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COUPLING MECHANICS AND TRANSPORT IN DISCRETE MESO-LEVEL MODEL: VERIFICATION

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Abstract. Cracking in concrete has a paramount impact on the durability of structures. The natural permeability of a healthy material is severely magnified in the presence of cracks. Cracks form a network of channels capable to transport a fluid that may chemically or physically interact with concrete constituents or the reinforcing steel, leading to deterioration of structural members or entire structures. Moreover, the presence of a pressurized fluid in cracks and pores leads to further crack development and therefore also to further increase in permeability.

In order to predict the behavior of fractured quasibrittle solids filled with a pressurized fluid, a robust mechanical model is needed to describe the crack widths, connectivity, tortuosity, spacing, etc. The mechanical model must be fully coupled with a transport model into a multiphysical solver. We present such a solver, and validate it by comparison with experimental data from literature. The model is discrete, allowing to easily embody cracks and the coupling mechanisms. Individual discrete units represent mineral aggregates while the inter-particle contacts account for matrix between them.

1 INTRODUCTION

Water permeability and chloride diffusivity of concrete are essential elements that govern durability and serviceability of concrete structures. For a sound concrete, permeability and diffusivity depend on interconnected porosity of mortar and microcracks in concrete. When cracking occurs under loading, a rapid permeability growth is caused by interconnecting macrocracks that eventually dominate the permeability of the specimen. Consequently, an increased amount of water or chemical content can penetrate into the material, causing mechanical or chemical deterioration. Therefore, it is necessary to properly capture the dependence of the permeability on the level of structural damage induced by mechanical loading.

Robust modeling approaches allowing to describe the effect of cracking on permeability are based on a detailed representation of the cracks in the material. One of such approaches, employed also in this contribution, is discrete mesoscale modeling. Concrete material is represented by ideally rigid particles (mineral aggregates) interconnected by soft contacts (matrix). Cracks may develop at these contacts by damaging them. This kind of mechanical models can easily describe the transition from distributed to localized cracking [1] or splitting cracks under compressive loads [2].

Mass transport through developed cracks in discrete models is then simulated by a dual network of conduit elements [3, 4]. Flow through the individual cracks is computed by Poiseuille equation, taking into account the width of the crack. A number of researchers employs this concept, for example [5, 6, 7]. Recently, the effect of short fiber reinforcement on permeability was added into the description of flow [8].

We developed a coupled mechanical and mass transport mesoscale discrete model by adopting the aforementioned concepts. The aim of the present contribution is to verify the ability of the model to capture the increase of permeability due to cracking within concrete by comparing the model results with experimental data.

2 BRAZILIAN DISC EXPERIMENTAL SETUP

In the present study, we simulate Brazilian disc experiments as conducted in [9] and subsequently in [10]. A water flow through a pre-cracked Brazilian disc specimen is measured in dependence on opening of cracks scattered throughout the specimen. The test setup is depicted in Figure 1. The tested specimens were concrete discs with the diameter $D = 100\,\mathrm{mm}$ and thickness $L = 25\,\mathrm{mm}$. Firstly, the specimens were mechanically loaded to reach a desired crack opening displacement (COD). Mechanical loading of the Brazilian splitting test was controlled by a closed-loop feedback system to get a desired value of the crack opening displacement as represented by transversal LVDT measurements, normal to the expected crack plane. Note that the measured transversal displacement is not identical to COD, especially before reachng the peak stress, i.e. before localization of the macrocrack. However, the desired crack widths are well beyond peak stress and transversal LVDT measurements can be conveniently used for representing of COD. During mechanical loading, the applied force, F, was recorded. The mechanical tensile stress is then calculated as:

$$\sigma = 2\,F/\pi LD \tag{1}$$

After unloading, water permeability tests were performed in unloaded state. The cumulative water flow through the specimen was measured. The water flow was induced by the 300 mm water column above the horizontally laid discs. After reaching a steady water flow through the specimen, the permeability coefficient, k, was calculated considering a falling water head.

3 NUMERICAL MODEL

The three-dimensional domain is discretized into convex polyhedral particles by (i) random placement of sites with minimum mutual distance $l_{\min}$ and (ii) computing Voronoi tessellation on those sites. This exact procedure was developed in [11]. These polyhedra represent concrete aggregates with surrounding cement matrix and are treated as ideally rigid bodies [12]. Smaller aggregates are not modeled explicitly, their influence is smeared within the constitutive material model in a phenomenological way.

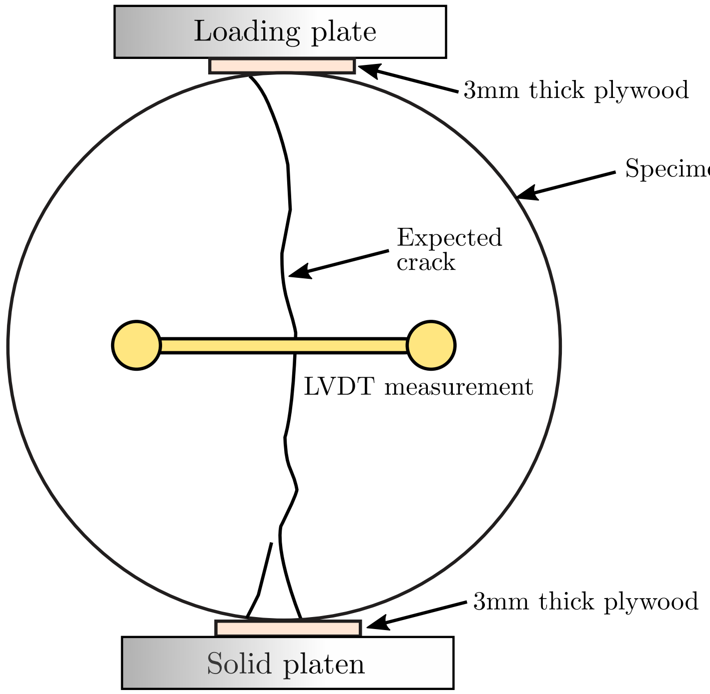

Figure 1: Brazilian disc splitting test setup.

Vectorial strains $\boldsymbol{e}$ are computed at contact facets between neighboring particles from displacement jump divided by distance between connected nodes and projected into local reference system with directions N (normal), M and L (tangential). The stress $\boldsymbol{s}$ is calculated using the meso-scale elastic modulus E_0, tangential-normal stiffness ratio α, and the internal damage variable ω

$$s_i = (1-\omega)E_i e_i \quad \text{for } i = N, M, L \tag{2}$$

where $E_N = E_0$ and $E_M = E_L = \alpha E_0$. Damage evolution laws are adopted from [13] and simplified as described in [14]. Only two additional material parameters are used for the nonlinear regime: fracture energy in tension G_t and tensile strength f_t. Other required material parameters are computed subsequently with relation to G_f and f_t.

Forces and moments acting on individual particles are obtained by integrating contact stresses. Force and moment balance equations are assembled for each particle and the resulting nonlinear system is solved by incremental Newton-Raphson method.

The transport part of the model is assembled from conduit elements running along the Voronoi edges. Pressure gradient g is defined as pressure difference divided by distance. Flux density j is provided by constitutive equation

$$j = \lambda(\boldsymbol{w})g \tag{3}$$

Permeability coefficient is composed from two parts, $\lambda = \lambda_0 + \lambda_\mathrm{c}$. λ_0 accounts for conductivity of the sound material while λ_{c} introduces an effect of crack [15]:

$$\lambda_0 = \frac{\kappa\rho}{\mu} \qquad \lambda_{\mathrm{c}} = \xi \frac{\rho}{12\mu S} \sum_{i=1}^{3} w_i^3 l_i \tag{4}$$

where S is the cross-sectional area of the conduit element, ρ is fluid density, μ is viscosity, κ is permeability of sound material, w and l are equivalent crack openings and crack lengths of associated mechanical elements, respectively. ξ is auxiliary model parameter accounting for crack tortuosity.

Mass balance equations for transport part of the model are steady-state. They are assembled for each Delaunay simplex individually by integrating fluxes on its surface and adding possible external sources or sinks.

4 RESULTS

Because the water pressure acting at the top disc surface is relatively small, the subsequent influence of water pressure on the crack opening can be neglected. Similarly to the physical experiment, indirect displacement control was applied to govern loading by the horizontal displacement (COD). The minimum aggregate size was set to be $l_{\mathrm{min}} = 2\,\mathrm{mm}$. The numerical analysis was conducted as steady state. The specimen can be therefore loaded with fluid pressure simultaneously with the mechanical loading.

Figure 2a shows the development of tensile stress, σ, in relation to COD during mechanical loading. The peak tensile stress is obtained at COD in the range from 25 to 60 μm. For the numerical model to reach the crack widths of 300 to 400 μm, a compromise had to be made between fitting material properties to match the immediate post-peak phase as well as the plateau beyond COD of 100 μm.

Figure 2b illustrates the effect of cracking on the permeability of the specimen, i.e. the relationship between COD and permeability coefficient. The COD values correspond with the target COD under loading. Note that unlike the numerical model, during the physical experiments, the specimens were unloaded prior the water permeability test. Permeability tests were conducted using specimens contracted to a lower COD due to unloading. However, the crack length and shape and the level of specimen damage corresponded to the history of loading up to the target COD. The resulting permeability measurements were afterwards converted back to the COD under loading. The results from physical experiments are therefore affected by this test procedure.

The numerical model confirms the behavior observed during the physical experiments. When the specimen is loaded to reach COD no greater than 50 μm, cracking has little to no effect on permeability. In the range of COD between 50 μm and 200 μm, the permeability increases rapidly with COD. For crack openings greater than 200 μm, the rate of permeability growth keeps increasing steadily. It can be concluded that the numerical model is well capable of capturing the evolution of permeability in dependence on crack opening displacement in all these described regimes.

Table 1 shows the mechanical and transport material properties used in numerical simulations to match the physical experiments.

Mechanical properties				Transport properties			
Young modulus	E_0	60×10^9	Pa	Density	ρ	1000	kg/m^3
Tang. to norm. ratio	α	0.3	[-]	Permeability	κ	1×10^{-16}	m^2
Tensile strength	f_t	4.5×10^6	Pa	Viscosity	μ	8.9×10^{-4}	$\mathrm{Pa}\cdot\mathrm{s}$
Fracture energy	G_t	65	N/m	Tortuosity	ξ	0.9	[-]

Table 1: Material properties used in numerical simulations.

5 CONCLUSIONS

The present contribution presents a verification of the developed discrete model of concrete using experimental data from literature. The mechanical model is coupled with the mass transport model. Detailed representation of cracks in the mechanical part is used in the transport part to update the material permeability. To verify the model, experimental data performed on Brazilian discs evaluating the relation between permeability and crack opening were selected. Material parameters of the mechanical model were set to provide a reasonable compromise between capturing the peak behavior and the post-peak plateau of the mechanical experimental response. Simultaneously with mechanics, the steady-state mass transport problem was simulated and water flux through the specimens was measured. Data provided by the model are in good agreement with experimentally obtained results. The implemented coupled discrete model is capable to simulate all the observed stages of the evolution of concrete permeability during cracking.

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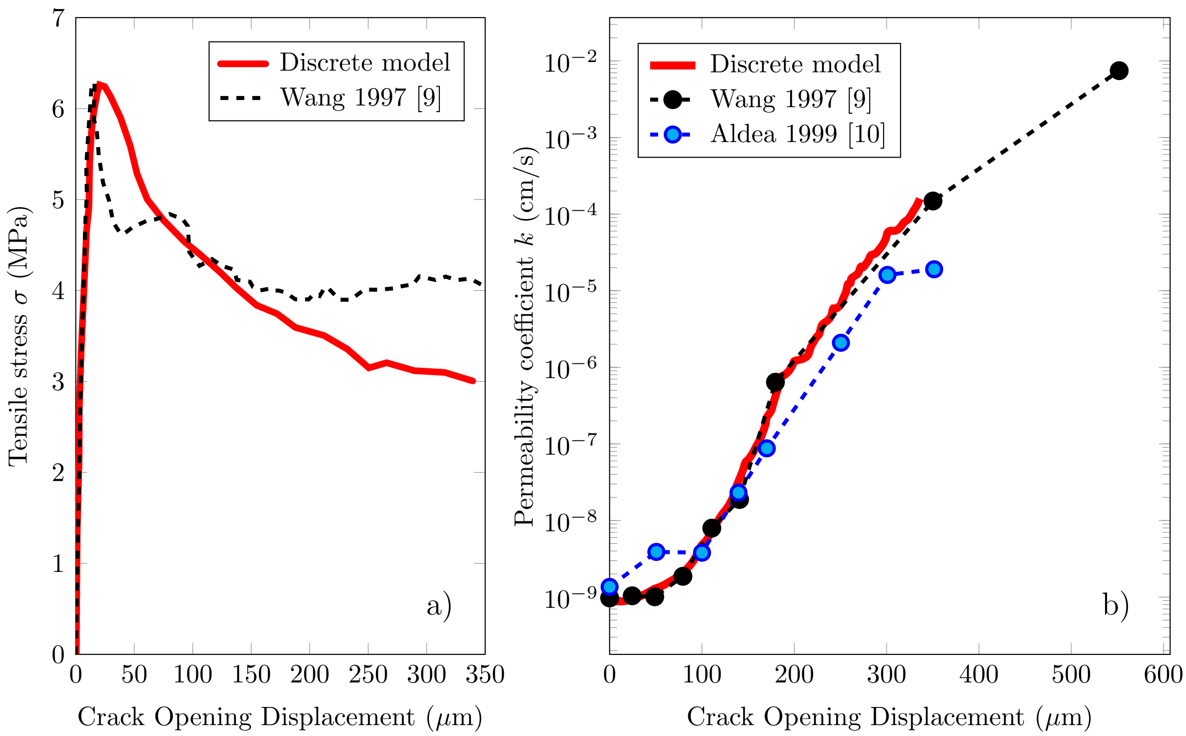

Figure 2: Relationship between crack width, tensile stress and permeability.

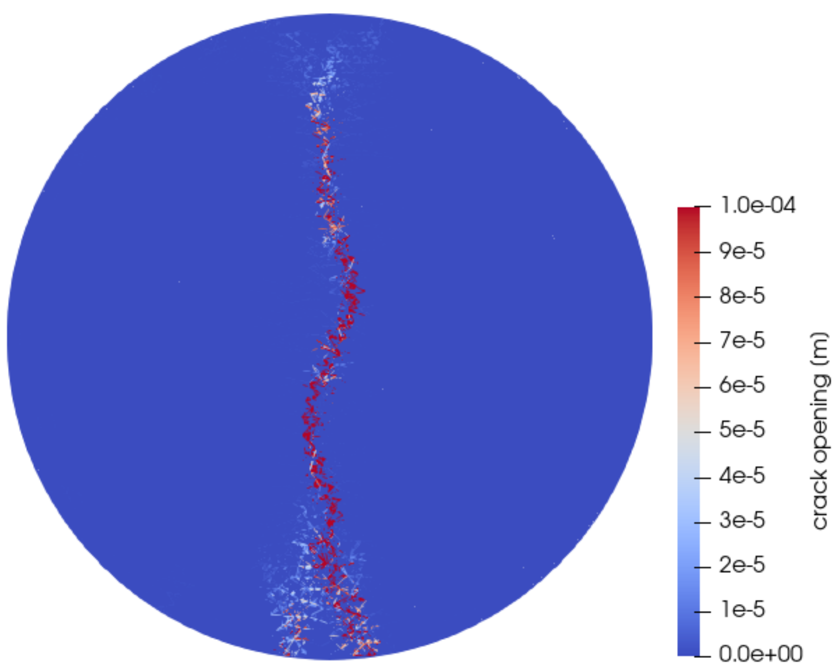

Figure 3: Crack in the discrete model at the final stage of the simulation.

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