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Rapid detection of alkanes and polycyclic aromatic hydrocarbons (PAH) in oil-contaminated soils using visible near-infrared spectroscopy and chemometrics

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The recent developments and applications of rapid measurement tools (RMT) such as visible near-infrared (vis-NR) spectroscopy can provide 'fit for purpose' and cost effective data for informing risk assessment and managing oil-contaminated sites. While vis-NIR spectroscopy has been used to detect and quantify on-site hydrocarbons in soils and sediments, it is not appropriate for the elucidation of hydrocarbon compound structures and therefore advanced chemometrics methods are needed to expand the applicability of vis-NIR spectroscopy. In the present study, 74 oil contaminated soil samples collected from the Niger Delta were scanned using an analytical spectral device spectrophotometer with a spectral range of 350-2500 nm. The vis-NIR signal for each soil sample was then analyzed using partial least squares regression (PLSR) and random forest (RF) regression. Reference alkanes and PAH fingerprints of the oil-contaminated samples were determined using sequential ultrasonic solvent extraction followed by gas chromatography- coupled to mass spectrometry (GC-MS) analysis. Prior to the model development, spectra were subjected to pre-processing including successively, noise cut, maximum normalization, first derivative and smoothing. The pre-processed spectra were divided into calibration (75%) and validation (25%) sets. The alkane and PAH concentrations determined by GC-MS and the vis-NIR based spectra were subjected to PLSR and RF with leave-one-out cross-validation (LOOCV) to establish calibration models. Results showed that RF calibration models for both alkanes and PAH outperformed PLSR, indicating that vis-NIR signal acquisition followed by RF can provide a rapid and cost effective means to inform risk assessment for oil-contaminated sites.

keywords: *Total petroleum hydrocarbons, vis-NIR spectroscopy, chemometric methods, site investigation*