Molecular and colloidal dynamics in acid mine waters

[a]Durães N, [b]Bobos I, [a,c]Ferreira da Silva E

Acid mine waters collected from the Lousal, Aljustrel and S. Domingos mine areas (Iberian Pyrite Belt) were studied by infrared spectroscopy and chemical analysed by ICP-MS.

The pH of these waters range from 1.5 to 4 and the electrical conductivity range from 1470 to 40840 µS.cm^{-1}. Chemistry of acid mine water corresponds to the Fe-Mg-SO_4-(Al) type, which well explains why Fe and Mg sulfates precipitate during evaporation. The amounts of sulfate and metals are considerably variable but far exceed the background values in several times: SO_4 (30 – 7500), Fe (11 – 159000), Al (170 – 43700), Cu (15 – 322000), Zn (30 – 101000), and Pb (1 – 2400). Zinc are the most mobile of the three metals considered and remains in waters in high amounts, instead of Pb^{2+} which is only stable in extreme acid pH values (pH<1.5).The ratio between the concentration (values in ppm) sediments:waters show a sequence Pb>Cu>Zn. The average concentrations in waters shows a sequence Zn>Cu>Pb, while in sediment are Zn>Pb>Cu.

Speciation calculus indicates the predominance of Cu^{2+}, Zn^{2+} and Pb^{2+} species in solution. The SO_4 concentration increases significantly at pH<2 and sulfate species become more important.

Attenuated total reflectance infrared spectroscopy (FTIR-ATR) allowed identifying in aqueous solution the S-O and Fe-O-OH (goethite) complexes. The divalent metals form complexes with Fe-O-OH and SO_{4-}Me. Two structural coordination forms were identified: monodentate (pH<2) and bidentate (pH <4) coordination. These complexes allow the precipitation of schwertmannite, goethite or simple sulfates during evaporation. The Fe-O-OH and SO_4^{2-} complexes form simple and complex sulfates, where both Cu^{2+} and Zn^{2+} from acid waters are sequester in their structure. Under high acidic conditions (pH ~ 1.5) jarosite is crystallized and the Pb is fixed in its structure, fact that is reinforced by the correlation of Pb with K.

[a] *GEOBIOTEC - Universidade de Aveiro, Campus de Santiago, 3810-193 Aveiro (nunomsduraes@gmail.com)*
[b] *Departamento de Geociências, Ambiente e Ordenamento do Território and Centro de Geologia da Universidade do Porto, Rua do Campo Alegre 687, 4169-007 Porto*
[c] *Departamento de Geociências, Universidade de Aveiro, Campus de Santiago, 3810-193 Aveiro*