Pore-Scale Controls on Calcite Dissolution using Direct Numerical Simulations

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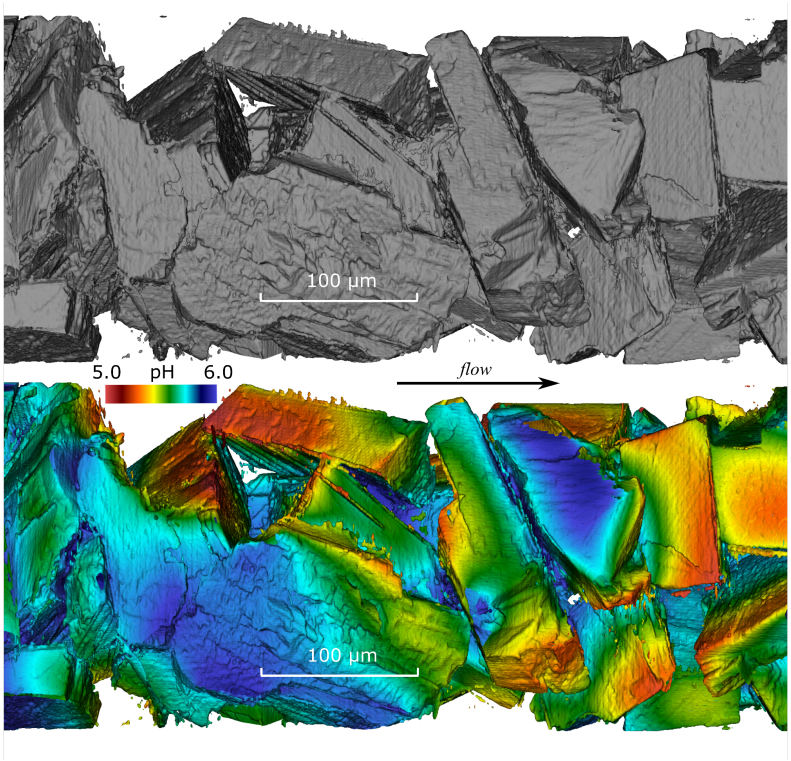

The complexity of pore geometry results in local variations of uid velocity that affect the interplay between advective and diffusive transport. Dissolution rates are a function of the solute concentrations that are in direct contact with the mineral surfaces. In the image, the variability of pH values on the mineral surfaces indicate the existence of distinct reactive transport regimes in areas in close proximity to each other (bottom). This result was obtained by simulating calcite dissolution driven by the flow of a high-CO2 solution using the code Chombo-Crunch. A 6144×512×512 grid was used to discretize the geometry of the crushed calcite grains packed in a 0.7 cm long 0.5 mm in-diameter capillary tube with 1.16 µm resolution. The domain geometry (top) was generated from X-ray computed microtomography data. High-resolution simulations of uid ow and reactive transport enable exploration of differences in geochemical conditions in the uid near mineral surfaces[1, 2].

[1] Molins, S., Trebotich, D., Steefel, C. I., & Shen, C. (2012). An investigation of the effect of pore scale flow on average geochemical reaction rates using direct numerical simulation. *Water Resources Research*, *48*(3). https://doi.org/10.1029/2011WR011404

[2] Molins, S., Trebotich, D., Yang, L., Ajo-Franklin, J. B., Ligocki, T. J., Shen, C., & Steefel, C. I. (2014). Pore-Scale Controls on Calcite Dissolution Rates from Flow-through Laboratory and Numerical Experiments. *Environmental Science & Technology*, *48*(13), 7453–7460. https://doi.org/10.1021/es5013438