A Microfluidic Experiment and Pore Scale Modelling for Assessing Mineral Precipitation and Dissolution in Confined Spaces

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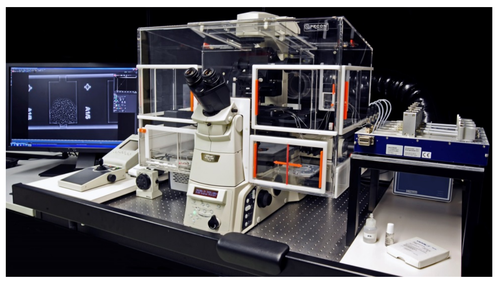
MOTIVATION

- Dissolution and precipitation processes control fundamental transport properties of porous media.
- These processes occur at different time and length scales, and are often not easily captured by a macroscopic continuum scale reactive transport model.
- For upscaling purposes, a mechanistic understanding and description of these processes in the pore space is a prerequisite, using state-of-the art experimental and modelling techniques.

Our approach: combination of microfluidic experiments with pore scale modelling

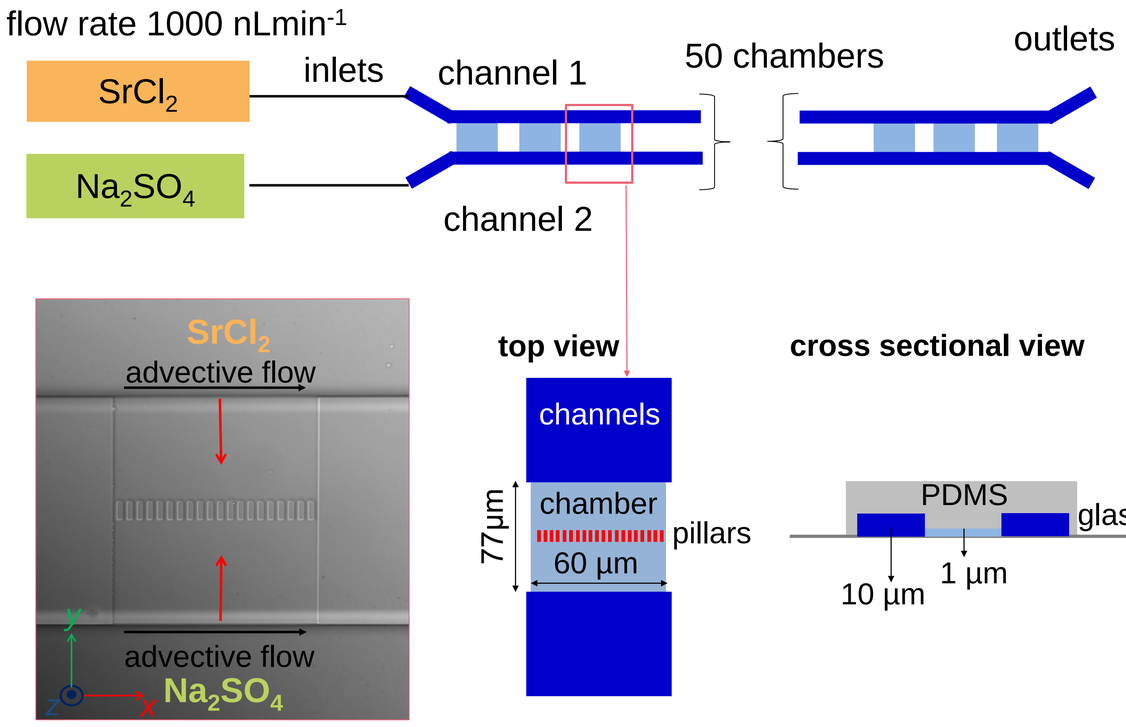


- idealized porous media with controlled pore shape
- feasibility of constant monitoring
- control on chemical system and environmental parameters (e.g. T)

EXPERIMENTAL SETUP AND MODELLING APPROACH

- A microfluidic reactor to precipitate celestine due to mixing of $SrCl_{2(aq)}$ and $Na_2SO_{4(aq)}$ $\quad SrCl_{2(aq)} + Na_2SO_{4(aq)} \rightarrow SrSO_{4(s)} + 2NaCl_{(aq)}$

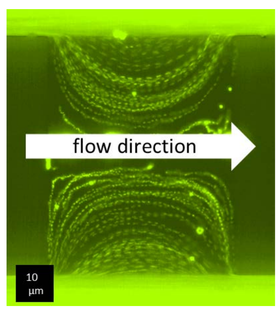
microfluidic reactor

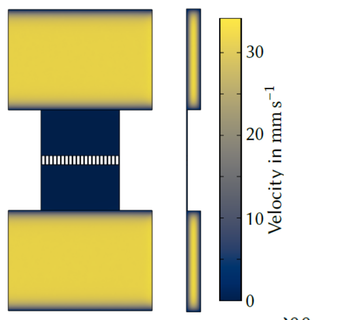


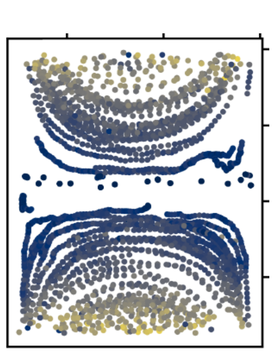
- Modelling of solute concentrations in the microfluidic reactor without chemical reaction using COMSOL Multiphysics 5.3a[1]
- Lattice Boltzmann method was used to investigate the reactive transport processes at the single chamber level, by transient calculation of solution composition and the local saturation indices using full speciation and by prediction of the induction time.

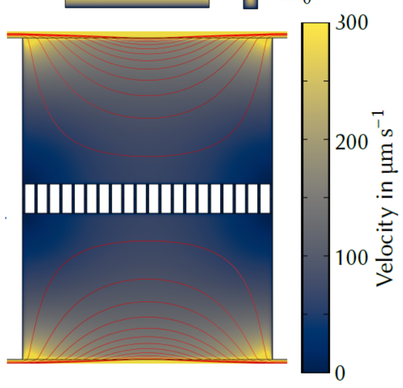
RESULTS : CHARACTERIZATION OF FLOW FIELD

- Injection of fluorescent beads for visualization of the flow field









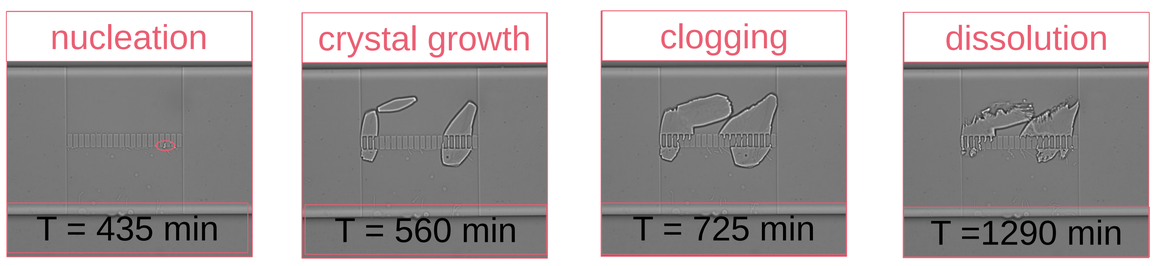
- Laminar flow develops in the channels, particles are dragged in the chambers
- Velocities decrease from channels towards center of chamber
- ➢ Transport inside the chamber by advection and diffusion
- ➢ Good agreement between experimental and modeled velocities

Solute transport along the reactor

- No concentration gradient (due to diffusion) along the channels at the chosen pumping rate
- ➢ Constant boundary conditions at the inlets of each chamber

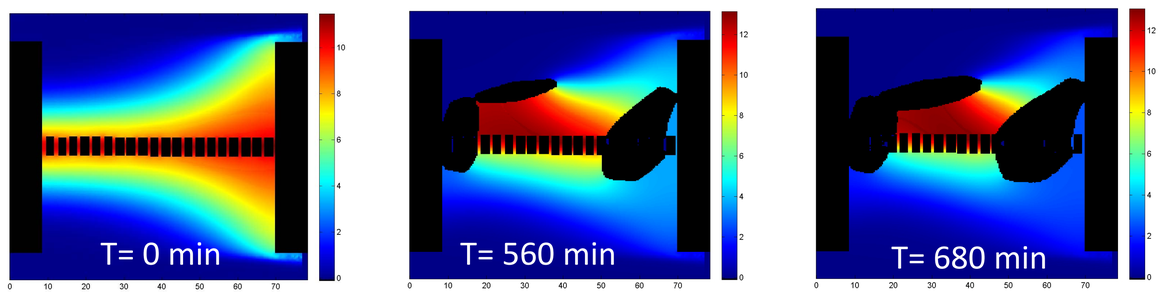
RESULTS : CELESTINE PRECIPITATION & DISSOLUTION

- The evolution can be described by four stages :



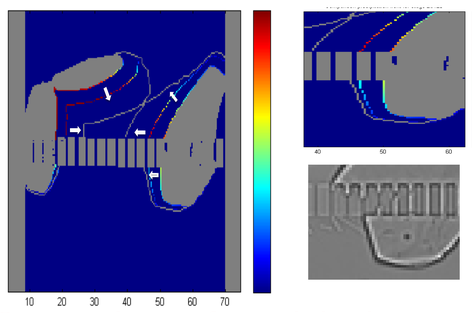
- The numerically predicted induction time for nucleation considering classical nucleation theory was in agreement with experimental observations

Evolution of the saturation ratio (Ω) with time



- Appearance of crystallites in regions of low velocities with highest Ω
- Growth favoured along boundaries with higher Ω
- ➢ Final shape of crystals controlled by the hydrodynamics of the system

Comparison of simulated and experimental precipitation fronts

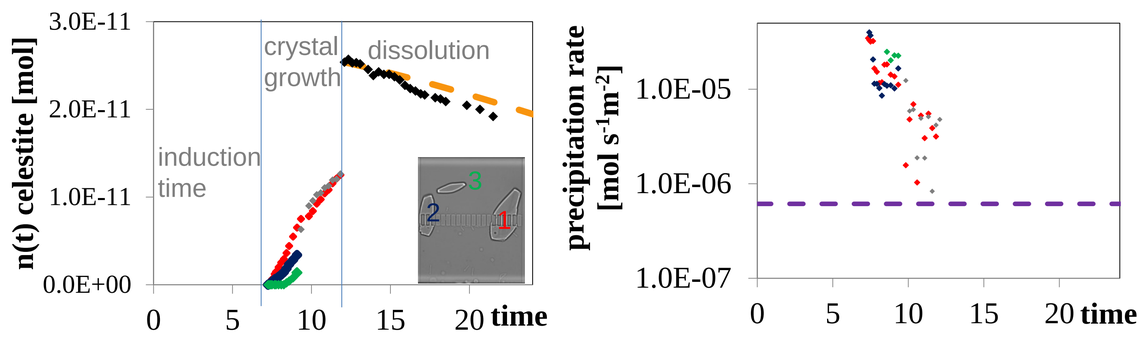


red → high speed of precipitation front

blue → low speed of precipitation front

- ➢ Good agreement between experimental observations and predictions

Comparison of precipitation and dissolution rates with literature data



- dashed line: dissolution rate following [2]
- dashed line: precipitation rate at log Ω 1.3 following [3]

- ➢ Good agreement of our experimental data with literature data

CONCLUSION

Establishment of a proof of concept approach combining microfluidics and pore scale modelling based on Lattice Boltzmann method to address fundamental geochemical processes: nucleation, precipitation and dissolution [4].

References:

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[4] Poonoosamy et al. 2019 Chem. Geo. doi.org/10.1016/j.chemgeo.2019.07.039

Acknowledgements:

The research leading to these results has received partial funding from the German Federal Ministry of Education and Research (BMBF, grant agreement 02NUK053A) and from the Initiative and Networking Fund of the Helmholtz Association (HGF grant SO-093) within the *iCross* project. MM, SVC, CE and NIP acknowledge partial support from Swiss National Science Foundation, SNSF project No: 200021_172618.