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Numerical homogenization approach for coupling of chemical and mechanical processes in the geological subsurface

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Reactive transport and related processes as dissolution and precipitation of minerals may substantially change rock composition, and consequently its geomechanical properties. However, this chemo-mechanical interaction is rarely considered in assessments of subsurface processes. An approach to determine the macroscopic stress-strain-relationship of a composite material, based on the mechanical characteristics of its constituents is provided by analytical homogenization models. This method is widely used within the field of materials sciences and highly promising for geoscientific applications. However, none of the analytical models can accurately determinate elastic parameters of the composite for the entire range of the inclusions mechanical properties, their specific volume fractions and aspect ratios.

Numerical 3D models allow for a more precise quantification and help to overcome the limitations of analytical solutions, especially regarding the spatial distribution of inclusions and their interaction. For a representative rock volume element, effective elastic properties are determined in our approach by taking into account the characteristic geomechanical parameters of all relevant mineral inclusions. We successfully validated our model against available analytical solutions and published experimental data. Sensitivity analyses indicate that the calculated elastic rock properties vary up to 28 % due to the spatial distribution of the inclusions within the rock matrix. Additionally, the developed numerical homogenization method enables an improved quantification of rock parameters: particularly for high inclusion-to-matrix-volume fractions and high mechanical property contrasts, the analytical solution deviates up to 58 % from the numerical results. In conclusion, the introduced homogenization approach provides an essential basis for coupling chemical and mechanical processes in numerical simulations related to the geological subsurface.