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Hydro-Mechanical-Chemical modelling of Brucite – Periclase (de)hydration reactions

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Metamorphic reactions involving hydration and dehydration frequently occur during orogenic cycles, for example, when ambient pressure and temperature conditions change due to subduction and subsequent exhumation, or when fluids infiltrate metastable mineral assemblages at constant ambient conditions. Such (de)hydration reactions can be associated with significant volume changes, which may cause significant differential stresses in the rock, potentially leading to fracturing. The impact of (de)hydration reactions on the rock's stress state and on the magnitudes of associated differential stresses is still controversially debated. One reason for the debate is due to the different theoretical models used to quantify and simulate (de)hydration reactions coupled with rock deformation. In many models, the rock deformation is frequently simplified, by either completely ignoring rock deformation or by considering volume deformation only. Additionally, the fluid flow is often simplified, by for example considering constant porosity. Here, we present a method to derive a system of governing equations to describe coupled Hydro-Mechanical-Chemical processes, which is suitable to quantify rock deformation coupled to (de)hydration reactions. Reactions are mainly treated as density changes whereby the density changes are determined by tabulated densities from thermodynamic Gibbs free energy minimizations in pressure, temperature and composition space. The rock deformation is quantified by the continuum mechanics force balance equations, here the Stokes equations. Considered flow laws describe either linear viscous deformation or dislocation and diffusion creep. Equations for reactions and rock deformation are coupled by several equations for the conservation of mass, such as total mass or mass of solid components stored in the solid. The governing system of equations is solved with a pseudo-transient finite difference method. For simplicity, we apply the numerical model here to several Brucite – Periclase (de)hydration reactions and show results of models with different levels of coupling, for example, constant or variable porosity. We also quantify the differential stresses associated with the (de)hydration reactions. Furthermore, we compare the modelled stresses with microstructural observations and stress estimates from high-resolution EBSD measurements in natural rock.