



Detection of hydrocarbons in clay soils: A laboratory experiment using spectroscopy in the mid- and thermal infrared

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ABSTRACT

Remote sensing has been used for direct and indirect detection of hydrocarbons. Most studies so far focused on indirect detection in vegetated areas. We investigated in this research the possibility of detecting hydrocarbons in bare soil through spectral analysis of laboratory samples in the short wave and thermal infrared regions. Soil/oil mixtures were spectrally measured in the laboratory. Analysis of spectra showed development of hydrocarbon absorption features as soils became progressively more contaminated. The future application of these results airborne seems to be a challenge as present and future sensors only cover the diagnostic regions to a limited extent.

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1. Introduction

Remote sensing in the near- and shortwave infrared can be used for direct and indirect detection of hydrocarbons. Previous research largely focused on direct spectral detection of hydrocarbons (e.g. Lammoglia and Filho, 2011; Bihong et al., 2007; van der Werff et al., 2006; Winkelmann, 2005; Kühn et al., 2004; Hörig et al., 2001; Malley et al., 1999). The presence of hydrocarbons in a soil can also lead to chemical and mineralogical alterations. Bacterial oxidation of hydrocarbons can establish anomalous redox zones that favour the development of a diverse array of chemical changes (Schumacher and Abrams, 1996). An overview of hydrocarbon-induced alterations, and consequences for remote sensing is given by van der Meer et al. (2002), Schumacher and Abrams (1996), and Cloutis (1989).

The aforementioned studies focused on natural hydrocarbon seepage and/or controlled experiments. Recent work, related to pipeline leakage, in the laboratory (Noomen et al., 2006; Smith et al., 2004), field (van der Meijde et al., 2009) and airborne (van der Werff et al., 2008), showed that indirect detection of hydrocarbons through analysis of vegetation reflectance is possible. These studies, however, focused only on areas with relatively dense vegetation cover, leaving areas with little or no vegetation unaccounted for.

In this research, we investigate the possibility of detecting hydrocarbons in bare soil through spectral analysis of the short wave and thermal infrared wavelength regions. Based on the discriminative wavelengths found and available thermal infrared sensors, a feasibility study shows that the direct applicability of such techniques for airborne based detection and monitoring is currently limited.

2. Methods

2.1. Laboratory experiment

The laboratory experiment consisted of two stages. At first, 10.00 g soil samples was created from a mixture of air-dried clay soil and a hydrocarbon (Shell mineral engine oil). The hydrocarbons were added to the soil in increments of 10% weight, from 10% till 100% hydrocarbon content. In the second stage, the air-dried clay soil was moistened (8.50 g soil to 1.50 g water) and well mixed to make it comparable to field conditions. The sample was prepared with hydrocarbon concentrations that ranged between 0 and 10% of the moistened soil weight, in increments of 1%. Directly following sample preparation spectral samples were measured thereby minimising the possibility of evaporation.

2.2. Instrument and spectral measurement set-up

Thermal and shortwave infra-red spectra were recorded with a Bruker Vertex 70 Fourier Transform Infrared (FTIR) spectrometer (Hecker et al., 2011). Diffuse Reflectance Infrared Fourier Transform (DRIFT) spectral measurements were recorded in the wavenumber

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range of 5000–500 cm^{-1} . For laboratory samples a spectral resolution of 2 cm^{-1} and 64 scans per sample was used. For field samples the number of scans was increased to 500 to enhance the signal-to-noise ratio. The sample was stirred in its cannister and a random sub-sample was drawn to fill the sample holder. The sub-sample was levelled to ensure a flat measurement surface and placed in the DRIFT compartment (following a background reference measure) to take a sample measurement. The sub-sample was then rotated 180° and measured again, thereby capturing brightness differences resulting from scattering due to soil structure. Thus, for each sub-sample two spectra were measured. A total of five sub-samples (10 spectra in total) were measured per sample.

2.3. Statistical analysis

Spectral data shows strong co-linearity between wavelengths, therefore analysis should consider how to account for this. The large sample size of the laboratory data set allowed for the application of a partial least squares regression (PLSR, Wold et al., 2001) to initially reduce the dimensionality of the data by identifying significantly contributing wavelengths and to reduce the impact of co-linearity on the modelling.

The FTIR dataset was split randomly into 75% for training and 25% for model validation. Applying PLSR (see Hecker et al. (2012) for an application of PLSR to thermal infrared spectra), latent variables were selected which reduced the prediction residual error sum of squares values observed in the training data. The summed absolute loadings of the selected latent variables were then used to identify which wavelengths contributed most to the derived model. Once the number of latent variables had been selected, the (absolute) loading values of these variables were summed, to determine which wavenumbers were contributing most. A major limitation is that the results of PLSR analysis are dependent on the hydrocarbon type it was trained for and the uncertainty estimates are only valid for a dataset that is compositionally comparable (in average as well as extreme values) to the training dataset.

To account for this limitation of the PLSR and in an attempt to create a model that can generalise to new data, we selected the 10 highest loading peaks identified in the PLSR modelling and applied a stepwise multiple linear regression (SMLR, Crawley, 2006; Grossman et al., 1996) to these wavelengths. Since the data has been strongly reduced and co-linearity already addressed in the PLSR modelling this can now deliver a model that is more

independent from the hydrocarbon type used. Prior to performing a forward/backward SMLR procedure it was verified that the data followed a non-normal distribution and these were therefore arc-sine transformed (Crawley, 2006). The SMLR models were then validated using the independent validation set.

3. Results

3.1. Trends in spectra

Analysis of both dry soil to oil mixtures (0–100% hydrocarbon contamination) as well as the moist soil to oil mixtures (0–10% hydrocarbon contamination) shows that there was development of hydrocarbon features and reduction in the soil features as soils became progressively more contaminated (see Fig. 1 for an example of the moist mixture). The most dominant and specific hydrocarbon features (Stuart, 2004) between 2850 and 2960 cm^{-1} were already visible from a hydrocarbon concentration of approximately 1%. Furthermore, an absorption feature is present in the C–H fingerprint region of 1000–1275 cm^{-1} which is becoming increasingly visible with increasing hydrocarbon content. Other spectral features are related to water content and/or soil composition and are getting smaller with increasing hydrocarbon content.

3.2. Modelling

The presence of water in soils can potentially reduce spectral detection capabilities. The results indicate, however, that hydrocarbons can be detected under moist conditions and for low concentrations. The modelling is therefore only done on the moist samples, since that provides a model that is close to reality. This results in a selection of 3 latent variables. The summed loading provides an overview of wavenumbers that contribute to the highest loadings in the PLSR model. The wavenumbers with highest loading are indicated in Fig. 1 and further used in the SMLR analysis.

The wavenumbers selected from the loading plot to be used as input into the SMLR modelling for moist soil/oil samples were: 1045, 1416, 1465, 1613, 1800, 1876, 2515, 2850, 2920, and 3158 cm^{-1} . Except for 3158 cm^{-1} , all wavenumbers can be associated with hydrocarbons. Wavenumber 3158 cm^{-1} is associated with a gaseous vibrational water molecule (Winkelmann, 2005) and therefore related to the moistened soil in this experiment. From this list, 1045, 1416, 1465, 1876, 2515, 2850, 2920 cm^{-1} were the

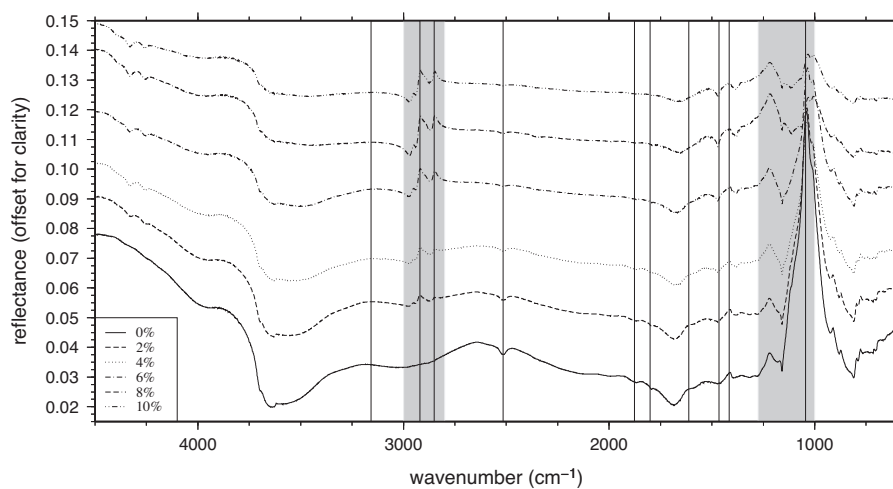


Fig. 1. Average spectrum for HC (oil) contaminated soil ranging between 0 and 10% contamination levels. For visualisation purposes only the even percentages pollution levels are shown and offset in steps of 0.02 with respect to the lowest concentration spectrum. The wavenumbers highlighted (vertical lines) are those selected in the PLSR analysis for inclusion in the SMLR modelling. Typical regions for C–H spectral features are indicated in grey (after Stuart (2004)).

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