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Numerical modeling of coupled diffusion/advection-, reaction- and deformation- processes

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In nature chemical weathering is a common process which changes the composition of rocks. Serpentinization and carbonation of peridotite is one process of interest, since it may be considered as a natural analogue for in-situ CO_2 sequestration in ultramafic rocks. The rate of the process is dependent on the feedback that the reaction creates. Chemical reaction processes acting on a material can cause volume changes, and make internal stresses build up and in turn potentially fracture/buckle the material. The reactants are transported by diffusion-advection processes from a surrounding mobile phase. The bulk rock density is generally decreasing with increasing degree of serpentinization and carbonation, and lead to changes also in porosity and permeability. These changes will feedback on the fluid flow and affect the solute transport and reactivity.

To study this a two-dimensional coupled mechanical and diffusion-advection model is developed. For the mechanical problem the model solves the Navier-Cauchy equations, where the extent of reaction is used to determine the internal stress, and the diffusion-advection is solved separately in each time step. The numerical model is developed in Matlab, and uses the FEM discretizations of mechanical and diffusion-advection problems. The model gives the stress states in the material as the reaction front propagates inwards and changes the volume of the material. An analytical solution for the stress state in a cylinder, with a simple diffusion process representing thermal stresses, is used to benchmark the numerical model.

From the stress states the model gives, we predict when the material will fracture/spall/buckle, and at what depth with respect to the reaction front. We have a particulare focus on feedback processes, because it has been demonstrated that as stresses build up during a reaction there is a possibility for the material properties to change [2]. And questions about how these feedbacks can lead to an acceleration of the reaction rate, are tried to be answered.

References

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