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## **Abstract**

Soil has been utilised in criminal investigations for some time because of its prevalence and transferability. It is usually the physical characteristics that are studied, however the research carried out here aims to make use of the chemical profile of soil samples.

It is thought that the land type a soil sample comes from can lead to a particular chemical profile being present, which may make it possible to identify which land type a sample of evidential soil may have come from such as woodland or river sites. This would limit the possibilities significantly and so narrow down the scope for comparison. It could also be used to limit the areas required to be searched in certain cases. The ideal scenario would be that there was a general profile found for each land type and a characteristic profile for each land type location that could be used to identify each specific type of soil and its location specifically.

The research we are presenting in this work used sieved (2mm) soil samples taken from the top soil layer (about 10cm) that were then analysed using Fourier Transform Infrared (FTIR) spectroscopy. The spectra obtained were used as raw data in Principal Component Analysis (PCA). Results showed that it was possible to discriminate between soil samples with different soil type and different origins and, with some degree of error, between samples with similar soil type and different origins.

Soil Analysis, Forensic Science, Principal Component Analysis.

## **INTRODUCTION**

Until fairly recently, most of the analysis of soil for comparison has been done using visual comparisons of the colour and texture, looking at the basic mineral content of the samples [1,2]. Over the past few years however, more and more studies have been carried out in attempting to utilize chemical profiles of soil using a wide variety of novel and quick analytical methods, such as FTIR [3].

The value of soil as evidence rests with its prevalence at crime scenes and its transferability between the scene and the criminal [1], and this is the main basis for all of the work that is carried out on soil within forensic applications. This can be of value for comparison if the scene of crime is known, but could also be so in the identification of a scene with the help of a geologist or maps showing the distribution of soil and rock types in the area [4].

The main basis for the comparison of sites to determine provenance is that soils vary from one place to another. This is also one of the major problems in the use of soil comparisons in legal cases, as this variation can occur both within a particular site and between sites, and the extent of this is as yet unknown. Projects such as the Soil Forensics University Network (SoilFUN) aim to set up a database of information on urban soil from across the UK to establish a base for comparison based on different chemical

and physical measurements [5]. A common problem identified for soil analysis is the lack of staff with the expertise and training to carry out reliable soil analysis. This problem indicates a need to find simpler methods that do not require quite such specialised experience. This is the aim of the present project developed at Lincoln University based on FTIR and multivariate analysis.

## METHODS AND MATERIALS

Soil samples were taken from a flowerbed site and a woodland site in the Lincoln, UK area. Map locations were accurately recorded for each location. At each site a transect was set-up using a tape measure and samples were taken to a depth of 10 cm along the transect at 50 cm intervals. Five samples were taken from each site and labelled a-e. The samples were air dried followed by removal of stones and vegetation, sieving (2 mm), grinding and finally sieving again (125  $\mu\text{m}$ ). Samples were measured directly on a Golden Gate Attenuated Total-internal Reflection (ATR) accessory (Specac) housed in a Perkin-Elmer Spectrum 100 Fourier Transform Infrared Spectrometer (FTIR). After recording the spectrum the soil was removed from the ATR and the lens was cleaned with a tissue (Kimwipe) and methanol. Instrument settings used were 128 scans; 4  $\text{cm}^{-1}$  resolution; range 4000-400  $\text{cm}^{-1}$ . Regular background spectra were performed and the cleanliness of the lens was checked between samples using the live spectra feature of the instrument. Spectra in ASCII format were exported into Excel for pre-processing before exporting into Tanagra © for multivariate analysis.

## RESULTS AND DISCUSSION

Fig. 1 shows the spectra obtained for different sampling locations at the same flowerbed site. The spectra are normalised by row scaling to constant total [6]. Of the many pre-processing techniques available this simple normalisation was chosen as the raw spectra showed little variation in baseline regions suggesting that variation seen in replicate spectra was mainly due to variation in the amount of material sampled on the ATR diamond lens. The most interesting region of the spectrum is the fingerprint region and so multivariate analysis of the data was carried out on the spectral region 1800-400  $\text{cm}^{-1}$ . This also resulted in a smaller set of data which significantly speeded up processing time.



Fig.1. Normalised spectra for samples taken at different sampling locations at the same flowerbed site.

PCA of the flowerbed site spectra show separation of locations a-e in the PC1/2 score plot (Fig.2). Site a and b are strongly correlated with positive values of PC1 whereas site d is correlated with negative values of PC1 and is negatively correlated with sites a and b. Sites a and c show positive correlation with positive values of PC2 and sites b and e are correlated with negative values of PC2. The PC loadings plot (Fig.3) shows that positive PC1 values are associated with the spectral regions 400-550, 900-1050  $\text{cm}^{-1}$  and negative values are associated with the region 1150-1550  $\text{cm}^{-1}$  which includes the peak at around 1430  $\text{cm}^{-1}$ . PC2 has positive values associated with the regions 550-675, 800-850  $\text{cm}^{-1}$  and 1600-1750  $\text{cm}^{-1}$  and negative values with the 1050-1150  $\text{cm}^{-1}$  region. These regions show spectroscopic changes that seem to be associated with the different sampling locations from the various sites. This suggests that it may be possible to differentiate between soils from the same site but from different locations.

[pic]

Fig.2. PC1(57 %)/PC2(29%) score plot for 1800-400  $\text{cm}^{-1}$  normalised spectra for replicate samples taken from locations a-e at the same flowerbed site.



Fig.3. PC1/2 loadings plot with spectra from flowerbed sampling locations a-e.

To investigate variation between different types of site, the data from the flowerbed site were combined with a similar data set from a woodland site. The data from the woodland set also demonstrated that a PC model could be used to discriminate between sampling locations at the same site showing separation of replicates from sampling locations a-e in the PC1/2 score plot. PCA of the combined data give separation of the two sites on the PC1/2 score plot (figure 4). The individual examples used are average sampling location spectra and it shows that the flowerbed locations show a good grouping. Woodland locations are much more widely spread. This seems largely due to site b which is closest to the flowerbed examples on PC1 and is also individually discriminated from the other examples (flowerbed and woodland) along PC2. The loadings plot for PC2 reveals negative values of PC2 are associated with regions 700-800 and 1050-1200  $\text{cm}^{-1}$ . W1b has a much higher absorbance in the spectral features shown in these regions. This needs to be investigated as a potential outlier.

[pic]

Fig.4. PC1(62%)/PC2(25%) score plot for combined flowerbed and woodland site data using average location spectra.

## CONCLUSION

It has been shown that a simple procedure using ATR-FTIR appears to be sufficiently sensitive to detect spectral differences between samples taken from a site that seem to relate to the sampling location within the site. This has been shown for two different locations. Analysis of the spectra from different sites shows that better separation is achieved between sites although the examples used here show that care needs to be taken with possible outliers. This is only a small data set but shows that it may be possible to discriminate between soil types for forensic investigations. Further work will concentrate on increasing the number of sample sites and locations to create a representative model for the soil types found in the Lincoln region. A classification model will be created with this data.

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