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A Phase-Field Discrete Element Method to study chemo-mechanical coupling in granular materials.

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Geochemical reactions are ubiquitous for subsurface energy extraction and storage applications, like geothermal electricity production or hydrogen storage, but also for other applications aiming at reducing climate change like underground CO_2 disposals [1]. Those reactions lead to mineral dissolution/precipitation that can modify the different properties of the reservoir rock and the caprock. For example, porosity of the porous material depends strongly on the dissolution/precipitation of the solid phase. It can thus affect the evolution of its permeability, a key parameter for most of those applications that involve the transport of a fluid through the reservoir. Moreover, the mechanical behavior and rupture of geomaterials is also strongly affected by dissolution/precipitation phenomena. In the case of cemented rocks, debonding can occur during weathering and strongly weakens the material [2]. This strength degradation has also been highlighted during oedometric tests in the case of granular materials presenting no cohesion [3]. In the case of underground storage applications, if a strength reduction is induced in the caprock, cracks can be created, leading to a migration pathway and leakage. It can also affect the behavior of faults in the vicinity of the reservoir and induce earthquakes [4]

Granular material (like in fault) or sedimentary rock can be modeled by the discrete element method (DEM). This method was first developed by Cundall and Strack to model the micromechanical behavior by reproducing more accurately the interactions in an assembly of grains. In the classical approach, grains are modeled as disks (2D) and spheres (3D), however, real particles can be highly irregular. These complex shapes of the grains influence greatly the macroscopic mechanical behavior of the material [5] and accurate models should aim at capturing this complexity. To do so, different approaches have been developed in the frame of DEM like particles cluster, ellipsoids, polygonal (2D) or polyhedral (3D) particles [6]. The latter is the most accurate solution, but it tends to overestimate the roundness of the particles and show some limitations to reproduce experimental results [7]. Recently, a level-set discrete element model was developed and allowed to capture the complex shape of the grains and reproduce experimental results [8].

To model grain dissolution/precipitation, discrete elements are often considered with a homogenous decrease/increase of the particle diameter. But in some cases, like pressure-solution, the dissolution/precipitation are localized. Hence, the dissolution occurs in the high-stress area, whereas the precipitation occurs in the low-stress area with a large solute concentration. This diffusive mass transfer is done within the pore fluid. Considering the granular material as a phase, the phase-field theory (PF) is a good candidate to model with physics-based laws an addition or reduction of the quantity of material locally. The dissolution at the contact is controlled by the introduction of mechanical and chemical energy into the Allen-Cahn formulation on the phase variables, whereas the precipitation and the mass conservation are verified by a coupled diffusion formulation on the solute concentration.

In this study, an extension to the discrete element method is developed to simulate the irregular shapes of particles in a granular material and their heterogeneous change using the phase-field variable as a particle's geometrical descriptor. This method, available on https://github.com/AlexSacMorane/PFDEM_ACS_MultiGrains, is applied to reproduce results from previous experiments on K_0 evolution [9]. The influence of the grain shape has been highlighted. Then, the model is used to investigate on the pressure-solution phenomenon at several grains level [10]. For example, a so-called Andrade creep law has been reproduced.

In conclusion, this new framework enables us to model chemo-mechanical couplings, considering the true shape of the grain. It is used to investigate the influence of the different physical phenomena (dissolution, precipitation or diffusion) controlling the rate of material compaction and of the macro properties evolutions, as the porosity, permeability or strength.

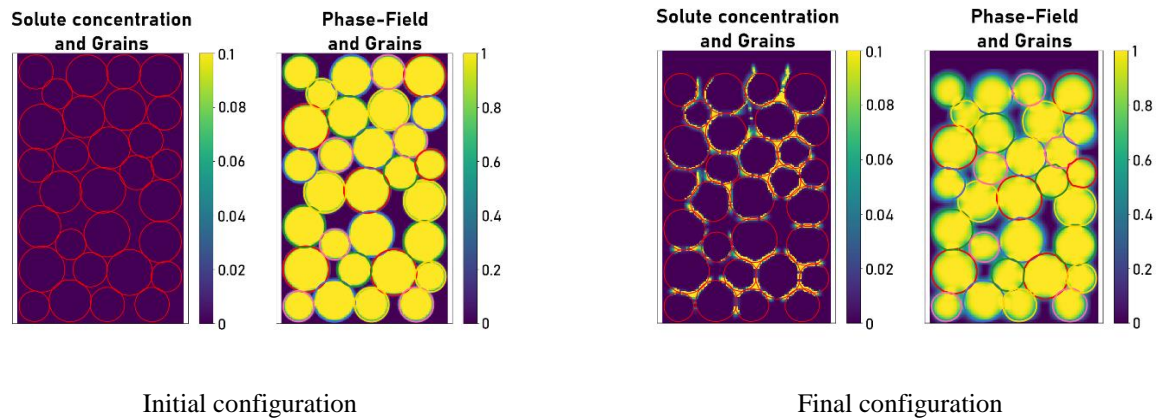Initial configuration   Final configuration

Figure 1: Pressure solution phenomena between multiple grains. For initial and final configurations, the left plot shows the position of the grains and the solute concentration, and the right plot shows the phase variables. Between the initial and the final steps, solute has been generated and the shape of the grains have become less and less spherical. The granular material becomes denser while the pressure-solution phenomenon occurs.

Contributor statement

Conceptualization: Hadrien Rattez and Manolis Veveakis; Investigation: Hadrien Rattez, Manolis Veveakis and Alexandre Sac--Morane; Software: Alexandre Sac--Morane; Supervision: Hadrien Rattez and Manolis Veveakis; Writing - Original Draft: Alexandre Sac--Morane; Writing – Review and Editing: Hadrien Rattez and Manolis Veveakis

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