Sequential extraction of Pb, Zn, Cd, and Cu in contaminated soils due to mining operation in Isfahan-Iran

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Sequential extraction was applied on 6 soil samples collected from metal contaminated site due to Gooshfil mining operation (20 km south west of Isfahan) to evaluate the level of contamination and bioavailability of Pb, Zn, Cd, and Cu. The sequential extraction method which was used in this research has been introduced by Tesser *et al*. in 1979 and modified by Salbu *et al*. in 1998. This method separates metals in six operationally defined fractions: water soluble, exchangeable, carbonate bonds, oxides bonds, organic bonds and residual fractions.

From the results of this study it can be concluded that the study area is contaminated with led. Zn is lower but near the contamination level. Mining operation in the area is the major source of metal contamination. The results obtained from the sequential extraction indicate that up to 90 % of metals in soil samples were associated to low soluble and high stable fraction such as oxide, organic and residual fraction. Metal distribution in soil samples generally followed the order oxide fraction> residual fraction> organic fraction> carbonate fraction> exchangeable> water-soluble.

Metal mobility and bioavailability

Ratio of relatively metal bioavailable and mobile fractions to stable and less mobile fractions is defined as mobility factor.

Metal mobility factor (Mf) defined as the following equation:

MF = (water-soluble + exchangeable + carbonate fraction)/ total metal content *100

The high MF values have been interpreted of relatively high biological availability and bioaccessibility of metals in soils. Mobility factor for six soil samples was determined by using the result of sequential extraction. Results are presented in Table 1.

Table 1: Mobility factor for metals

Soil	Pb	Cd	Zn	Cu
S1	1.8	7.8	1.7	2.0
S2	0.7	6.9	0.6	0.7
S3	3.0	9.7	1.0	3.6
S4	3.9	10.2	1.4	8.1
S5	1.9	9.7	2.0	7.1
S6	3.1	10.2	1.0	4.1

Bioavailability for metals found to be very low. Metal mobility factor for four studied metals were lower than 12%. The highest mobility was measured for cadmium and the lowest obtained for Zn. The results of bioavailability and mobility factor for the studied metals in the soil samples generally show the following order: Cd>> Cu> Pb> Zn

Viscosity of MgO-SiO_2 melt system from first principles simulations

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Transport properties of silicate melts are crucial to our understanding of chemical and thermal evolution of Earth. In recent years, we have performed density functional theory-based molecular dynamics simulations to study from first principles several key properties including viscosity (η) of relevant melts in the MgO-SiO_2 system. Numerous simulations of durations from a couple of tens of picoseconds to a few nanoseconds were completed to sample the pressure-temperature-composition (P-T-X) space accurately. The calculated results show that the viscosity is strongly dependent on pressure and temperature showing large deviation from the normal Arrhenian behaviour. The melt viscosity varies by two to three orders of magnitude across the entire mantle pressure regime. The predicted anomaly (i.e. viscosity increasing on compression) becomes more pronounced in silica-richer melts. Such dynamical changes can be associated to the structural changes. The simulations results were used to derive a viscosity model, η (PTX), applicable for the parameter space considered. The predicted viscosities compare favourably with the available measured data.