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Linking microscale and macroscale dissolution rates in carbonates with X-ray tomography data and numerical modelling

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Investigations of mineral surface reactivity have recently challenged the classical approach of determining dissolution rates from mineral powders as crystals or more generally mineral-fluid interfaces often exhibit heterogeneous and/or anisotropic reactivity. Here, we provide a detailed characterization of the dissolution kinetics of carbonate materials in 3D using X-ray microtomography with a resolution below 1 μm. The local dissolution rates determined at crystal faces, edges and corners from calcite dissolution experiments [1,2] are then used to constrain a stochastic numerical model based on the probability of detachment. In the model, the carbonate solid is divided into equally shaped voxels. The model identifies the number of free surfaces for each voxel and uses this information to classify which voxels are considered corners, edges or faces. Based on the estimated detachment probability for each class of voxels, a selection of voxels is removed at each time step too mimic a dissolution process. The number of removed voxels at each time step is dependent on the sample shape. Thus, the dissolution of carbonate samples with complex geometry is simulated from a pre-defined shape measured experimentally with 3D X-ray microtomography. The user can also build its own crystal shape as an input for the dissolution model. The model is first tested on Kossel-like crystals and then extended to more complex dissolution cases in natural rocks. By tracking the topography and voxel detachments at several time steps, we demonstrate that the model reproduces fairly well the observed topographic evolution of the fluid-mineral or fluid-rock interface in carbonate materials. This modelling approach provides a new tool to link dissolution rates at the microscale of fluid-mineral interfaces to macroscopic dissolution rates measured on bulk samples.

[1] Noiriel, Oursin, Saldi & Haberthür (2019), *ACS Earth and Space Chemistry* 3(1), 101-108.

[2] Noiriel, Oursin, & Daval (2020), *Geochimica et Cosmochimica Acta* 273, 1-25.