Using equilibrium thermodynamics to estimate pressure and porosity changes during reactive transport

Benjamin Malvoisin (1,2), Yury Podladchikov (2), and Johannes Vrijmoed (3)
(1) UNINe Neuchâtel, CHYN, Neuchâtel, Switzerland (benjamin.malvoisin@gmail.com), (2) UNIL Lausanne, Institute of Earth Sciences, Lausanne, Switzerland, (3) ETH, Zurich, Switzerland

Mineralogical reactions play a key role during transport in porous media by generating or consuming fluids and modifying the fluid pathways through volume changes. Here, we used a theoretical and numerical approach to determine the interplays between reaction, transport and deformation during metamorphic reactions. Mass conservation equations were written for a reacting system and a system of equations was obtained to describe the relationships between fluid pressure, porosity and three thermodynamic parameters (the density of the fluid, the density of the non-volatile solid and a function of the volume change). Thermodynamic parameters were calculated by energy minimization with Perple_X for three lithologies found in subduction zones: sedimentary, mafic and ultramafic rocks. The evolution of porosity and fluid pressure was predicted in several cases. First, the maximum pressure changes associated with volume change during reaction was estimated for univariant reactions. Then, multi-variant reactions were considered and the system of equations was solved with several assumptions. Typical equations for porosity waves were obtained by simplifying the system with a solid density as a simple function of pressure or with the assumption of a constant amount of non-volatile species. Numerical models were finally used to solve these equations for three cases: the dehydration of chlorite in mafic rocks (positive Clapeyron slope), the dehydration of serpentine in ultramafic rocks (negative Clapeyron slope) and the decarbonation of calcite (positive Clapeyron slope with a $\text{H}_2\text{O}-\text{CO}_2$ fluid). Such kind of models take into account the complexity of mineralogical reactions and allow to better understand the generation of fluid pathways in metamorphic rocks.