THE USE OF AVAILABLE CHEMICAL EQUILIBRIA SOFTWARE FOR THE PREDICTION OF THE PERFORMANCE OF EKR

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Risk assessment aims for the prediction of the mobility of contaminants, and these are usually based in lab essays together with mathematical modelling. Also the feasibility studies of most techniques, require similar tools. Frequently the lab characterization is based in the chemical fractionation of the contaminants based on their mobility under different chemical reagents. Probably the most frequent fractionation technique for heavy metal contaminated soils is the BCR [1].

The use of chemical equilibria software helps to understand the processes involved in the contaminant transport during electrokinetic remediation. Most mathematical models used for the simulation of electrokinetic decontamination assume local equilibrium between the chemicals present in the aqueous phase. In other cases also equilibrium is supposed between the chemical species present in the aqueous phase and the solid matrix.

In this work, we compare the results of batch extraction experiments with those obtained using Visual MINTEQ [2]. This is a free software that allows a reliable simulation of the chemical processes involved in the water-soil systems such as solubility, sorption, etc.

We found that even when the main contaminant behaviour is in accordance with the local equilibrium assumption, the mobilization of other metals, such as Ca and Mg, that are also present in important concentrations, are affected by kinetic limitations. These kinetic limitations have important effects in the overall behaviour of the system. Thus, if ignored, important flaws will appear in the predictions of the model with respect to those toxic species that could be considered to behave under local equilibrium.

[1] M. Villen-Guzman, J.M. Paz-Garcia, J.M. Rodriguez-Maroto, C. Gomez-Lahoz and F. Garcia-Herruzo. Acid Enhanced Electrokinetic Remediation of a Contaminated Soil Using Constant Current Density: Strong vs. Weak Acid. Separation Science and Technology (in press; DOI 10.1080/01496395.2014.898306).

[2] J.P. Gustafsson, Visual MINTEQ ver. 3.0beta. KTH Royal Institute of Technology, Dept. of Land and Water Resources Engineering, Stockholm, Sweden. (2010) http://www2.lwr.kth.se/English/OurSoftware/vminteq/index.html