

# In-situ determination of total petroleum hydrocarbon (TPH) contamination: A quick infrared spectroscopic test for TPH at contaminated sites

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## Background

Currently most soil analyses for TPH use extractive techniques combined with instrumentation; gas chromatograph (GC-MS, GC-FID), UV fluorescence, attenuated total reflectance (ATR) infrared. A more simple and rapid alternative technique for screening contaminated sites for TPH would be desirable.

## Objective

To develop a rapid *in situ* screening technique for TPH.

## Experimental

Spectra were obtained with a hand-held field portable FTIR instrument *in situ* at TPH contaminated sites (Figure 1). The soils were collected and sub-sampled for laboratory analysis by GC for TPH and scanning with a bench top FTIR, using diffuse reflectance (DRIFT). Partial least-squares (PLS) cross-validation was used for modelling TPH concentration in the samples, and the development of predictive models for in-field use.

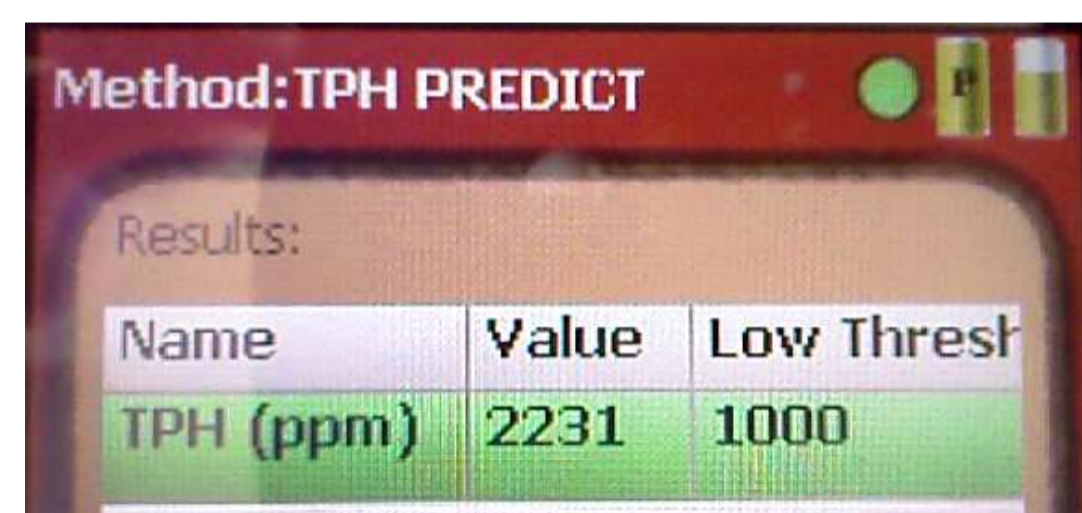


Figure 1: Field use of the hand-held MIR spectrometer, and an output display on the instrument.

## Results and Discussion

### Mid-infrared DRIFT spectra (Figure 2)

DRIFT spectra of soils from a lab bench-top (1 min. scan) and field-portable instrument (20 sec. scan) were very similar. Hydrocarbon peaks characteristic of alkyl-CH<sub>3</sub> and -CH<sub>2</sub> stretching vibrations are seen in the 3000-2700 cm<sup>-1</sup> range.

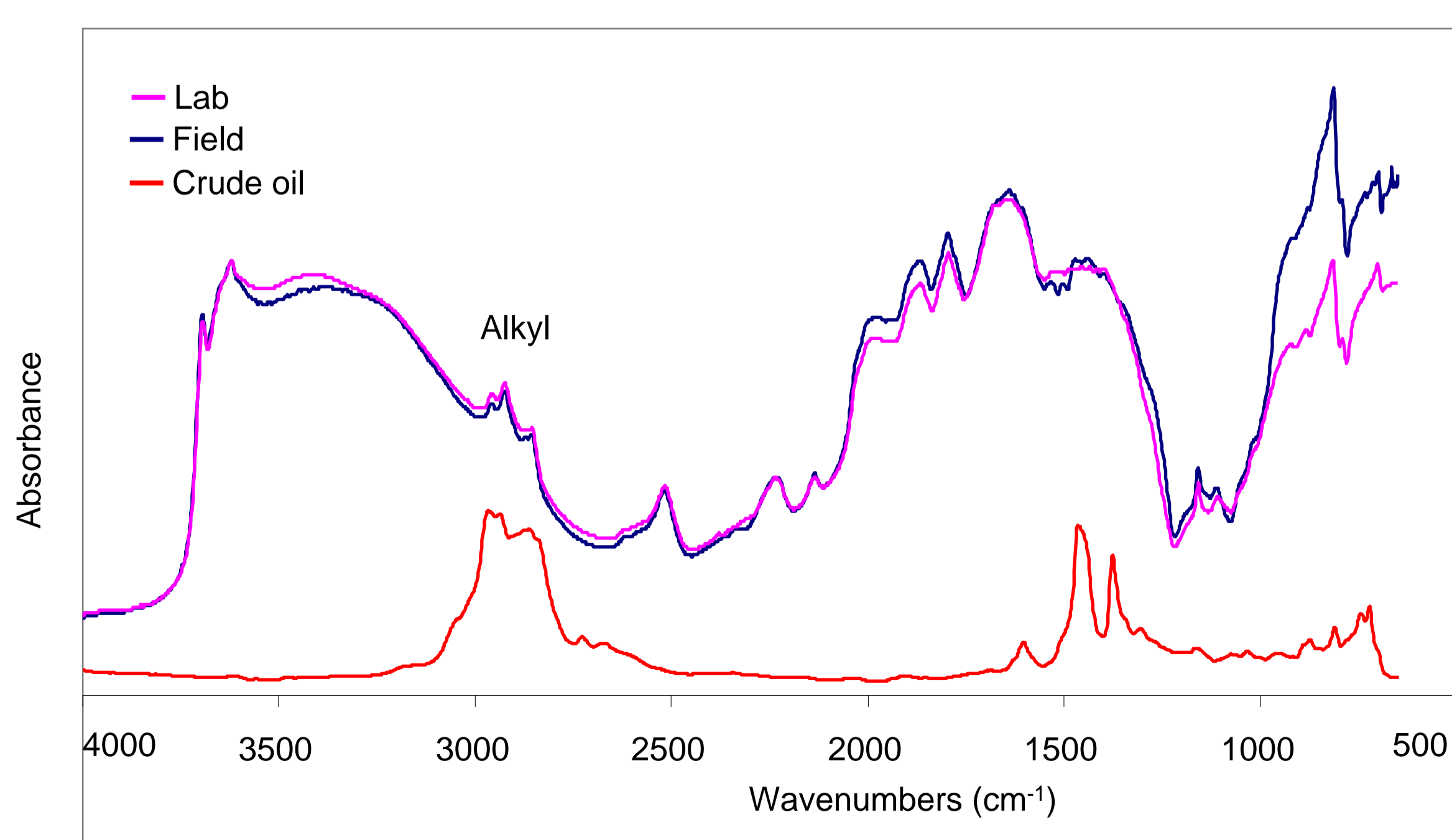


Figure 2: DRIFT mid-infrared spectra of a soil, scanned with a laboratory bench-top and the hand-held field-portable instrument, are shown together with a spectrum of crude oil. The oil shows peaks characteristic of TPH.

## PLS regression analysis

PLS cross-validation for TPH predictions for field soils at contaminated sites are depicted in Figure 3. Total TPH concentrations ranged from 0 - 11000 mg/kg giving an RMSECV=759 mg/kg (Lab) and 903 mg/kg (Portable).

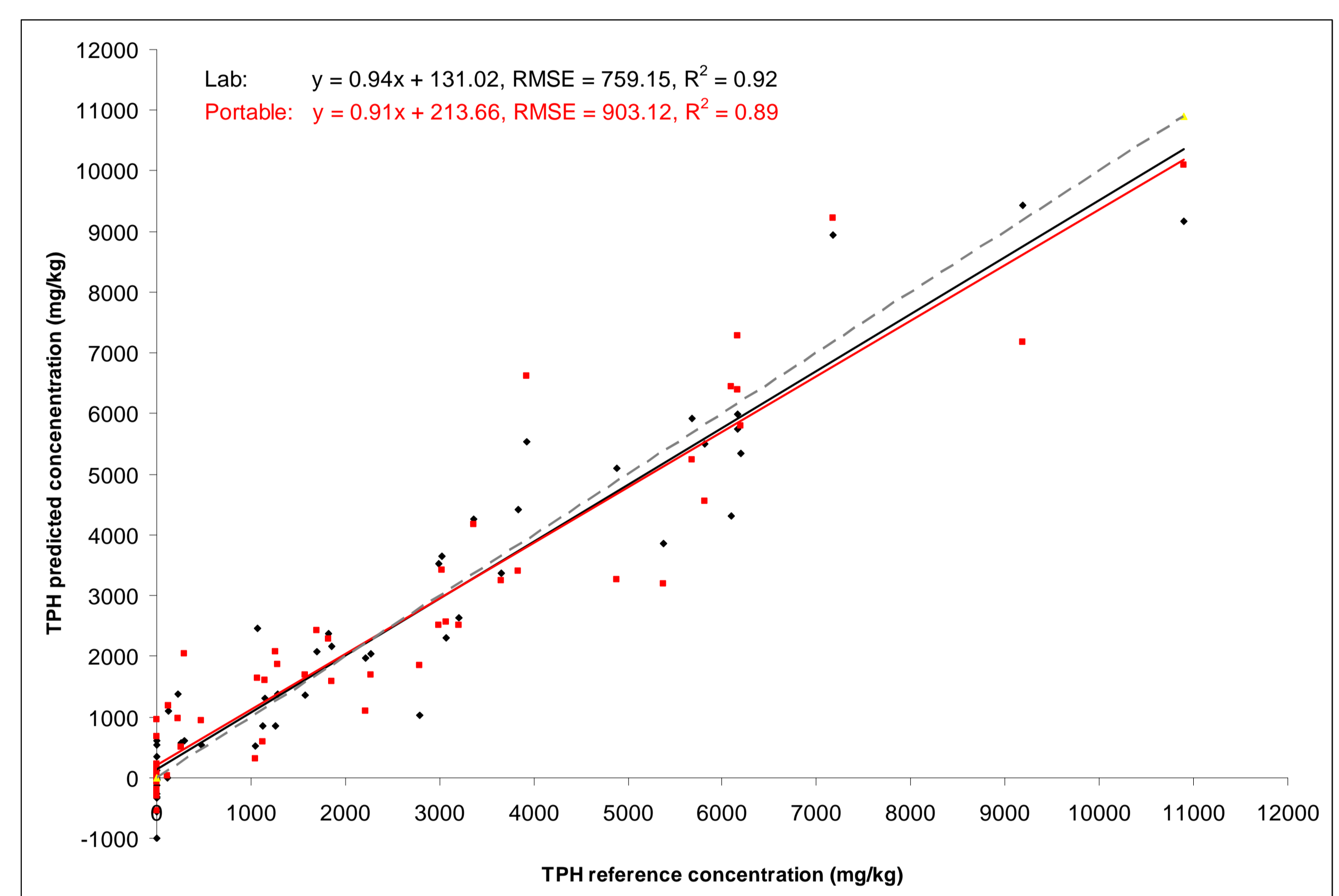


Figure 3: FT-MIR PLS cross-validation for total TPH in soil samples.

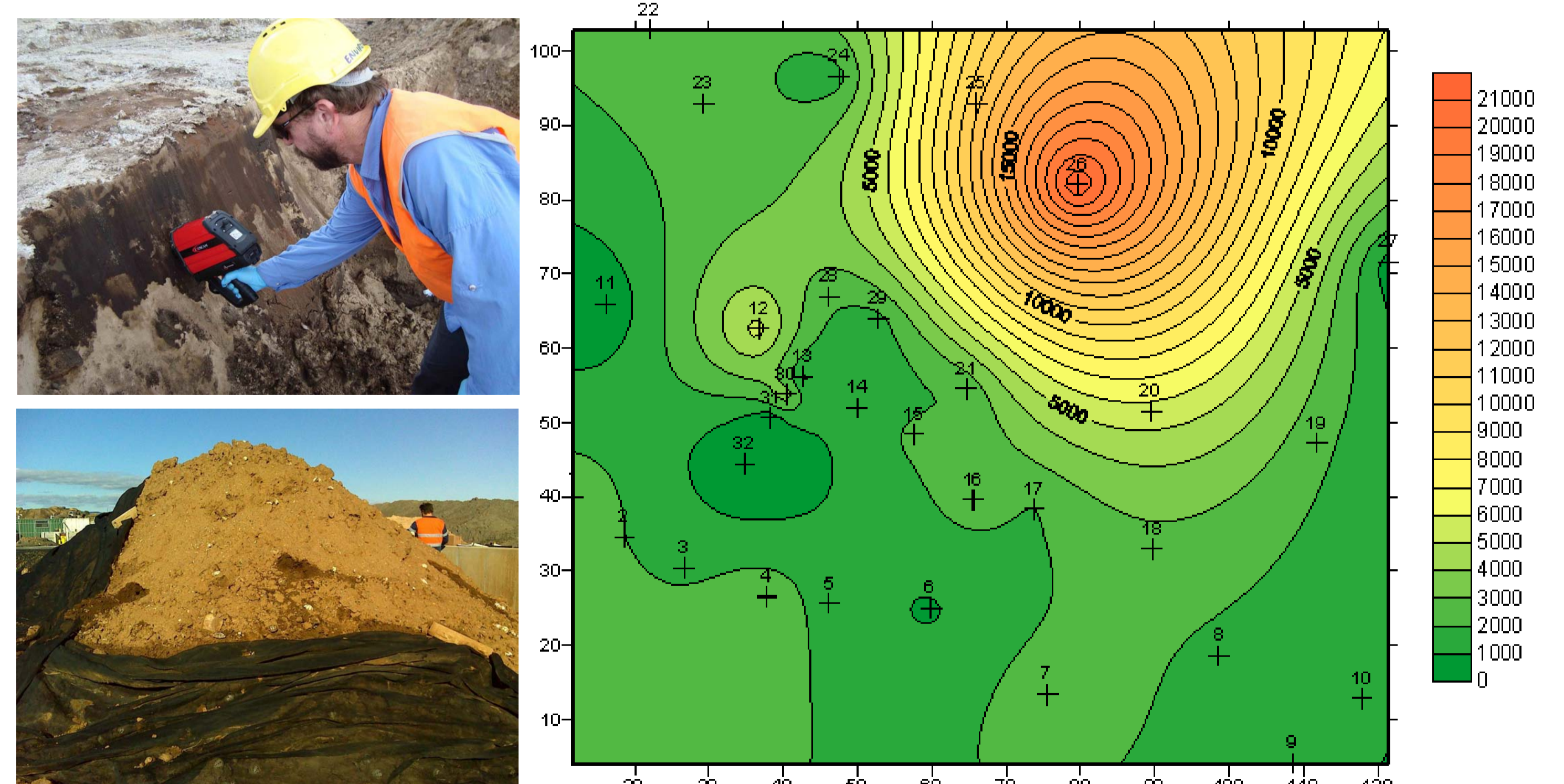


Figure 4: Clockwise from top: Field use of the hand-held MIR spectrometer, site survey map of predicted TPH ppm at a contaminated site, contaminated soil at a soil remediation processing plant.

## Conclusion

DRIFT with PLS regression analysis satisfies the accuracy requirements for rapid screening, provided that the model uses the most effective spectral signatures. The predicted TPH values for in-field screening can also be normalised by reference laboratory control data. An encouraging finding of this study was the possibility of being able to discriminate between TPH and SOM. This study suggests that, with recent availability of truly field portable IR spectrometers, the *in situ* measurement of petroleum contaminants in soils is now possible.

