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Reactive transport modelling of calcium carbonate formation in a Lab-on-a-Chip device at 25°C

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A mechanistic kinetic law for the successive formation of amorphous calcium carbonate (ACC) and calcite is developed at room temperature. It relies on a detailed description of aqueous speciation and a combination of transition-state-theory (TST) and surface complexation model (SCM) equations [1]. The proposed law aims at describing several inter-related mechanisms: *i*) formation of ACC seeds with the creation of surface complexation sites, *ii*) formation of calcite initiated by surface complexation and creation of new surface complexation sites, *iii*) growth of calcite at the expense of ACC, *iv*) progressive disappearance of ACC.

The TST-SCM equations are implemented in the geochemical calculation software PhreeqC-3 [2] which allows managing complex kinetic laws. The calibration of the model is first performed on published data acquired on batch experiments [3]. Then, it is applied to a dynamic system which consists in the simultaneous injection of two aqueous solutions of CaCl₂ and Na₂CO₃, respectively, into a micro-channel. The dimensions of the system and the conditions of injection are representative of a recently published experimental work [4] performed on a Lab-On-a-Chip device. The reactive transport modelling is done using the PHAST software [5] since it is full coupled with PhreeqC.

The numerical simulations could satisfactorily describe these observations. Obviously, there is room for further improvements like the use of more adequate flow equations (i.e. Navier-Stokes), as well as the implementation of the transport of particles.

Bibliographic references

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