Migration of small organic molecules in dense clay systems

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^{14}C is an important contributor to the annual radioactive dose predicted in performance assessment of a low- and intermediate-level radioactive waste repository in Switzerland. Corrosion of activated steel can release ^{14}C-labelled organic molecules.

The migration/retention behaviour in clay material of a suite of organic model compounds was studied using an infiltration technique. A pulse of tracers (carboxylic acids and alcohols) was injected into a column of compacted clay (illite and kaolinite). Their breakthrough was monitored and compared with a non-sorbing tracer, tritiated water (HTO). The effluent concentrations were measured with ion chromatography and the activity of HTO was measured by liquid scintillation counting.

For illite, the breakthrough times of non-hydroxylated acids (for example, propanoate) and HTO were identical. Hydroxylated acids were generally retarded, with alpha hydroxy acids showing a more significant retardation than beta hydroxy acids. The non-hydroxylated carboxylic acids were found to be more retarded in kaolinite than illite. For currently unknown reasons, hydroxylated acids could not be recovered in the effluents from kaolinite. A weak retardation of alcohols was observed in both illite and kaolinite.

The breakthrough of the individual tracers is modelled with a 1D advection/diffusion model implemented in COMSOL Multiphysics.

The strong sorption of hydroxylated acids might be explained by chelation of the alpha/beta-hydroxo group with the metal cations on the clay surface. The alpha-hydroxo group possibly has a stronger chelating power. This is being currently investigated by using attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) and nuclear magnetic resonance (NMR) techniques.