Reactive transport modeling of in-situ arsenic removal systems in Jianghan Plain, China

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In situ chemical oxidation (ISCO) can be used as a technique for in-situ arsenic (As) removal from groundwater. NaClO as an oxidant was intermittently injected into the anoxic aquifer, typical of high-As and high-Fe aquifer in Jianghan Plain, to promote the formation of Fe oxides/hydroxides and to oxidize As(III) to As(V), thus removing aqueous As via adsorption and/or co-precipitation. A three-dimensional reactive transport model (RTM) was developed using GMS to determine the hydrogeochemical process responsible for As (im)mobilization during field experiment. Based on the field hydrogeological test, a flow model equivalent to the natural flow field was built in the MODFLOW module. Oxidation of Fe(II) and As(III) were simulated using kinetic-rate expressions in PHREEQC database. Cation exchange and formation of new chemical species were modeled as equlibrium reactions. Adsorption of As, HCO_3^-, Fe(II), SO_4^{2-}, F, Mg, Mn and Si on the surface of Fe(III) hydroxide was equivalent to surface complexation reactions. It was determined the oxidative hydrolysis production of Fe(II) in field experiment was ferrihydrite, by comparing the calculation results when different form of Fe(III) hydroxide (goethite and ferrihydrite (HFO)) was regarded as a surface specie. As concentration was mainly affected by HFO content and concentration of competitive adsorption ions in groundwater. The natural flow field led to a difference in the concentration of HFO between upstream and downstream of the injection well, and the higher content of HFO, the lower concentration of As. HCO_3^- was the dominant surface species affectting adsorption of As by HFO, other less competitive ions in the early stage gradually showed an advantage in response to the decrease of As and Fe concentration. Reactive transport model gives a reasonable match with observed concentrations of the main ions, indicating that the model has a reasonable modeling of the crucial chemical processes in the in-situ remediation test, which can provide technical guidance for similar remediation operation.