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Predicting macroscopic elastic rock properties requires detailed information on microstructure

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Abstract

Predicting variations in macroscopic mechanical rock behaviour due to microstructural changes, driven by mineral precipitation and dissolution is necessary to couple chemo-mechanical processes in geological subsurface simulations. We apply 3D numerical homogenization models to estimate Young's moduli for five synthetic microstructures, and successfully validate our results for comparable geometries with the analytical Mori-Tanaka approach. Further, we demonstrate that considering specific rock microstructures is of paramount importance, since calculated elastic properties may deviate by up to 230 % for the same mineral composition. Moreover, agreement between simulated and experimentally determined Young's moduli is significantly improved, when detailed spatial information are employed.

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Keywords: digital rock physics; effective elastic properties; numerical homogenization, Young's modulus, micromechanics, geomaterials

1. Introduction

Prediction of macroscopic mechanical rock properties based on their microstructure and mineralogical composition has a wide practical importance. Particularly regarding changes due to thermal or chemical processes within the context of risk assessments for various types of subsurface utilization or improving the understanding of

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geogenic processes. A variety of homogenization models can be used to relate macroscopic elastic rock behaviour to the mechanical characteristics of its microstructure and mineralogical composition. For a representative elementary volume (REV), effective elastic properties can be determined, e.g., by analytical homogenization methods. The first approaches by Voigt [1] and Reuss [2] predict upper and lower strength bounds by averaging elastic rock parameters of the mineralogical components. Many mean-field homogenization schemes consider inclusion geometries based on the Eshelby solution [3] of an ellipsoidal inhomogeneity embedded in an infinite medium. In this context, most popular concepts are the dilute scheme [4], the self-consistent approximation [5], the differential scheme [6] as well as the Mori-Tanaka approach [7]. Further models consider certain types of rocks, characterized by a particular microstructure [8,9]. However, none of the analytical models can determine elastic rock parameters for complex multi-component systems and the full range of possible pore network geometries.

Several numerical approaches are employed to estimate rock elasticity, either for synthetic geometries finding an adequate specific analytical solution [10,11] or to improve the understanding of geological processes at REV scale [12]. Characteristic microstructures derived from digital images are taken into account within the field of digital rock physics to estimate permeability, conductivity or effective elastic moduli [13–15]. Despite their higher computational demand in comparison to analytical methods, numerical models provide significant benefits, including consideration of various rock types and their characteristic microstructures. Also, these models can be extended for internal stresses occurring within the rock matrix due to swelling, shrinking, crystallization or changes in pore fluid pressure. Additionally, the presented approach allows for chemo-mechanical coupling within a simulation framework [16]: elastic rock properties can be determined depending on chemical changes, such as mineral dissolution and precipitation, and further upscaled from REV to reservoir scale (Fig. 1). This kind of approach is of particular relevance, since a direct chemo-mechanical feedback is rarely considered in studies regarding subsurface process assessments [17,18], while spatial heterogeneity at different scales significantly affects geochemistry, and thus reactive transport [19].

The calculated rock properties depend on three essential input parameters: (1) elastic properties and (2) volume fractions of the mineral components as well as (3) microstructure of the inclusions. This study particularly investigates the effects of (2) and (3), comparing a widely-used analytical approach with a numerical one. For a range of elastic rock parameters, the presented numerical homogenization model considers five different inclusion geometries to examine the impact of the microstructure. Moreover, elastic parameters of the synthetically generated geometries are modelled and compared with experimental data from the literature, considering the same mineralogical rock composition. Aim of this study is to determine the main influencing factors of the numerical estimation of macroscopic elastic rock properties.

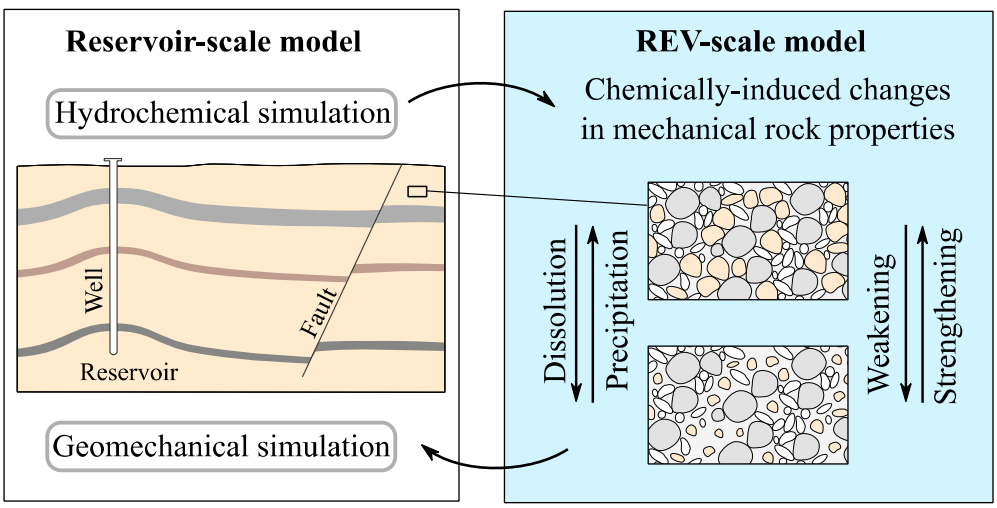

Fig. 1. Prediction of macroscopic mechanical rock properties based on their microstructure within the concept of chemo-mechanical coupling: changes in mineralogical composition can significantly strengthen or weaken rocks.