0.845**	0.361	0.101	-0.098	-0.104	0.116	0.888
Ni	**0.859**	0.362	0.166	-0.187	-0.054	-0.018	0.935
Pb	0.234	0.192	**0.751**	-0.141	-0.222	0.158	0.75
Rb	**0.929**	-0.015	0.189	-0.132	-0.108	-0.107	0.939
Sb	0.129	-0.035	0.654	0.006	0.085	-0.03	0.453
Sc	**0.806**	0.2	0.048	-0.191	-0.196	-0.046	0.768
Se	0.427	0.018	0.127	-0.022	-0.609	-0.277	0.648
Sn	0.21	0.087	**0.703**	-0.016	-0.173	-0.023	0.577
Sr	0.613	0.494	0.021	-0.343	-0.172	0.12	0.782
Th	**0.920**	0.157	0.125	-0.017	-0.095	0.171	0.924
U	0.479	-0.044	-0.183	0.249	-0.403	0.118	0.504
V	**0.900**	0.183	0.133	-0.207	-0.156	-0.1	0.939
W	0.677	-0.048	0.188	0.192	-0.055	0.102	0.546
Y	**0.835**	0.33	0.122	0.03	-0.093	0.239	0.887
Zn	0.721	0.354	0.426	-0.073	-0.172	-0.18	0.894
Zr	-0.155	-0.055	-0.095	**0.913**	-0.009	0.114	0.882
Al$_2$O$_3$	**0.946**	-0.022	0.135	-0.139	-0.171	-0.042	0.964
CaO	0.44	**0.618**	-0.021	-0.323	-0.169	-0.134	0.727
Fe$_2$O$_3$	**0.867**	0.245	0.244	-0.072	-0.065	-0.076	0.887
K$_2$O	**0.898**	0.062	0.143	-0.105	-0.084	0.224	0.899
MnO	0.409	**0.597**	0.079	-0.044	0.228	0.451	0.787
Na$_2$O	0.119	-0.091	-0.02	0.19	-0.023	**0.895**	0.86
P$_2$O$_5$	-0.133	**0.695**	0.239	0.106	-0.048	-0.223	0.621
SiO$_2$	-0.388	-0.539	0.124	0.438	**0.278**	-0.108	0.738
TiO$_2$	**0.947**	-0.065	0.155	0.013	-0.116	0.135	0.956
Variance	18.735	3.412	2.667	2.63	2.043	1.907	31.393
% Var	0.468	0.085	0.067	0.066	0.051	0.048	0.785

Images in Figure 8 show the distribution of loadings and scores of variables for the first two factors. An important image is the scree (Eigenvalue) plot as it can be used to set the cut-off at the number of factors to compute as factors with low Eigenvalues contribute only little to the explanation of variances. In this study the maximum of Factors was set to six.
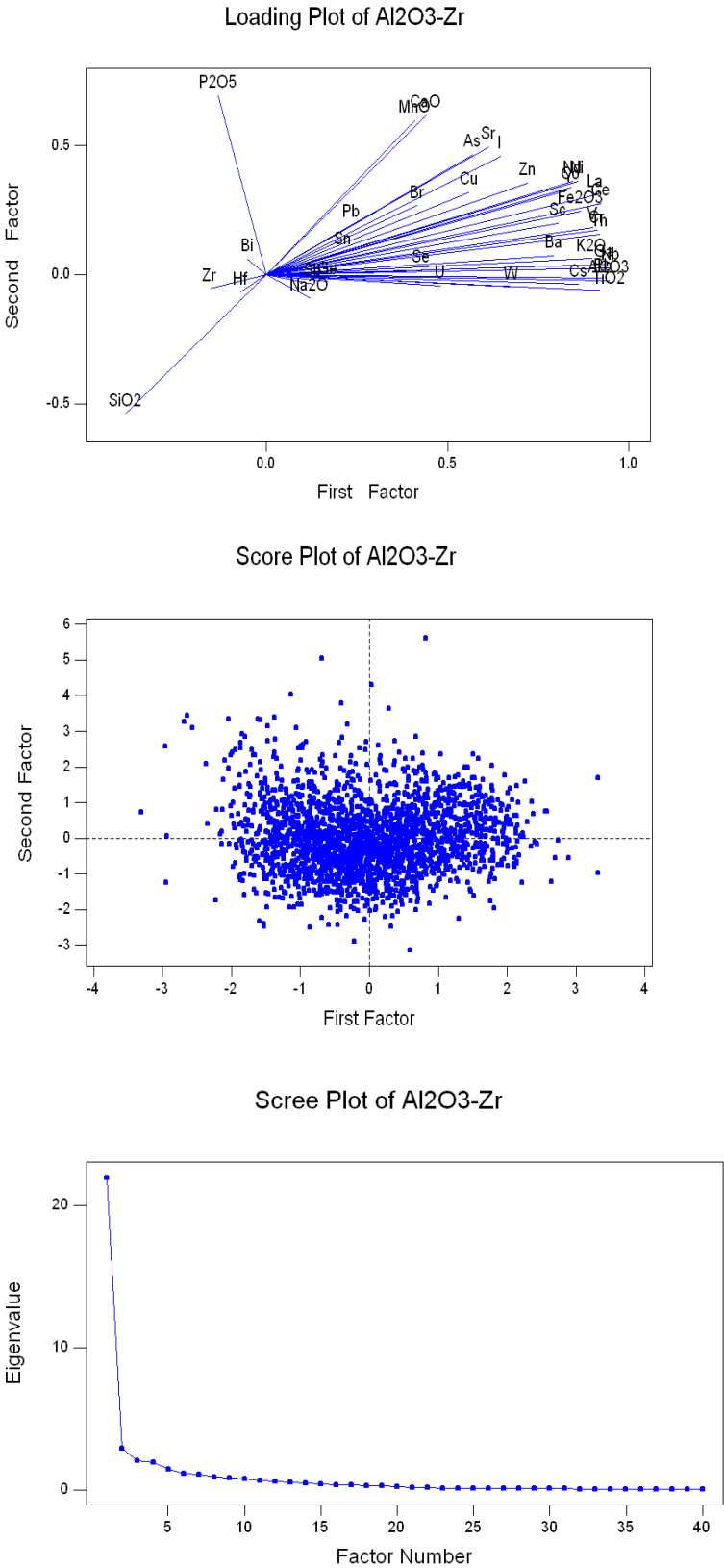

Figure 8: Loading and score plots for Factor 1 and 2 and scree (Eigenvalue) plot

14

3.1   FACTOR 1

Factor 1 is the strongest factor accounting for 18.74 % of the total variance with an Eigenvalue of 21.12. Table 4 lists a wide range of elements with very strong, strong and moderate loadings associated in Factor 1. Weakest loadings are counted for Pb, Sn, Ge, Na_2O, Sb, Sn and negative loadings for Bi, Hf, P_2O_5, SiO_2 and Zr.

Table 4: Determinant associations for Factor 1

Factor loadings class	Determinant association
0.99 to 0.70	Al_2O_3, Ba, Ce, Co, Cr, Cs, Fe_2O_3, Ga, K_2O, La, Nb, Nd, Ni, Rb, Sc, Th, TiO_2, V, Y, Zn
0.69 to 0.50	As, Cu, I, Sr, W,
0.49 to 0.30	Br, CaO, MnO, Se, U
0.29 to 0.20	Pb, Sn
< 0.19	Ge, Na_2O, Sb, Sn
negative loadings	Bi, Hf, P_2O_5, SiO_2, Zr

Highest scores of Factor 1 associated elements are predominantly located on tills in the southern part of East Anglia, just south of Bury St. Edmunds, leaving the northern half almost completely unrepresented by Factor 1. The strongest signature can be found in the south east around Haverhill. Figure 9 below, shows clearly this division of the Lowestoft Till Formation.
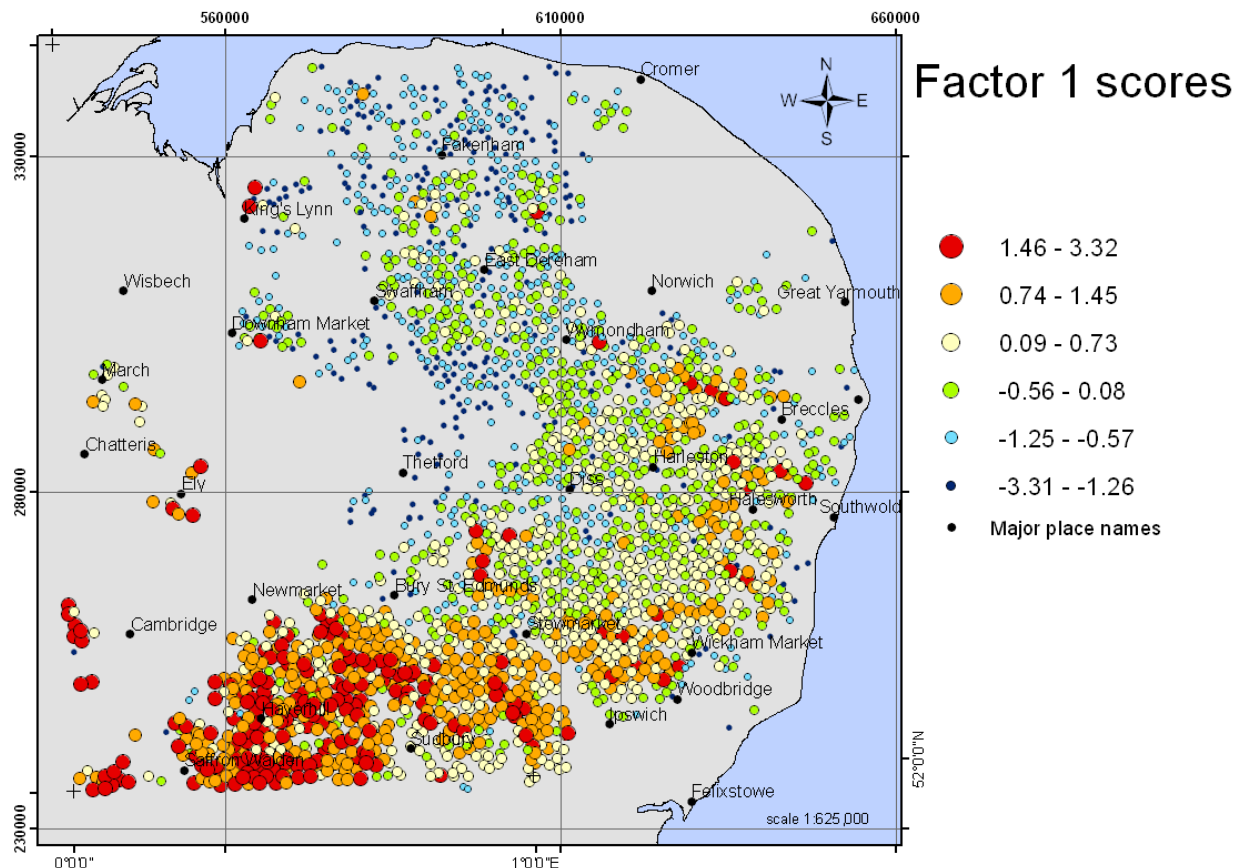

Figure 9: Distribution of Factor 1 scores (n = 2258)

15

3.2 FACTOR 2

Factor 2 is the second strongest factor accounting for 3.41 % of the total variance with an Eigenvalue of 2.91. Table 5 shows that Factor 2 represents strong loadings for CaO, MnO and P_2O_5 and moderate strength of As, Co, Cu, I, La, Nd, Ni, Sr, Y and Zn.

Table 5: Determinant associations for Factor 2

Factor loadings class	Determinant association
0.99 to 0.70	
0.69 to 0.50	CaO, MnO, P_2O_5,
0.49 to 0.30	As, Co, Cu, I, La, Nd, Ni, Sr, Y, Zn
0.29 to 0.20	Br, Ce, Fe_2O_3, Sc,
< 0.19	Ba, Bi, Cr, Ga, K_2O, Nb, Pb, Se, Sn, Th, V,
negative loadings	Al_2O_3, Cs, Ge, Hf, Na_2O, Rb, Sb, SiO_2, TiO_2, U, W, Zr

The distribution map in Figure 10 shows that highest loadings of Factor 2 occur mainly along the western edge of the till deposits. Locations of lowest scores for Factor 2 are located in the centre and along the eastern edge of the till belt.
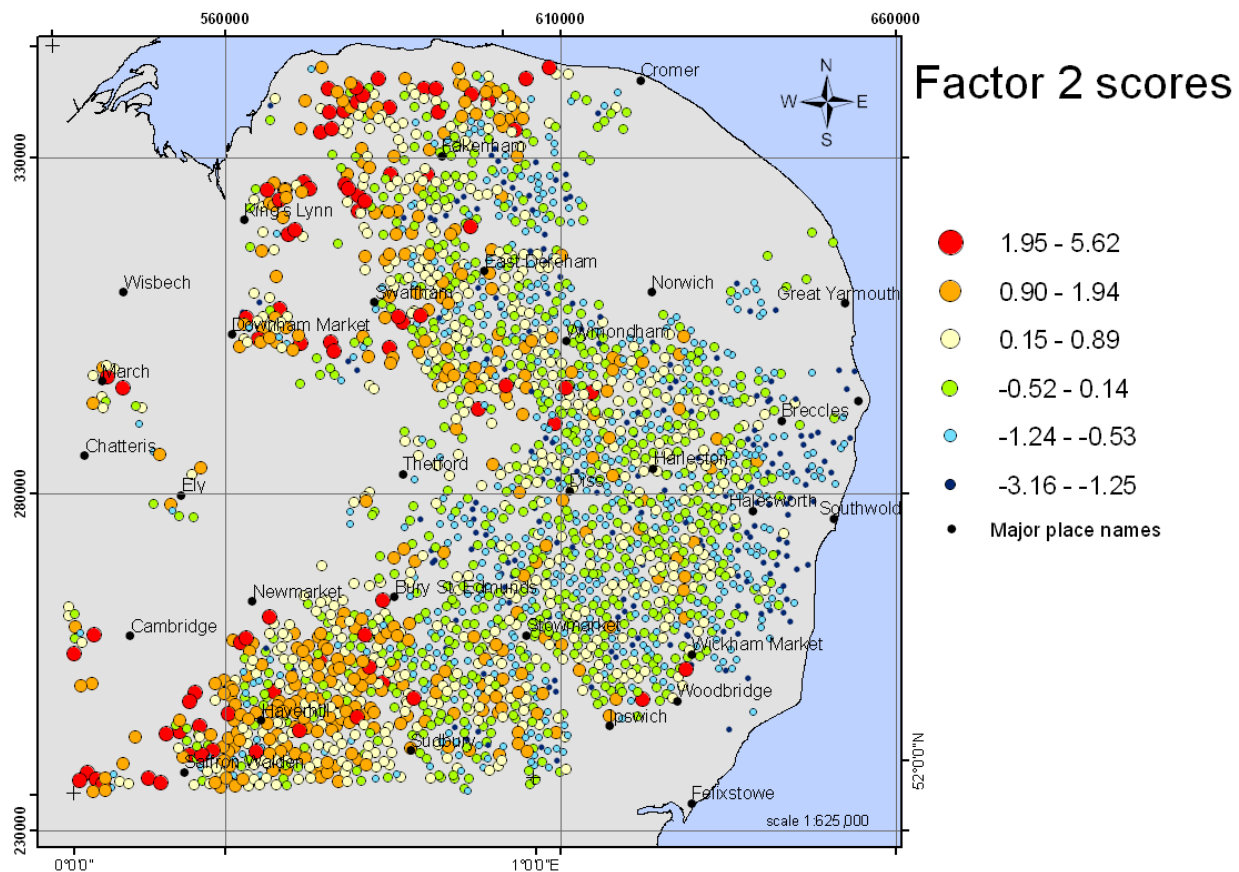

Figure 10: Distribution of Factor 2 scores (n = 2258)

16

3.3   FACTOR 3

Factor 3 is the third strongest factor, accounting for 2.67 % of the total variance with an Eigenvalue of 2.02. Table 6 shows that factor 3 represents heavy metals with very strong loadings of Pb and Sn, strong loadings of Cu and Sb and moderate loadings of Zn.

Table 6: Determinant associations for Factor 3

Factor loadings class	Determinant association
0.99 to 0.70	Pb, Sn
0.69 to 0.50	Cu, Sb
0.49 to 0.30	Zn
0.29 to 0.20	Fe_2O_3, Ge, P_2O_5, Sr, V
< 0.19	Al_2O_3, As, Ba, Bi, Br, Ce, Co, Cr, Cs, Ga, I, K_2O, La, MnO, Nb, Nd, Ni, Rb, Sc, Se, SiO_2, Sr, Th, TiO_2, V, W, Y
negative loadings	CaO, Hf, Na_2O, U, Zr

Figure 11 shows the distribution of factor 3 scores relative to their sampling location. The occurrence of very high loadings of heavy metals is indicated by red dots on the map below. Elevated concentrations of heavy metals are clearly correlated with urban areas in East Anglia; this may be due to higher anthropogenic and urban activity.
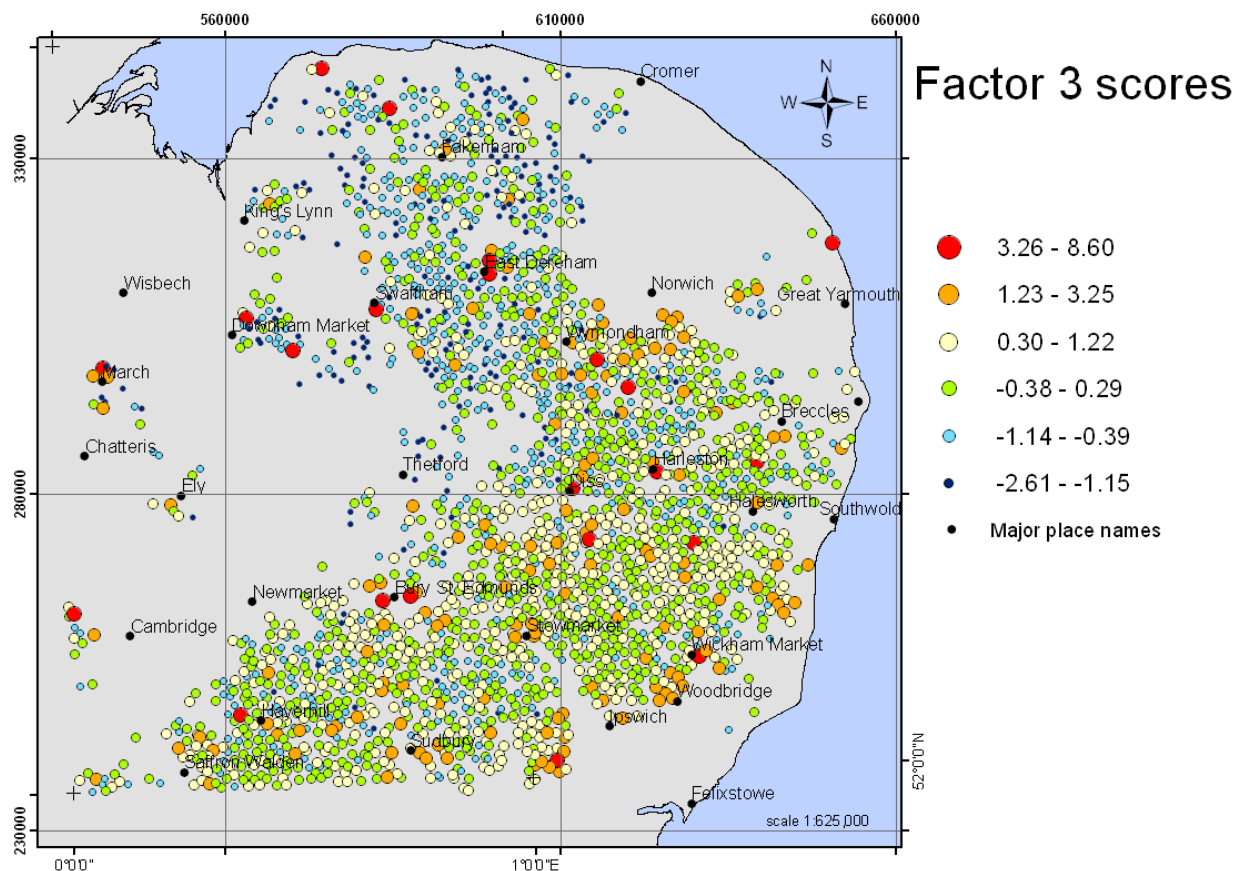

Figure 11: Distribution of Factor 3 scores (n = 2258)

This could be confirmed, in the case of Pb, by investigating stable Pb isotope ratios, which could display Pb signature from a fossil fuel source. These sample locations and results could be treated as outliers as they are not representative of the natural geochemical baseline.

17

3.4   FACTOR 4

The fourth strongest factor accounting for 2.63 % of the total variance is Factor 4 with an Eigenvalue of 1.86. It associates Hf and Zr with very strong loadings followed by moderate to strong loadings of SiO_2.

Table 7: Determinant associations for Factor 4

Factor loadings class	Determinant association
0.99 to 0.70	Hf, Zr
0.69 to 0.50	
0.49 to 0.30	SiO_2,
0.29 to 0.20	U
< 0.19	Ba, Bi, Na_2O, P_2O_5, Sb, TiO_2, W, Y
negative loadings	Al_2O_3, As, Br, CaO, Ce, Co, Cr, Cs, Cu, Fe_2O_3, Ga, Ge, I, K_2O, La, MnO, Nb, Nd, Ni, Pb, Rb, Sc, Se, Sn, Sr, Th, V, Zn

Figure 12 shows that highest Factor 4 scores are located in the centre of East Anglia and the till belt. They are scattered around Thetford, stretching from Bury St. Edmunds in the south to Swaffham in north and Diss in the east. Some other high scores are located to the southeast of Sudbury.
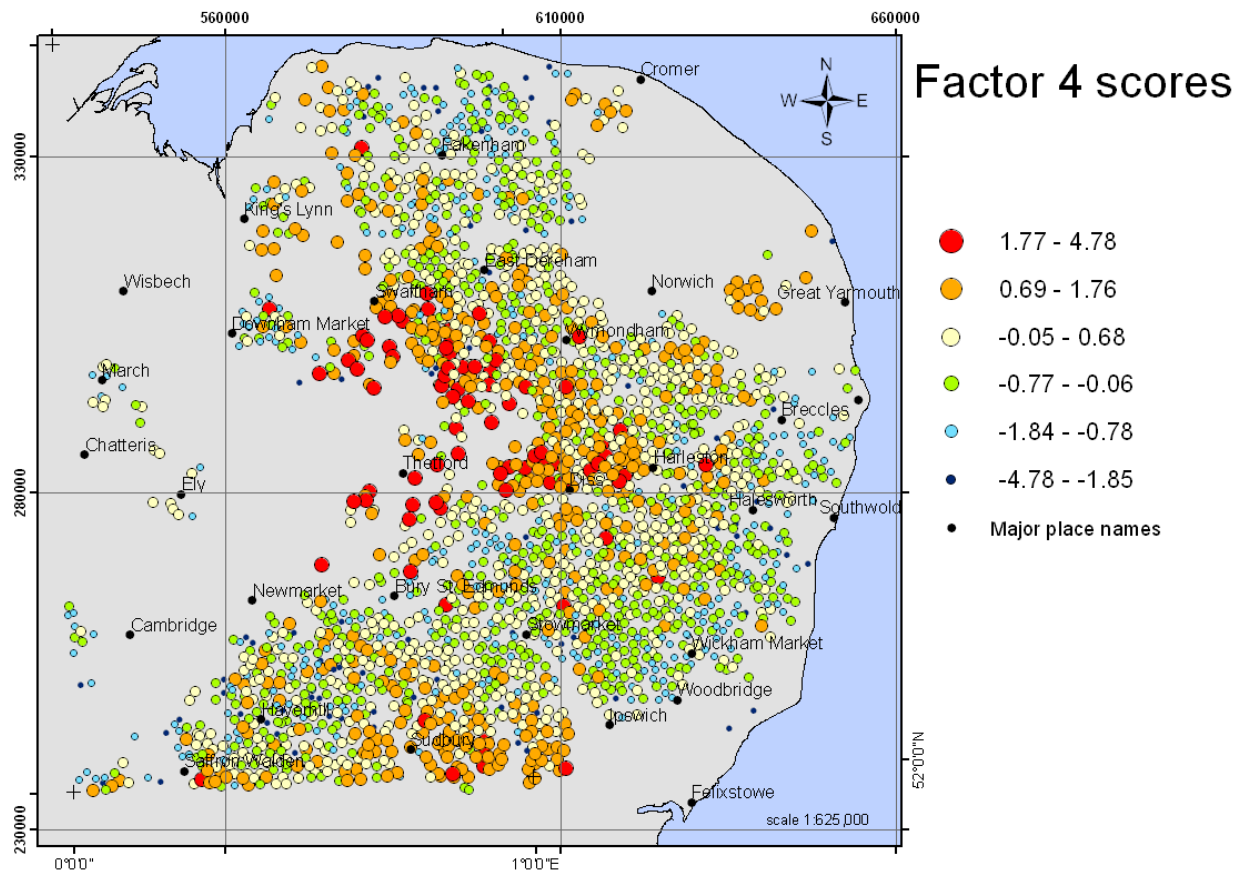
Figure 12: Distribution of Factor 4 scores (n = 2258)

18

The very strong concentration of Hf, Zr and SiO$_2$ in topsoils of this area may result from the presence of aeolian sand deposits in the Thetford area, and a combination of unmapped aeolian sands and glaciofluvial sand and gravel intercalations within the Till elsewhere.

3.5   FACTOR 5

Factor 5 accounts for 2.04 % of the total variance with an Eigenvalue of 1.42 and represents only weak association of MnO and SiO$_2$.

Table 8: Determinant associations for Factor 5

Factor loadings class	Determinant association
0.99 to 0.70	
0.69 to 0.50	
0.49 to 0.30	
0.29 to 0.20	MnO, SiO$_2$
< 0.19	Co, Sb
negative loadings	Al$_2$O$_3$, As, Ba, Bi, Br, CaO, Ce, Cr, Cs, Cu, Fe$_2$O$_3$, Ga, Ge, Hf, I, K$_2$O, La, , Na$_2$O, Nb, Nd, Ni, P$_2$O$_5$, Pb, Rb, Se, Sc, Sn, Sr, Th, TiO$_2$, U, V, W, Y, Zn, Zr
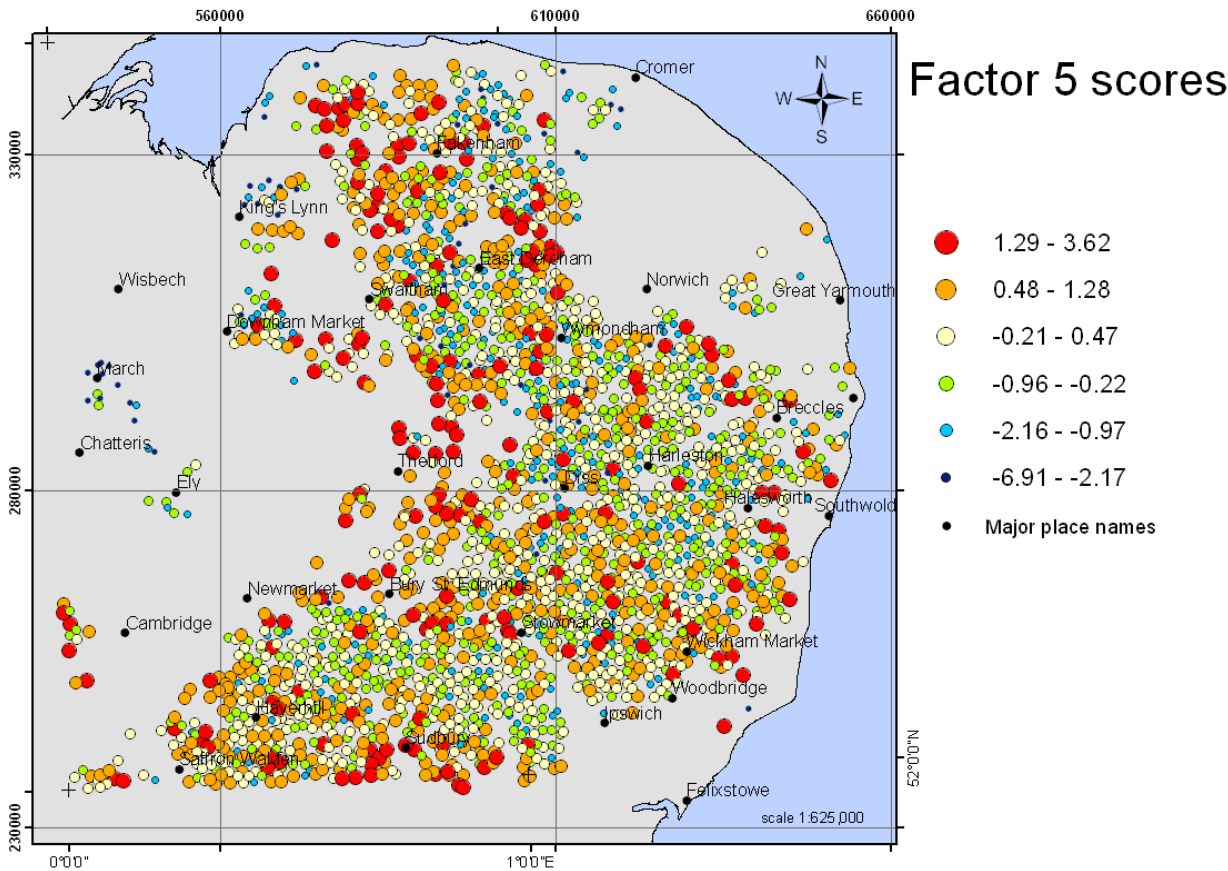
Figure 13: Distribution of Factor 5 scores (n = 2258)

19

3.6 FACTOR 6

Factor 6 is accounts for 1.91 % of the total variance with an Eigenvalue of 1.11. The strongest element associated in Factor 6 is Na_2O, followed by moderately strong loadings of Ba and MnO.

Table 9: Determinant associations for Factor 6

Factor loadings class	Determinant association
0.99 to 0.70	Na_2O
0.69 to 0.50	
0.49 to 0.30	Ba, MnO
0.29 to 0.20	K_2O, Y
< 0.19	As, Bi, Ce, Co, Cr, Ge, Hf, I, La, Nb, Nd, Pb, Sr, Th, TiO_2, U, W, Zr
negative loadings	Al_2O_3, Br, CaO, Cs, Cu, Fe_2O_3, Ga, Ni, P_2O_5, Rb, Sb, Sc, Se, SiO_2, Sn, V, Zn

The distribution of scores for Factor 6 (Figure 14) shows the greatest contrast of all previous factor score maps. The highest factor scores are located in the north and south of mapped till deposits whilst the lowest scores are found in the centre of the till belt.

Figure 14: Distribution of Factor 6 scores (n = 2258)

20

4 Discussion and Conclusions

Results of FA, presented in Section 3, presents some very interesting geochemical distribution patterns and associations of elements within the soils.
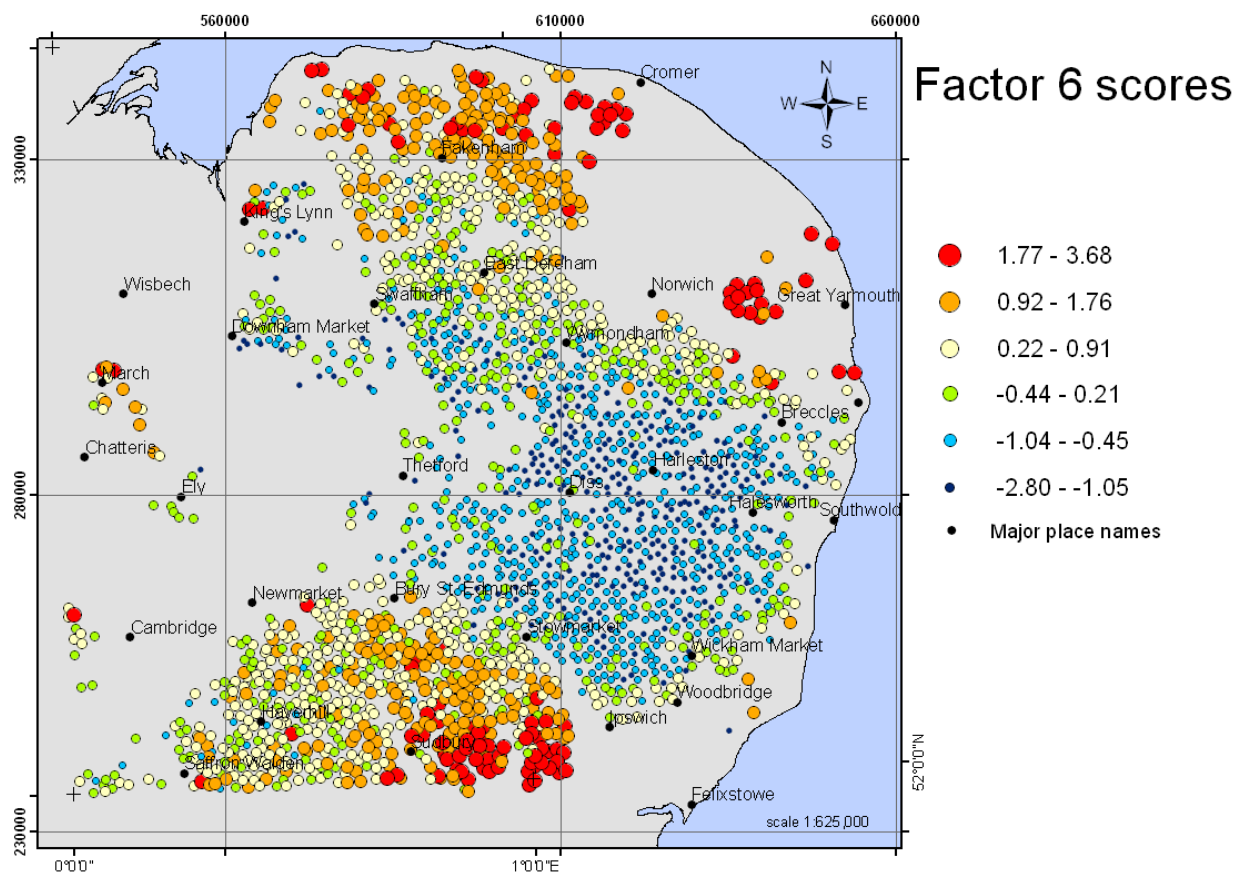
Element association of Factor 1 is mainly controlled by clay and clastic lithologies with a non-carbonate signature and occurs very strongly in the southeast of the study area. This suggest, that the material of the Lowestoft Formation of this area has derived from a clay rich source rock from the west of East Anglia. Deposits in the northern area, which are very weakly represented by Factor 1 and its element association, may have had a different source of material and direction of transport. There are also significant changes in bedrock topography and lithology types in this area. Additionally, the Factor 1 scores increase towards the most southern limit of the Anglian glaciation.

The distribution of Factor 2 scores suggest that the results are Chalk controlled. Highest scores are (as shown in Figure 10) located along the western contact of the Till deposits with the Upper Chalk. A possible explanation for this pattern is that the western margin of the till is underlain by Cretaceous Chalk and in this vicinity the till cover is thinner and more heavily dissected by drainage than to the east (see Figure 4). It is possible that bedrock influence or increased fragmental bedrock material content (high in calcite) is present here.

Factor 3 scores show a classic urban signature of heavy metals, which coincide with the location of urban areas in East Anglia, even when extreme, contaminated samples have already been removed from the dataset.

The association of Hf and Zr in Factor 4 and the locations of high scores in the central area of East Anglia suggest an influence of the Thetford Sands. Soil geochemistry is therefore controlled by more recent Holocene aeolian sand deposits rather than by Pleistocene Tills in this particular area.

Factor 5 is probably the least indicative of all Factors presented and might have been caused by a silica dilution effect. There is no apparent spatial correlation.

Factor 6 shows a very significant distribution pattern of Na_2O with highest scores located in the north and south of the study area. There are numerous possible causes for this distribution pattern. Firstly, Na_2O determined by XRFS has to be used cautiously, because of high analytical variance when determining "light" elements by XRFS. It does not seem that there is an analytical batch relationship (see Appendix 4) as locations of high scores do not follow distribution patterns of the batch IDs. A comparison with the interpolated geochemistry map of Na_2O (Appendix 5) for whole East Anglia shows that highest Na_2O values of the 90 %ile class are located in the same areas as the high factor scores of Factor 5. This would support that the distribution patterns shown in Figure 14 are natural.

Natural causes could be that the southern-most anomaly may reflect the influence of the underlying bedrock (London Clays), whilst the northern anomaly may be the result of glacial reworking of material and possible intercalation of Loess deposits into the Till units. The variation is perpendicular to the accepted direction of ice flow across the area, and appears to demonstrate a marked stratification of chemistry within the till sheet.

A more likely explanation is that the soil chemistry in these areas is influenced by marine ingression. The Broads and wider area between Cromer and Great Yarmouth is naturally low lying (Appendix 6) and has also been indicated as coastal flood plain by a report of the Forest Research (2002). These areas would have been flooded by an event such as the storm surge in 1953. This major storm surge coincided with a naturally high spring tide resulting in an elevated sea level rising almost 3 meters (at King's Lynn) above normal high water marks. This event

overtopped sea defences along the east coast and flooded approximately 730 km^2 (www.metoffice.gov.uk).

Overall, these geochemical patterns suggest that the till deposit can be separated into a south eastern and central northern area, whilst the most western edge of the deposits being influenced by the Lower Chalk and the central area by cover sands.

This study has shown that despite their heterogeneous character and differing origin, Pleistocene tills of East Anglia and their derived soils can have strong spatial geochemical distribution patterns.

Multivariate analysis, such as Factor Analysis, of geochemical soil data can be a helpful aid to quickly describe and group tills and other superficial deposits, which may aid a better understanding of their origin, substrate composition and distribution.

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Appendix 1 Cumulative Probability Plots of Determinants
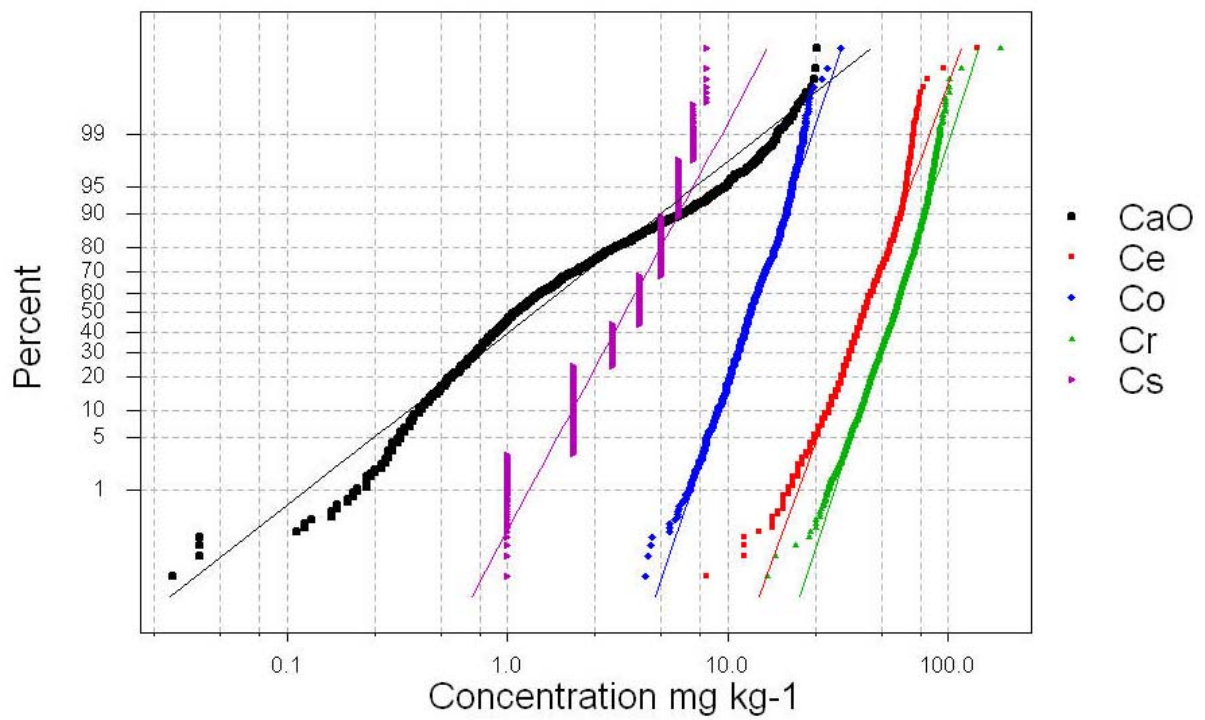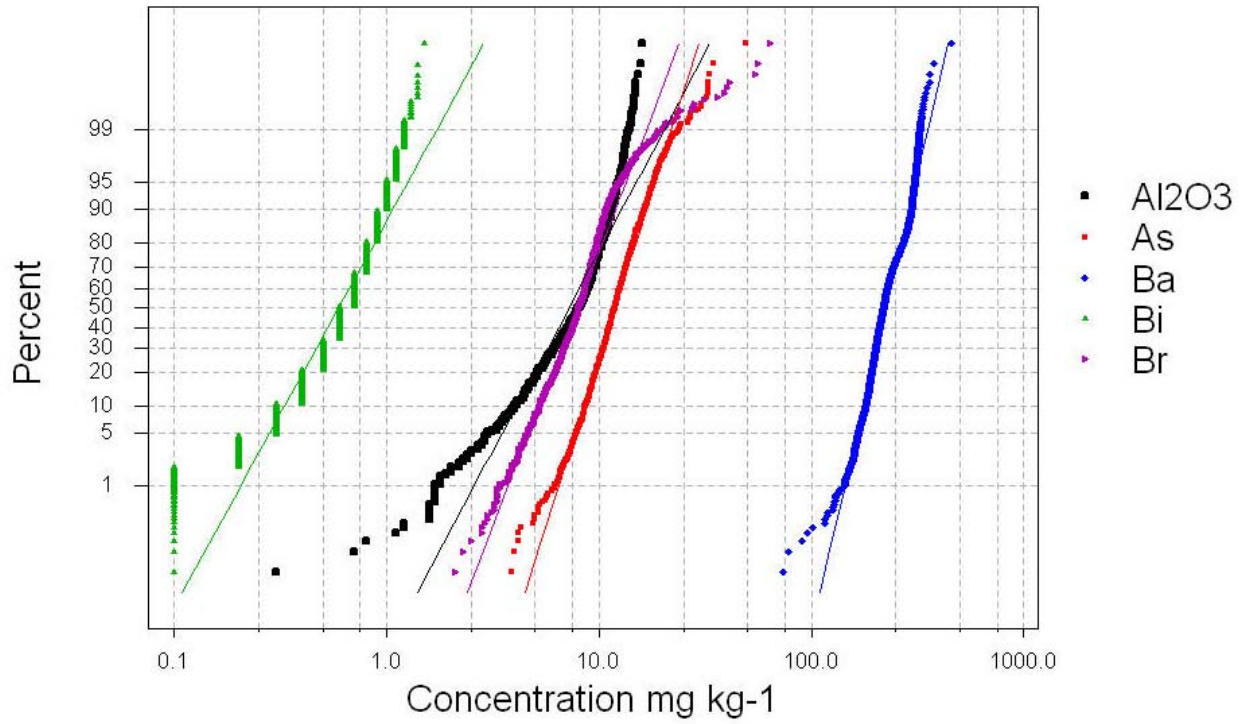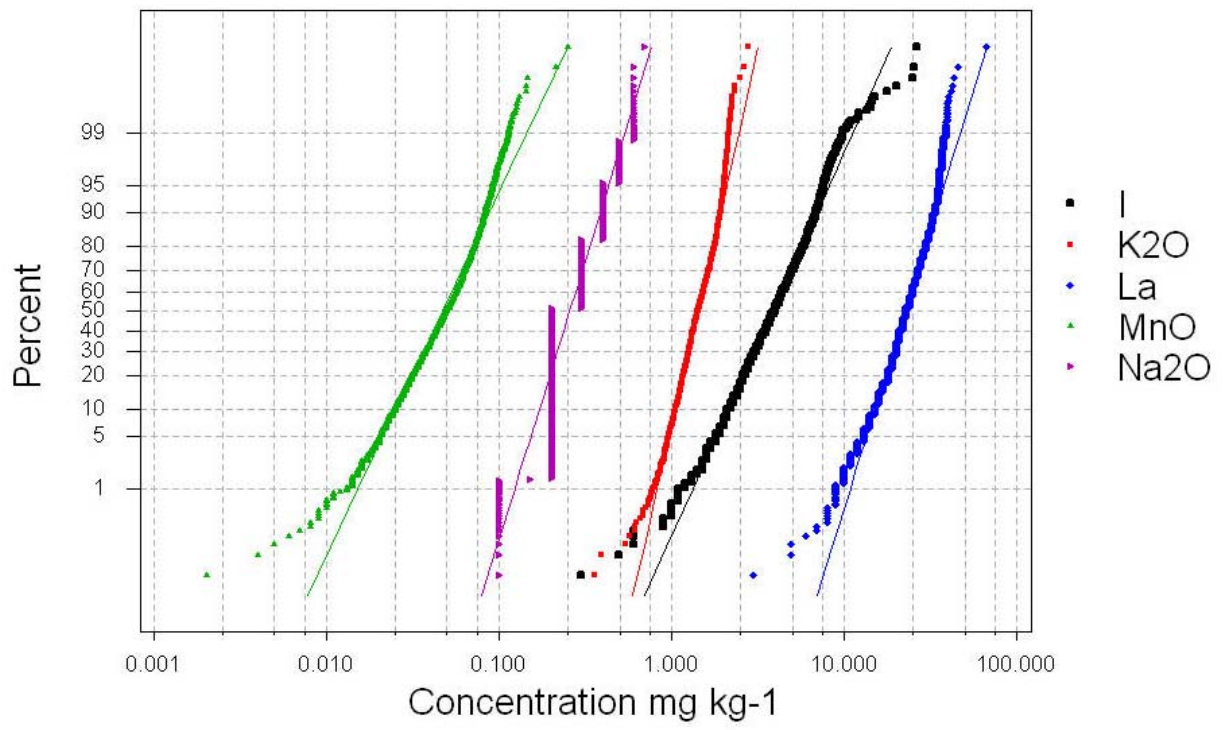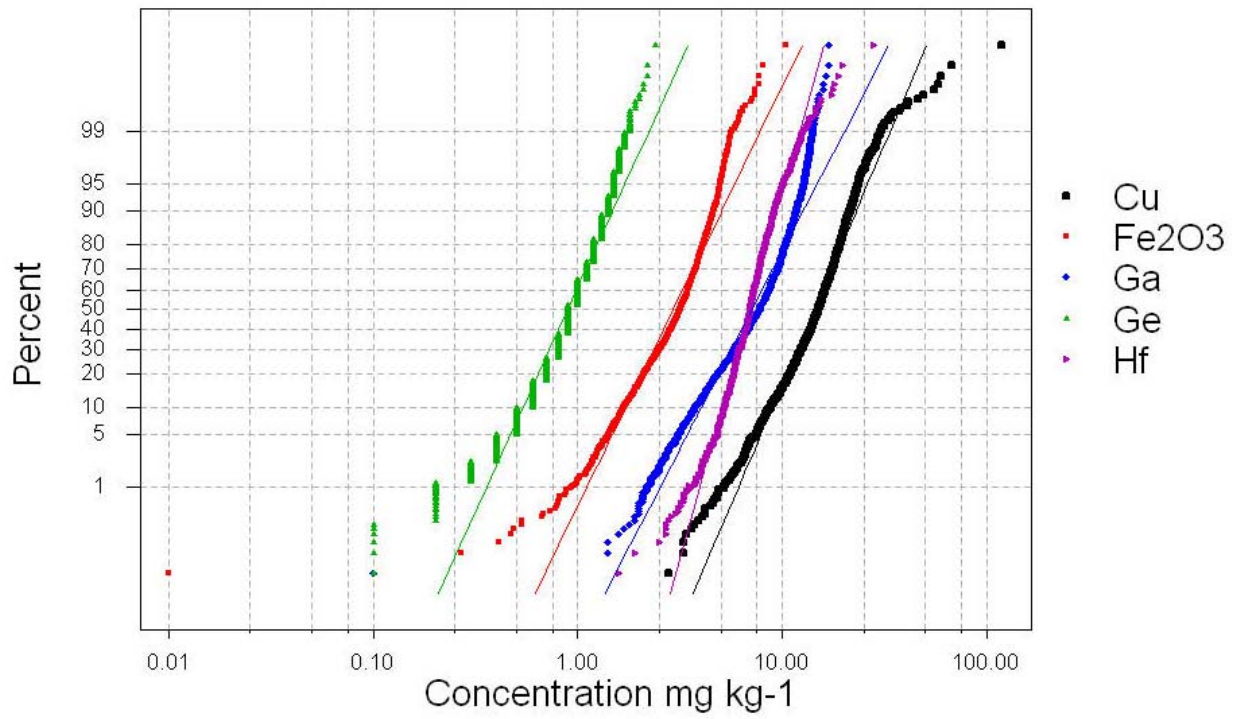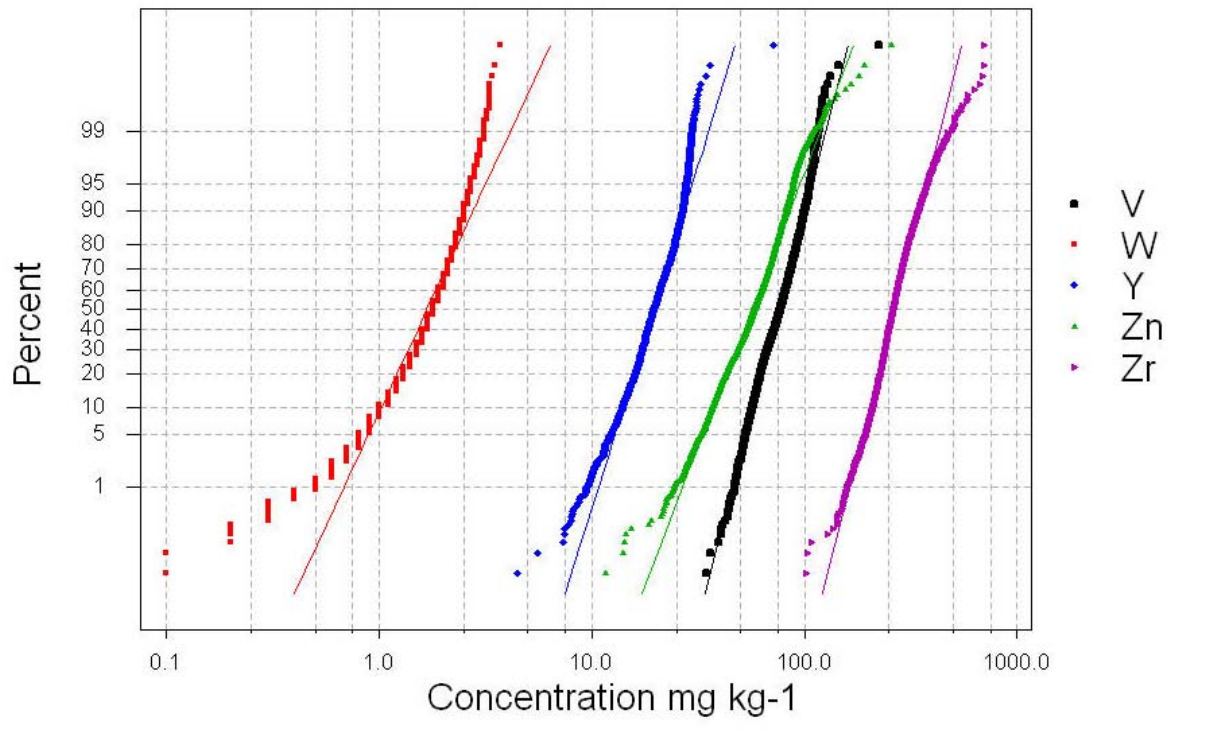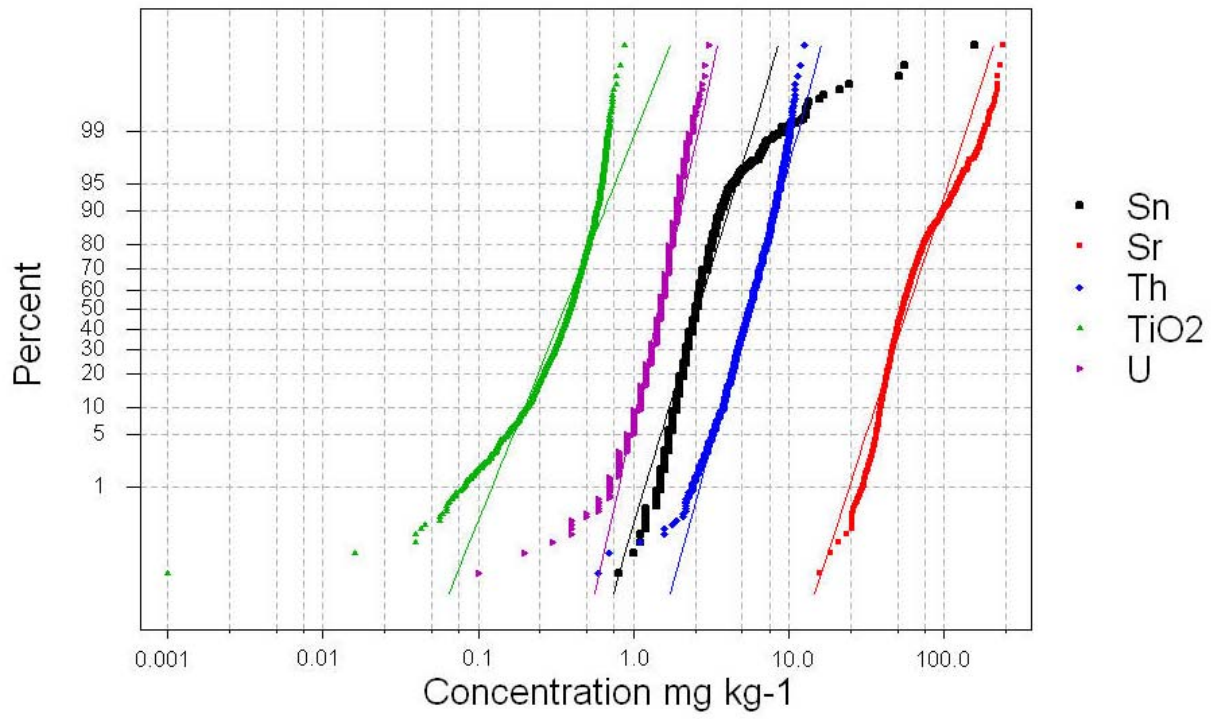
Appendix 2   Factor Score Coefficients

| Variable	Factor1	Factor2	Factor3	Factor4	Factor5	Factor6
Al_2O_3	0.083	-0.119	-0.016	-0.026	-0.004	-0.053
As	-0.005	0.149	0.02	0.022	0.027	0.035
Ba	0.027	-0.066	0.048	-0.012	-0.018	0.239
Bi	-0.076	0.005	0.005	0.013	-0.374	0.071
Br	-0.054	0.03	-0.042	-0.069	-0.36	0.05
CaO	-0.016	0.226	-0.098	-0.034	-0.024	-0.092
Ce	0.058	0.037	-0.021	0.037	0.059	0.023
Co	0.047	0.063	0.002	-0.013	0.128	0.041
Cr	0.062	-0.017	-0.042	0.013	-0.014	-0.025
Cs	0.092	-0.114	-0.022	-0.032	0.031	-0.177
Cu	-0.005	0.076	0.203	0.056	0.046	-0.112
Fe_2O_3	0.061	0.029	0.031	0.044	0.086	-0.099
Ga	0.076	-0.09	-0.014	-0.024	-0.004	-0.07
Ge	-0.059	-0.075	0.136	-0.02	-0.282	0.095
Hf	0.037	0.099	-0.028	0.439	-0.022	-0.085
I	-0.015	0.133	-0.076	0.02	-0.166	0.053
K_2O	0.06	-0.081	0.008	-0.04	0.029	0.097
La	0.054	0.053	-0.032	0.031	0.05	0.007
MnO	-0.015	0.235	0.007	0.011	0.199	0.197
Na_2O	-0.044	-0.083	0.041	-0.048	-0.107	0.526
Nb	0.078	-0.087	-0.007	0.013	0.02	0.014
Nd	0.041	0.08	-0.038	0.021	0.035	0.013
Ni	0.049	0.073	-0.01	-0.004	0.09	-0.059
P_2O_5	-0.073	0.363	0.071	0.173	0.021	-0.166
Pb	-0.098	-0.015	0.371	-0.078	-0.113	0.166
Rb	0.088	-0.109	0.011	-0.014	0.05	-0.098
Sb	-0.026	-0.064	0.338	-0.009	0.103	0.008
Sc	0.051	-0.001	-0.064	-0.024	-0.03	-0.054
Se	-0.01	-0.051	-0.014	0.05	-0.357	-0.13
SiO_2	0.045	-0.161	0.127	0.14	0.145	-0.09
Sn	-0.062	-0.03	0.34	-0.002	-0.067	0.034
Sr	-0.011	0.13	-0.065	-0.093	-0.039	0.066
Th	0.064	-0.02	-0.016	0.028	0.034	0.043
TiO_2	0.083	-0.127	0.008	0.017	0.015	0.032
U	0.033	-0.04	-0.15	0.129	-0.259	0.031
V	0.065	-0.019	-0.028	-0.025	0.019	-0.09
W	0.065	-0.07	0.043	0.102	0.034	0
Y	0.037	0.075	-0.018	0.062	0.027	0.073
Zn	0.015	0.083	0.121	0.063	0.015	-0.134
Zr	0.026	0.113	-0.051	0.431	-0.043	-0.058

Appendix 3　Values for Percentile Classes

Percentile	Al2O3	As	Ba	Bi	Br	CaO	Ce	Co	Cr	Cs	Cu	Fe2O3	Ga
	wt. %	mg kg-1	mg kg-1	mg kg-1	mg kg-1	wt. %	mg kg-1	mg kg-1	mg kg-1	mg kg-1	mg kg-1	wt. %	mg kg-1
5	3.0	7.8	168	0.3	4.6	0.33	25	8.2	35.7	2	7.5	1.42	3.1
10	4.0	8.7	182	0.3	5.3	0.40	29	9.1	40.2	2	8.8	1.68	3.8
15	4.7	9.3	189	0.4	5.8	0.49	31	9.9	42.9	2	10.0	1.92	4.4
25	5.7	10.1	200	0.5	6.6	0.65	35	10.8	47.3	3	11.8	2.30	5.4
50	8.1	11.9	221	0.6	8.1	1.09	42	12.8	57.6	4	15.1	3.18	7.8
75	9.9	13.9	258	0.8	9.4	2.47	52	15.7	67.9	5	18.3	3.92	9.9
90	11.5	16.4	299	0.9	10.8	6.15	61	18.7	78.2	6	21.5	4.62	11.8
95	12.3	18.2	310	1.0	12.6	9.76	65	19.8	83.4	6	23.7	4.99	12.8
99	13.8	23.7	328	1.2	19.1	16.88	70	22.3	92.1	7	30.4	5.66	14.1

	Ge	Hf	I	K2O	La	MnO	Na2O	Nb	Nd	Ni	P2O5	Pb	Rb
	mg kg-1	mg kg-1	mg kg-1	wt. %	mg kg-1	wt. %	wt. %	mg kg-1	mg kg-1	mg kg-1	wt. %	mg kg-1	mg kg-1
5	0.4	4.8	1.8	0.96	13	0.020	0.2	5.0	8.5	8.7	0.13	17.2	29.2
10	0.6	5.2	2.1	1.06	15	0.025	0.2	5.8	10.6	10.7	0.15	19.2	35.3
15	0.6	5.5	2.4	1.13	17	0.028	0.2	6.4	12.1	12.5	0.16	20.6	39.4
25	0.7	6.0	2.9	1.22	19	0.035	0.2	7.2	14.4	14.7	0.17	22.7	47.3
50	0.9	7.0	3.9	1.42	23	0.049	0.2	9.0	18.3	20.2	0.20	26.3	64.6
75	1.2	7.9	5.3	1.70	28	0.067	0.3	11.0	23.4	27.0	0.23	30.7	79.8
90	1.4	9.2	6.8	1.92	33	0.082	0.4	13.1	28.0	34.1	0.28	36.1	91.2
95	1.5	10.1	7.6	2.01	36	0.091	0.4	14.1	29.9	36.9	0.32	42.5	97.4
99	1.7	12.6	9.9	2.14	39	0.113	0.6	15.6	33.1	41.8	0.40	80.8	110.2

	Sb	Sc	Se	SiO2	Sn	Sr	Th	TiO2	U	V	W	Y	Zn	Zr
	mg kg-1	mg kg-1	mg kg-1	wt. %	mg kg-1	mg kg-1	mg kg-1	wt. %	mg kg-1	mg kg-1	mg kg-1	mg kg-1	mg kg-1	mg kg-1
5	0.6	2.6	0.1	48.5	1.7	36.8	3.3	0.152	0.9	53.2	0.8	12.4	32.7	194.7
10	0.7	3.3	0.2	53.4	1.9	39.4	3.8	0.208	1.1	57.1	1.0	14.1	37.1	210.6
15	0.8	3.9	0.2	56.5	2.0	41.5	4.1	0.238	1.1	60.1	1.2	15.2	40.2	220.7
25	0.8	4.8	0.2	60.9	2.2	45.3	4.6	0.286	1.3	64.9	1.4	16.9	45.9	234.9
50	0.9	6.7	0.3	67.9	2.5	54.2	5.6	0.388	1.5	77.2	1.8	19.7	58.5	262.8
75	1.1	8.6	0.4	74.0	3.1	69.0	6.8	0.484	1.7	89.2	2.2	23.7	71.0	298.1
90	1.2	10.5	0.5	81.1	3.6	98.4	8.2	0.573	1.9	100.2	2.5	27.0	81.8	344.7
95	1.3	11.5	0.6	83.9	4.3	123.2	8.9	0.623	2.0	107.1	2.7	28.1	88.6	379.2
99	1.5	13.0	0.8	90.0	8.9	180.2	10.3	0.687	2.4	116.6	3.1	29.8	109.5	474.7

Appendix 4 Distribution of Analytical Batches in East Anglia
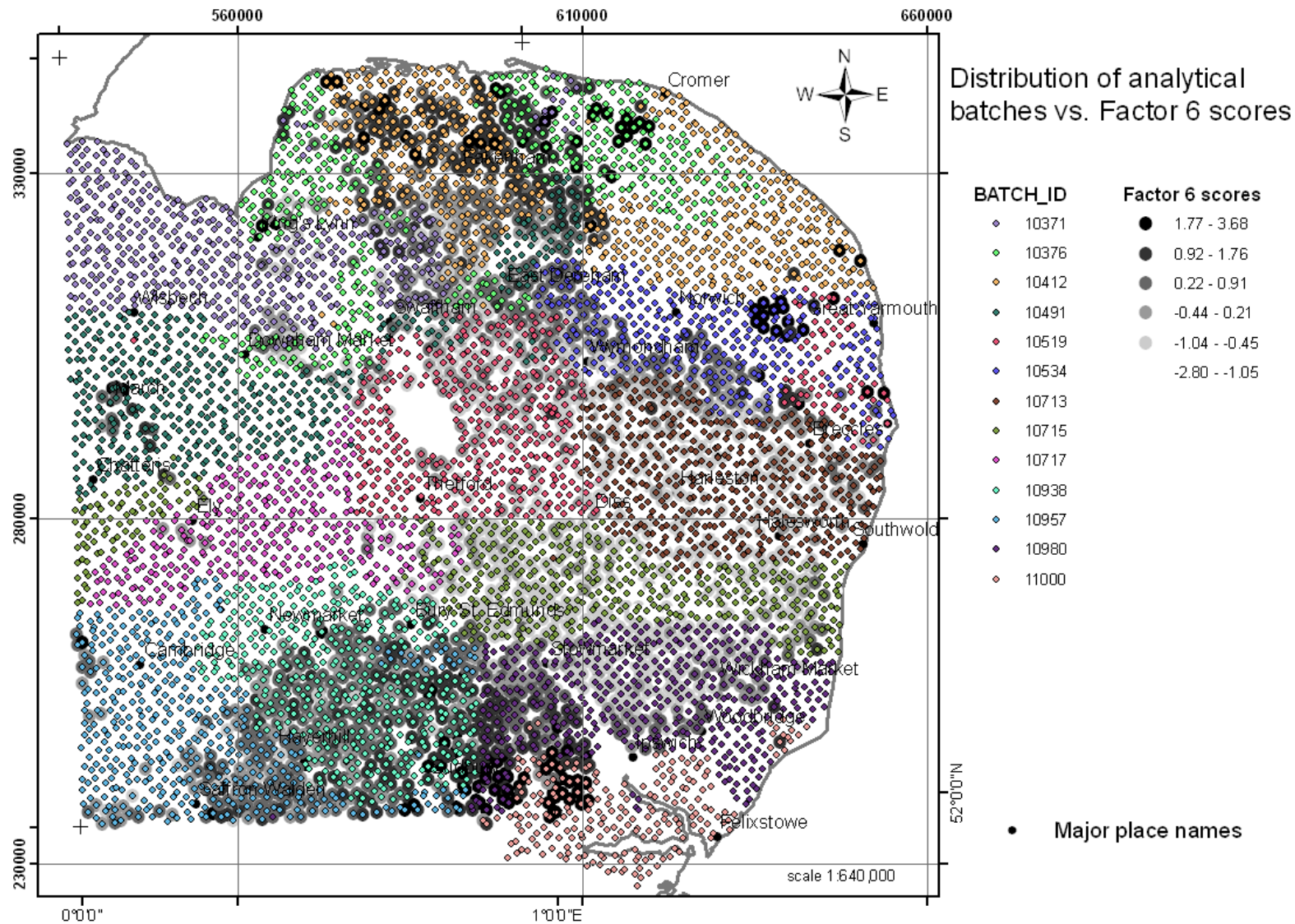
Appendix 5 Geochemistry of Na₂O in Soils of East Anglia
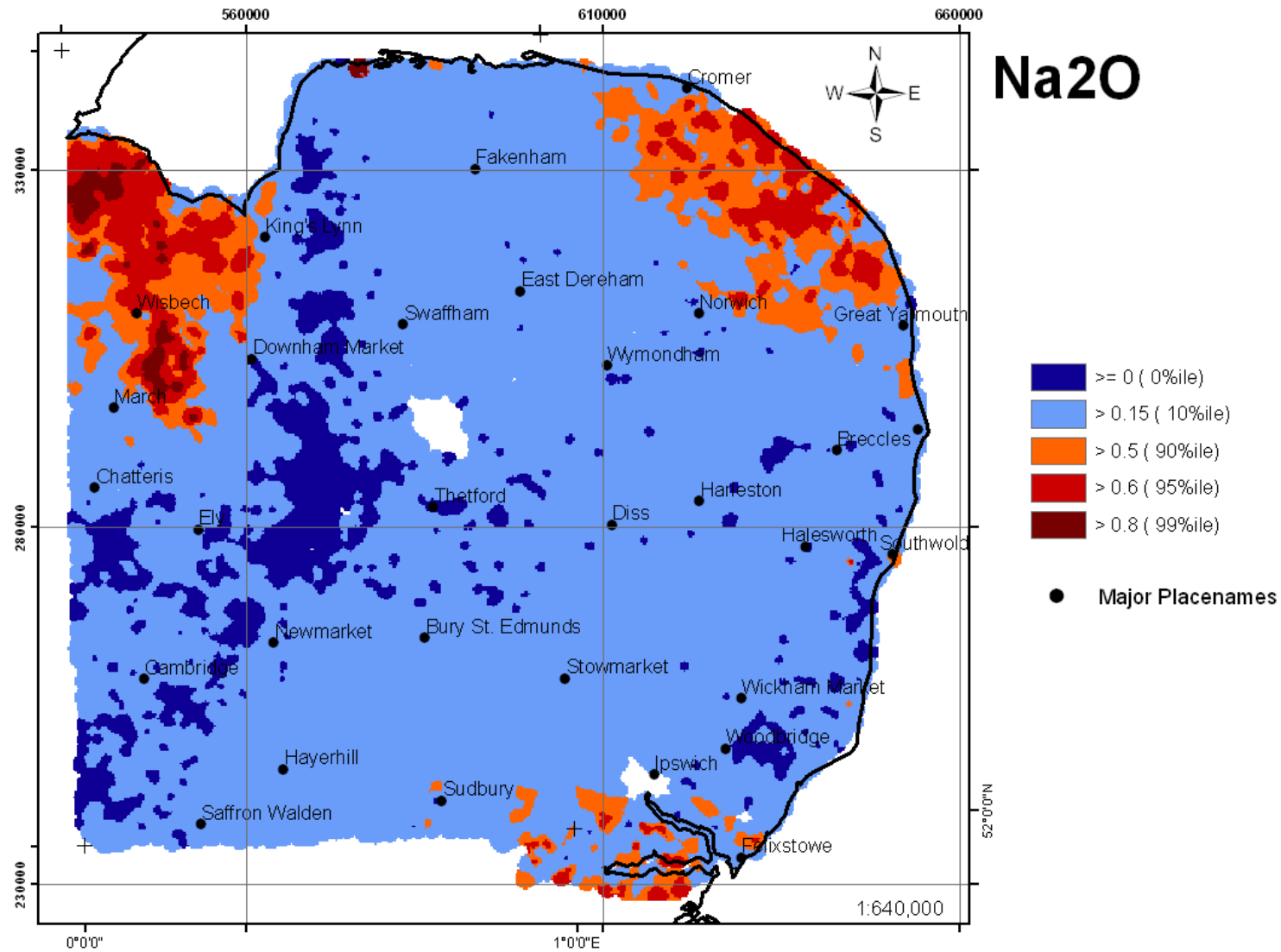
Appendix 6   Terrain Elevation of East Anglia