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A THMC approach to model the appearance and evolution of cracks within reactive porous media under various hydrogeochemical and mechanical loadings

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Coupled Thermal-Hydraulic-Mechanical-Chemical (THMC) approaches are crucial for a wide range of engineering and geosciences applications. Hence, their development have been the subject of numerous research projects over the past 20 years. However, due to the intrinsic complexity associated to simultaneously describe flow, species transport, chemical and mechanical effects together, no thorough dynamic two-way feedback between these processes have yielded satisfactory results. We present a novel approach to overcome past limitations by coupling two state-of-the-art simulators. Our numerical approach rests on a sequential non iterative coupling between Hytec, a reactive transport algorithm and Cast3M, a mechanical code. Hytec computes the evolution of hydraulic and mineralogical fields allowing to compute the micromechanical properties (e.g. Young modulus). The mineral reactions and drying processes generate tensile stresses and change in capillary pressure. Cast3M computes the associated strain tensors and induced damage. The damage model allows to account for the evolution of a crack network whose transport properties are computed based on the crack apertures. In the case of crack appearance, Cast3M thus imposes the increase of a double porosity in Hytec, which accelerates the subsequent reactive transport processes. We validate our method on the accelerated unsaturated carbonation of cementitious materials by comparing the predicted crack network and degradation depths with microtomographic images. We demonstrate that the shape of the degradation front results from the coupled impacts of chemistry and mechanics together which predominantly act along the sample edges, where crack apertures are the most important. Based on its physical basis, our approach can be extended to different hydro-chemo-mechanical loadings. For example, it could be used to study a wide range of concrete pathologies, including sulfate attack and alkali-silica reactions. Also, coupled mechanical and chemical processes involved in the opening or sealing of fractures associated to the induced seismicity of CO2 sequestration or geothermal energy constitute further potential applications of our method.