

## Evaluating magnetic susceptibility as a rapid scoping tool for assessing trace metal contaminated soils

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The widespread association in many soils of various trace metals with nano- or micro-particulate grains of magnetic Fe-O-H phases has led to the proposal (Bityukova *et al.*, 1999) that the magnetic susceptibility,  $\chi$ , of soils might be used as a proxy for trace metal concentrations, particularly concentrations of bioavailable trace metals, in contaminated soils. The utility of such measurements in areas of trace metal contamination has been tested here using field and laboratory magnetic susceptibility measurements and a variety of chemical and mineralogical analyses: ICP-AES, XAS, sequential extraction, EPMA, XRD and XRF. Three contaminated sites, two in Greece (Kozani – a disused power station; Thessaloniki – the site of a tannery) and one in the UK (Potters Hill, Bolton – site of a former chromate works) were selected for study.

Good correlation of Zn and Cu with field-based  $\chi$  data was found, however a very poor correlation was found between Fe and Cr and field-based  $\chi$  data. This suggests that whilst Zn and Cu are predominately associated with phases contributing to  $\chi$ , Fe and Cr occur in substantial proportions in phases with contrasting magnetic susceptibilities. EPMA mapping confirmed the existence of all of Fe-rich, Cr-rich and Fe+Cr-phases. XANES and EXAFS data were consistent with the occurrence in the soils of the Cr(III) phases with the following stoichiometries: CrO<sub>3</sub>, Cr(OH)<sub>3</sub> and FeCr<sub>2</sub>O<sub>4</sub>.

Whilst field-based  $\chi$  measurements are both cheaper and faster than chemical analysis of bulk soil or soil extracts and thereby have the potential to be a useful scoping tool, the relationship between  $\chi$  and metal concentrations may be critically dependent on the solid phase speciation of the trace metals of interest, necessitating careful consideration of data on a site-by-site basis.

## Novel corresponding - states principle approach for calculating the isotopic properties of water under elevated temperatures and pressures

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The isotopic properties of geologic fluids under geologic conditions are of geochemical interest. For this reason, we developed a corresponding-state principal (CSP) formulation for expressing the equation of state (EOS) of isotopologues of molecular fluids in terms of the dimensionless three-parameter equation (Polyakov *et al.*, 2007):

$$Z(\tau, \delta, \omega) = Z_0(\tau, \delta, \omega_0) + \left. \frac{\partial Z_0(\tau, \delta, \omega)}{\partial \omega} \right|_{\omega=\omega_0} (\omega - \omega_0)$$

where  $Z$  is the compressibility factor;  $\tau$  and  $\delta$  are dimensionless temperature and pressure, respectively;  $\omega$  is the Pitzer acentric factor; subscript “0” refers to the major isotopologue. Using this CSP formulation for minor isotopologues, we further developed a general EOS-based approach for calculating the reduced isotope partition function ratio (RIPFR) for “real-gas” fluids under elevated temperatures and pressures presented by Polyakov *et al.* (2006).

This novel approach was applied to the isotopologues of water (HDO and H<sub>2</sub><sup>18</sup>O), using experimental data (e.g. liquid-vapor fractionation and molar volume isotope effects). The RIPFR of water calculated from our approach show contrasting behaviors for HDO and H<sub>2</sub><sup>18</sup>O. The D/H exhibits an overall decrease of 5‰ with increasing pressure to 1 kb, which is in agreement with experimental results for brucite - water system (Horita *et al.*, 2002). In contrast, the RIPFR for H<sub>2</sub><sup>18</sup>O increases by 1‰ with pressure to 1 kb. The significant pressure effects on the isotopic properties of water obtained from this study have important geochemical implications.

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