

Modelling of Pb and Zn transport during phase transformation of monohydrocalcite: Preliminary results

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A simple model has been developed to examine Pb and Zn transport during phase transformation of monohydrocalcite. Monohydrocalcite is a nano-mineral with a diameter of ~100 nm and is metastable, being transformed to aragonite (several micrometer) in a few days. Accordingly, metals initially adsorbed on monohydrocalcite are redistributed between solution and solid during transformation, which affects metal transport. The model was made based on the results of Pb and Zn sorption experiments during transformation of monohydrocalcite (unpublished study). The model calculates changes in the concentrations of monohydrocalcite and aragonite and those of Pb and Zn sorbed to the solids and dissolved in solution with time at a given point in a water flow.

Major factors that the model considers are (i) transformation rate, (ii) change in metal distribution during transformation, (iii) change in particle size during transformation, (iv) sedimentation rate, and (v) water flow rate. The model calculations are made for the following cases: (1) with different transformation rate (e.g., retardation and inhibition) and without transformation, (2) with change in water flow rate, (3) with change in particle size of monohydrocalcite, and (4) with difference between metal redistribution mechanisms.

Metal transport is slower with transformation than without transformation because of the transformation and the subsequent sedimentation of aragonite with much larger size than monohydrocalcite. When the transformation rate is retarded, metal transport becomes faster than that with transformation, indicating important effects of transformation rate on metal transport. With slower water flow rate, metal transport is slower depending on transformation rate. The difference in particle size of hypothesized monohydrocalcite (10 and 100 nm) makes little difference when the water flow is fast. The difference in metal redistribution mechanisms (i.e., between only sorption and combination of sorption and metal precipitation) affects metal transport.

Keywords: monohydrocalcite, phase transformation, transport modelling