FTIR WITH MULTIVARIATE ANALYSIS

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INTRODUCTION

Over the past few years more and more studies have been carried out in an attempt to utilize chemical profiles of soil using a wide variety of analytical methods. The value of soil as evidence rests with its prevalence at crime scenes and its transferability between the scene and the criminal. 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. The main basis for the comparison of sites to determine provenance is that soils vary from one place to another. The aim of this work is to find simple methods to identify soil provenance based on FTIR and multivariate analysis

MATERIALS AND METHODS

Soil samples were taken from a flowerbed site and a woodland site in Lincoln (UK). At each site samples were taken to a depth of 10 cm using a soil corer along the transect at 50 cm intervals (Fig.1) . Five samples were taken from each site. The samples were air dried followed by sieving (2 mm), grinding and sieved again (125 µm). 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).

Fig.1. Sampling at the woodland site

RESULTS

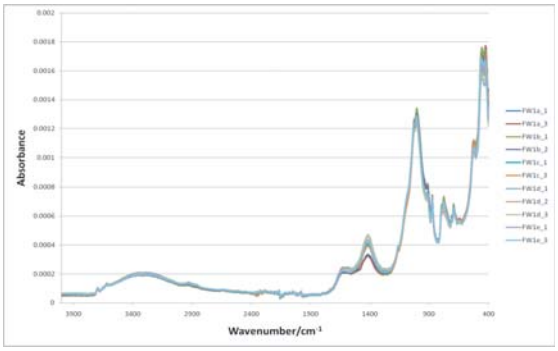

Fig.2. Normalised spectra for samples taken at different locations at the same flowerbed site.

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 cm-1. PCA of the flowerbed site spectra show good separation of locations a-e in the PC1/2 score plot (figure 3). 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

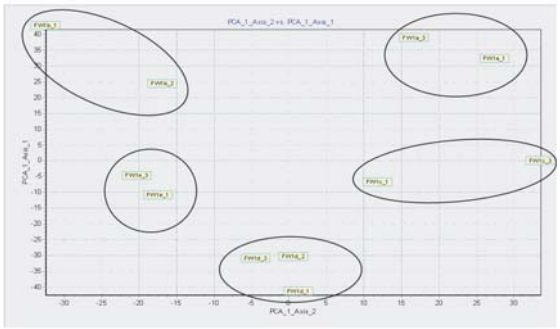

Fig.3. PC1(57 %)/PC2(29%) score plot for different locations at the same flowerbed site

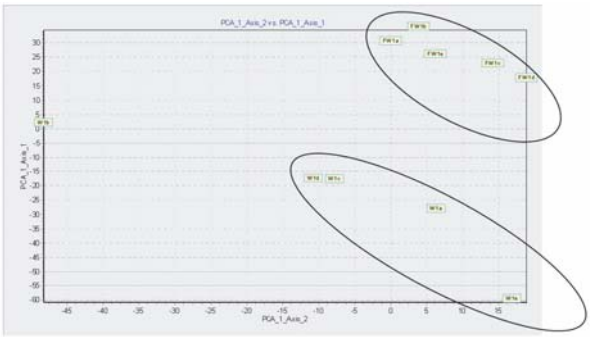

Fig.4. PC1(62%)/PC2(25%) score plot for combined flowerbed and woodland site data (averages)

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

CONCLUSIONS

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. 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.