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A novel coupled DEM-CFD approach to modelling of capillary driven two-phase water flow in unsaturated concrete

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Abstract:

Concrete is a strongly heterogeneous, discontinuous and porous material. It may be considered at the meso-scale as a composite material with four key phases: aggregates, cement matrix, interfacial transition zones (ITZs) between aggregates and cement matrix and macro-pores and ITZs, that are adjacent to aggregates, reveal pronounced compositional differences as compared to the cement matrix. ITZs include more and larger pores, smaller particles and less anhydrous cement and C-S-H (calcium silicate hydrate) gel what causes higher transport properties (i.e. permeability, diffusivity and conductivity) as compared to the cement paste. ITZs facilitate ingress and penetration of external aggressive agents into concrete what deteriorates both concrete and reinforcement.

A novel coupled approach to modelling of capillary driven two-phase water flow in unsaturated concrete was developed. The process of capillary driven two-phase water flow in unsaturated concrete was numerically analyzed in two-dimensional (2D) conditions by combining the discrete element method (DEM) [1] with the computational fluid dynamics (CFD) [2] under isothermal conditions. The mechanical behaviour of concrete was simulated with DEM, and CFD was used for describing the behaviour of laminar two-phase fracturing fluid (water and gas) flow in concrete. The geometry changes of pores in concrete were precisely reproduced. The capillary pressure was calculated by taking the interfacial tension, contact angle and throat radius into account. The DEM/CFD calculations were performed for the pure cement matrix, cement matrix including aggregates and cement matrix including aggregates and ITZs of a defined thickness. Thus, the effect of ITZs on the water permeability was evaluated. In addition, the effect of the external pressure direction, saturation volume and gas content on the water permeability was studied. The pure DEM represented by spheres was calibrated with the aid of simple uniaxial compression and tension tests while the pure CFD was calibrated with the aid of a permeability test. The main characteristics of capillary driven two-phase water flow in concrete were realistically reproduced with a proposed approach.

[1] Nitka, M. and Tejchman, J. (2020) Meso-mechanical modelling of damage in concrete using discrete element method with porous ITZs of defined width around aggregates. *Engineering Fracture Mechanics* 231, 107029.

[2] Krzaczek, M., Nitka, M. and Tejchman, J. (2020). Effect of gas content in macro-pores on hydraulic fracturing in rocks using a fully coupled DEM/CFD approach. *Int J Numer Anal Methods Geomech*. 1–31, https://doi.org/10.1002/nag.3160.