

## **Limitation of simple 1D-reactive transport simulations: the example of calcite dissolution**

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Over the last decades, numerous studies about mineral dissolution have revealed huge discrepancies (several orders of magnitude) between the rates measured in laboratory and those observed in the field, also referred to as “the laboratory-field discrepancy”. However, dissolution rate laws determined from laboratory experiments are usually used to implement reaction terms in geochemical models. Hence, it is crucial to improve the understanding of this discrepancy in order to make realistic extrapolations to the field.

Among the potential explanations for these differences, the role of intrinsic or extrinsic factors can be investigated. This study was dedicated to understand the effect of the chemical homogeneity of the aqueous fluid surrounding the mineral. Several experiments were run in flow-through reactors continuously stirred to obtain a dissolution rate law for (104) calcite face dissolution as a function of solution saturation. In our conditions, the results are not consistent with the transition state theory. A second experiment consisted in studying the dissolution of single crystals of calcite exposing their (104) face to the fluid in a column filled with zirconia beads to mimic a non-reactive porous medium (first step to understand the role of fluid chemical heterogeneity on the dissolution rate). The results highlighted a decrease of the dissolution rate compared to experiments carried out in continuously stirred reactors, and a dramatic difference between the reactivity of faces with identical orientations but either positioned face or back to the flow.

Finally, the comparison between the results obtained in the chemically non-homogeneous (porous) medium and a simple 1D reactive-transport model with a dissolution term based on the rate law derived from experiments conducted in continuously stirred reactors failed to fit the data of this experiment. Furthermore, the model failed to account for the significant differences between the dissolution rates of the two faces of a same mineral. Possible improvements of this model and consequences for natural settings will be discussed.