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modeling microbial and geochemical reactive transport : model development and applications to arsenic mobility

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The geochemistry of natural system, as old mine site, is influenced by biological activity. Only informatics tools taking into account geochemistry, hydrodynamic and microbiology will be able to analyze, and then predict, this complex system evolution. For about ten years, numeric tools, as CHESS and HYTEC, are able to take into account most of the geochemical and hydrodynamical process present in soil. The goal of this work is to extend this tools to the microbiological activities.

CHESS find the geochemical equilibrium speciation using a modified Newton-Raphson process. The same method of resolution is extended to the calculation of reactions mechanism containing biological kinetics. Most of the biological kinetics laws can now be used: Monod law, inhibition law, thermodynamic law. Moreover, others options of this tools are maintained, in particular, the coupling with transport process (HYTEC).

The code implementation is first verified by the calculation of several cases from literature. The tool is then used to analyse data from an experimental study realized at the BRGM, involving a bacterial consortium responsible of the reductive dissolution of an hydrous ferric oxide enriched in arsenic. The non-congruent mobilization of iron and arsenic is explained by the absorption on hydrous ferric oxide and the activity of two bacterial metabolisms which degrades organic matter and reduce Fe(III) and As(V).

A second application of the modeling tool deals with the old site mine of Carnoules (Gard, French). Experiments, realized at the university of Montpelier, permitted to study the natural biogeochemical evolution of natural acid mine drainage. The calcu-

lation take into account the biological oxidations of iron and arsenic by atmospheric oxygen, and the precipitation of amorphous Fe(III)-As(V)gel. The thermodynamic and kinetics parameters are then used in a hydrodynamical simulation at the field scale, in order to understand the geochemical evolution of acid drainage water.

Several applications prove the interest of computational tools in the water-mineral interface understanding, which is often colonize by bacterias implies in precipitation-dissolution processes. Moreover this two applications, CHESS and HYTEC extension of biological activity permitted to considerably extend the fields of applications.