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Comparison between reactive-transport simulations and calcite dissolution experiments highlights the importance of fluid flow in upscaling studies.

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Mineral dissolution kinetics is studied since decades because of its importance for many biogeochemical cycles and industrial concerns. However, despite the large range of studies, the upscaling from laboratory experiments to the field is still challenging since dissolution rates measured in laboratory are several order of magnitude greater than those measured in the field under similar conditions, leading to the so-called "field-lab discrepancy". Whether the field-lab discrepancy could be ascribed to the kinetic rate laws that are used, or to the poorly understood groundwater circulation is still debated. In this study, mixed-flow reactor experiments are used to revisit the calcite dissolution rate law that is implemented in classical reactive transport models. In agreement with several recent studies, we showed that the stepwave model (SWM) should be preferred over the transition state theory (TST). We then conducted a simple column experiment containing an inert porous medium and calcite samples radially centered and regularly placed along the column height, and compared the results to the outputs of simulations using a reactive-transport code run in either 1D, 2D or 3D geometry.
The comparison demonstrates that 1D simulations greatly overestimate the dissolution rates measured in the column by Vertical Scanning Interferometry and the importance of using more complex 2D or 3D models in order to reproduce as well as possible the flow characteristics (path, dispersion...). Finally, this study highlights that the difference between the results obtained in 2D simulations' outputs using TST or SWM are not significant (in our chemical conditions) compared to the importance of the systems' hydrology.
This study represents one of the multiple upscaling processes to understand the laboratory-field discrepancy.