Reactive transport modelling of calcium carbonate formation in a Lab-on-a-Chip device at 25°C
Arnault Lassin, Laurent André, Nicolas Devau, Adeline Lach, Thomas Beuvier, Alain Gibaud, Stéphane Gaboreau, Mohamed Azaroual

To cite this version:
Arnault Lassin, Laurent André, Nicolas Devau, Adeline Lach, Thomas Beuvier, et al.. Reactive transport modelling of calcium carbonate formation in a Lab-on-a-Chip device at 25°C. Goldschmidt Conference 2017, Aug 2017, Paris, France. hal-01500330

HAL Id: hal-01500330
https://hal-brgm.archives-ouvertes.fr/hal-01500330
Submitted on 3 Apr 2017

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Reactive transport modelling of calcium carbonate formation in a Lab-on-a-Chip device at 25°C


1BRGM, 3 av. C. Guillemin, 45060 Orléans, France; a.lassin@brgm.fr, n.devau@brgm.fr, a.lach@brgm.fr, s.gaboreau@brgm.fr
2Université d’Orléans-CNRS/INSU-BRGM, UMR ISTO 7327, 45071 Orléans, France; l.andre@brgm.fr, m.azaroual@brgm.fr
3LUNAM-Univ. Maine-IMMM, UMR CNRS 6283, av. O. Messiaen, 72085 Le Mans, France; tbeuvier@yahoo.fr, Alain.Gibaud@univ-lemans.fr

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 expanse 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 CaCl$_2$ and Na$_2$CO$_3$, 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**