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Modeling Pore-Scale Calcite Dissolution Kinetics

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Introduction

The study of the kinetics of heterogeneous solid-fluid reactions, such as dissolution-precipitation reactions is difficult due to the characterization of the solid-fluid interphase properties, and the possibility for the reaction rate to be limited by different phenomena, such as pore diffusion, surface kinetics, or electric double layer repulsion. Herein, a model for the porous scale dissolution of a calcite particle summited to an incident flow containing certain level of acidity is presented.

Use of COMSOL Multiphysics

First, the Chemical Reaction Engineering physics has been used to model the set of chemical
reactions defining the chemical problem, including the surface of the calcite particle, $CaCO_3(s)$, and the aqueous species Ca^{2+}, CO_3^{2-}, HCO_3^-, H_2CO_3, H^+ and OH^-. Then, a "*space-dependent model*" has been created to include coupling with the Transport of Dilute Species and Laminar Flow physics. Additionally, the physics "Secondary Current Distribution" has also been used in this model to use the functionalities of the "Deforming Electrode Surface", and modeling the surface of the calcite particle as a non-faradic reaction. This way, the changes of volume of the solid particle, due to the dissolution process, has been incorporated. The model is kinetically controlled by the surface reaction rate, and the diffusion – convection rates. Aqueous species aremodelled as instantaneous reversible (equilibrium) reactions.

Results

The fully-coupled reactive transport model is able to predict the dissolution of the calcite particle and the corresponding size change. Figure 1 shows the results for the pH variations around the dissolving particle, as well as the change of the volume of the particle (referred to the initial)
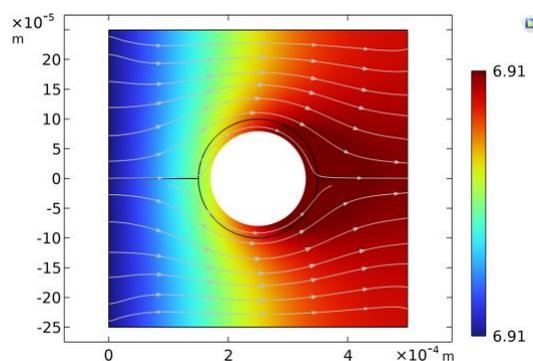

Figure 1. pH around the surface and streamlines for proton concentration.

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By changing the concentration and the flow-rate of the incident acidic current, it is possible to control the dissolution rate. Furthermore, if strong concentration gradients are created between the front and the back of the particle, the dissolution results in a deformation of the circular geometry.

Conclusion

Depending on the incident current flow-rate and concentration and the pore size and the particle sizes, the process may be controlled by either the surface kinetics, the diffusion or the convection rates. Validation with experimental results will allow the quantification of the chemical kinetics constant for a predictive use of the model.

References

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