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Transport properties of microcracked porous materials: Micromechanics models and mesoscale simulations

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Micro Abstract
In the presentation, using a combination of analytical micromechanics models and direct numerical simulations, the effective diffusivity of microcracked porous REVs for various isotropic and anisotropic microcrack configurations are investigated. Furthermore, the level of applied external loading on the effective diffusivity of a fracturing material is simulated by an element-erosion based mesoscale pixel-FE model for fracture coupled with diffusion using selected numerical experiments.

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Introduction

The degradation of porous materials, namely the reduction of strength and stiffness characterized by distributed microcracking and its influence on the overall transport properties of such materials are of relevance in a number of engineering problems. In concrete structures, the diffusion of water and hazardous ionic substances into the material adversely affect the integrity of the material. In subsurface engineering, the knowledge of the overall transport properties of rocks is required for the design and construction of tunnels, caverns or underground storage systems and for the exploitation of oil, gas and geothermal energy.

1 Characteristics of diffusion in microcracked porous materials

Let Ω_{REV} be the domain of a Representative Elementary Volume (REV) of a microcracked porous material whose characteristic size is much larger that of the microcracks and the pores. Microscopic diffusion in the REV can be described by the FICK'S law as $\mathbf{j}\left(\mathbf{z}\right) = -\mathbf{D}\left(\mathbf{z}\right)\cdot\mathbf{g}\left(\mathbf{z}\right)\ \forall\mathbf{z} \in \Omega_{REV}$. Here, $\mathbf{j}$ and $\mathbf{g}$ are the microscopic flux and the microscopic concentration gradients respectively and $\mathbf{D}(\mathbf{z})$ is the inhomogeneous microscopic diffusivity that is characterized by the microstructure of the microcracked porous material. The corresponding macroscopic flux $\mathbf{J}$ is related to the macroscopic concentration gradient $\mathbf{G}$ as $\mathbf{J} = -\mathbf{D}_{eff}\cdot\mathbf{G}$. Using mean-field homogenization, the macroscopic diffusivity $\mathbf{D}_{eff}$ of a microcracked porous REV idealized as a material with penny-shaped microcracks with diffusivity D_c embedded in a homogeneous material with diffusivity D_{int} (representing the homogenized porous material) has the form $\mathbf{D}_{eff} = \mathbf{f}(D_c, D_{int}, \mathbf{A}_i, \varphi_c, X)$. The tensors $\mathbf{A}_i$ are the so-called localization tensors [2, 4] that can be obtained by solving the classical ESHELBY problem, φ_c is the volume fraction of microcracks and X is the aspect ratio of the microcracks. The function $\mathbf{f}$ is characterized by the homogenization scheme. For porous materials with a high density microcrack morphology, the prediction by the recursive cascade continuum micromechanics model (see [3] for a lattice description of a microcracked porous material) at the self-similar limit is equivalent to the self-consistent solution. For isotropically distributed penny-shaped microcracks of half-length/radius a and half-width w, the model also predicts that the critical microcrack density $N^\star$ at which the distributed microcracks in the material would form a continuous network is [5]:

$$N^\star = \frac{4}{\pi(a^2 + 6aw + w^2)} \tag{1}$$

As one would expect, according to the above equation, longer the microcracks, smaller is the microcrack density required to form a connected microcrack network. The significance of this number can be illustrated using the following computational experiment. Consider the 5 microcracked porous specimens shown in the top row of Fig.1 with microcrack densities of 100, 200, 300, 400 and 500 microcracks of width $2w = 25\mu m$ and length $2a = 1000\mu m$ distributed in a domain of size $1cm \times 1cm$. The matrix material is almost impermeable. This diffusivity is assumed to be 100000 times smaller than that of the diffusivity in the microcracks. The right hand side of the specimens is in contact with a reservoir of a constant concentration of a particular species. The initial concentration of the species in all the specimens is assumed to be zero. Due to the difference in the concentration, the species will diffuse into the microcracked porous specimens. Shown in the lower row of Fig.1 is the depth of ingress of the diffusing species in all the 5 different specimens after a certain period of time. According to the computational simulations, there is a larger depth of ingress of the diffusing species in the specimen with 500 microcracks. This is a consequence of a large flux due to a connected microcrack network that spans the specimen. Here, transport is mainly driven by the microcrack network. For the specimens with 400 microcracks and less, the depth of ingress of the diffusing species is not significant as the overall flux is in comparison small. Even though the microcrack distribution in the specimens with 400 and 500 microcracks looks very similar, only one of them has a connected microcrack network that spans the specimen. If the prediction according to Eq.1 is correct, the value for $N^\star$ must lie between 400 and 500 microcracks. Substituting for $a = 500\mu m$ and $w = 12.5\mu m$ in Eq.1 gives a value of 442 microcracks !

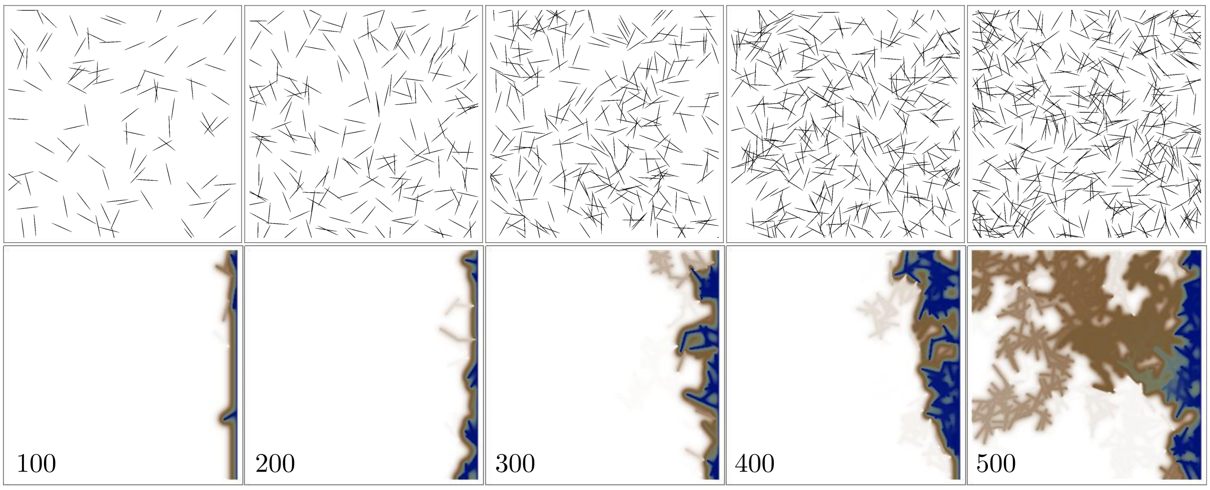

Figure 1. Pixel-FE simulation of diffusion in a porous specimens of size $1cm \times 1cm$ with 100, 200, 300, 400 and 500 microcracks of length $1000\mu m$ and width $25\mu m$. Upper row: morphology of the microcracked material. Lower row: depth of ingress of a diffusing species in all the specimens after a certain period of time

2 Modeling material degradation and its influence on diffusion

In the previous section, the origin of distributed microcracking was not relevant. In this section, we model initiation and evolution of distributed microcracking upto catastrophic failure of the material. We assume that the the definition of strength on the scale of observation. At the microscale, the material is assumed to have a heterogeneous distribution of strength due to the disorder in the material. The consequences of such a description of the strength at the microscale on the overall macroscopic failure of the material can be illustrated using the fiber-bundle analogy [1]. Consider a bundle of fibers assumed to have different breaking thresholds (strengths). This distribution of strengths is described by a probability density function $p(\sigma)$. When this bundle is subjected to an applied stress σ, the *weakest* fibers in the bundle will fail. The stresses released on breakage of these fibers are assumed to be distributed equally among the rest of the intact fibers. However after redistributing the loads, the local fiber stresses increases and thus leads to a cascade of fiber breaking that leads to catastrophic failure of the whole fiber bundle. For a uniform distribution with $p(\sigma) = 1/\sigma_{max}$, the recursion equation for the fraction of intact fibers in the bundle is given by $\phi^{(n+1)} = 1 - \sigma/(\sigma_{max}\phi^{(n)})$ and can be written as a differential equation $\dot{\phi}(t) = 1 - \phi(t) - \sigma/(\sigma_{max}\phi(t))$. This differential equation can be solved for $\phi(t)$ from which, the time to catastrophic failure of the whole bundle t_c can be computed by solving $\phi(t_c) = 0$ for t_c that reads $t_c = 2\left(4\frac{\sigma}{\sigma_{max}} - 1\right)^{-\frac{1}{2}} \tan^{-1}\left[\left(4\frac{\sigma}{\sigma_{max}} - 1\right)^{-\frac{1}{2}}\right]$. This simplified

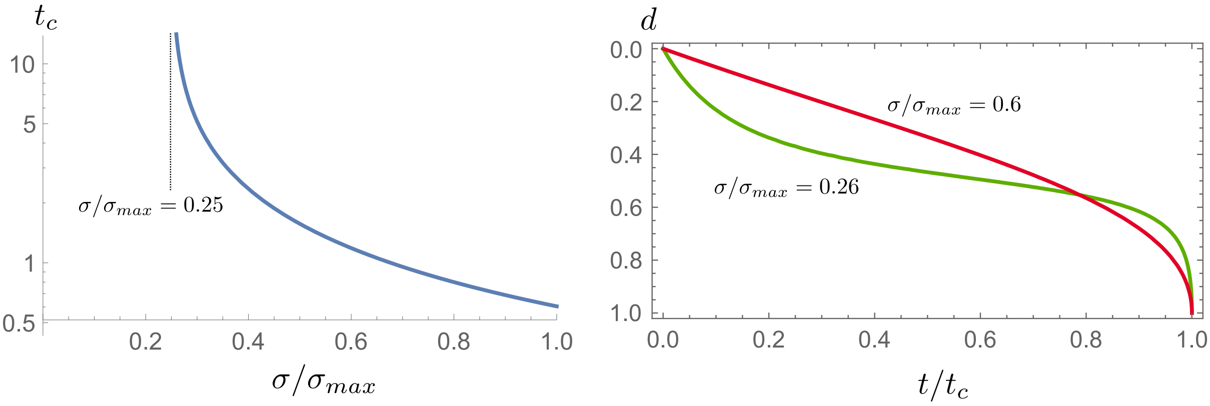

Figure 2. Left: Critical time to failure t_c vs the applied stress level $\frac{\sigma}{\sigma_{max}}$. Right: Evolution of damage d as a function of the normalized time to failure

1D model for characterizing macroscopic damage of a material with a disordered distribution of microscale strengths shows that any stress less than $\frac{1}{4}\sigma_{max}$ will take infinite time to fail (see Fig.2 - left). Fig.2 - right shows the evolution of macroscopic damage $d(t) = 1 - \phi(t)$ for two different applied normalized loads $\sigma/\sigma_{max} = 0.26$ and 0.6, i.e the applied stress is 26% and 60% of the maximum microscale strength. It must be noted that this macroscopic behavior is a characteristic of the material and is described by the microscale strength distribution. In order to estimate the effective transport properties of a cementitious material ($D_{int} = 0.001D_c$) during degradation, the aforementioned mechanics of failure is implemented withing a numerical FE framework in which deterioration is characterized by the erosion of finite elements (represented in terms of pixels) whose stresses are larger than the strength associated with that pixel-finite-element. Fig.3 shows the results of the overall macroscopic mechanical and transport properties of a material with a WEIBULL distribution of strength at the microscale described by $f(\sigma \geq 0; \alpha, \beta) = \frac{\alpha}{\beta}\left(\frac{\sigma}{\beta}\right)^{\alpha-1} e^{-(\sigma/\beta)^{\alpha}}$ with shape parameter α and scale parameter β. The mechanical behavior is shown in terms of the macroscopic strength normalized stress $\overline{\Sigma}$ and strain $\overline{E}$. The material degradation is characterized first by an isotropic distribution of defects and microcracks (the white pixels) (Fig.3 Right (b)) that evolve into microcracks oriented normal to the direction of loading and finally the percolation of microcracks that lead to localization and macroscopic failure.

Conclusions

In this extended abstract, we have investigated the influence of material degradation on diffusion in porous materials. In the first part of the paper, the critical microcrack density for establishing a continuous network of microcracks was characterized using the cascade continuum micromechanics model. Model predictions have been confirmed by explicit Pixel-FE simulations. In the second part of the paper, the mechanics of material degradation in disordered porous materials has been

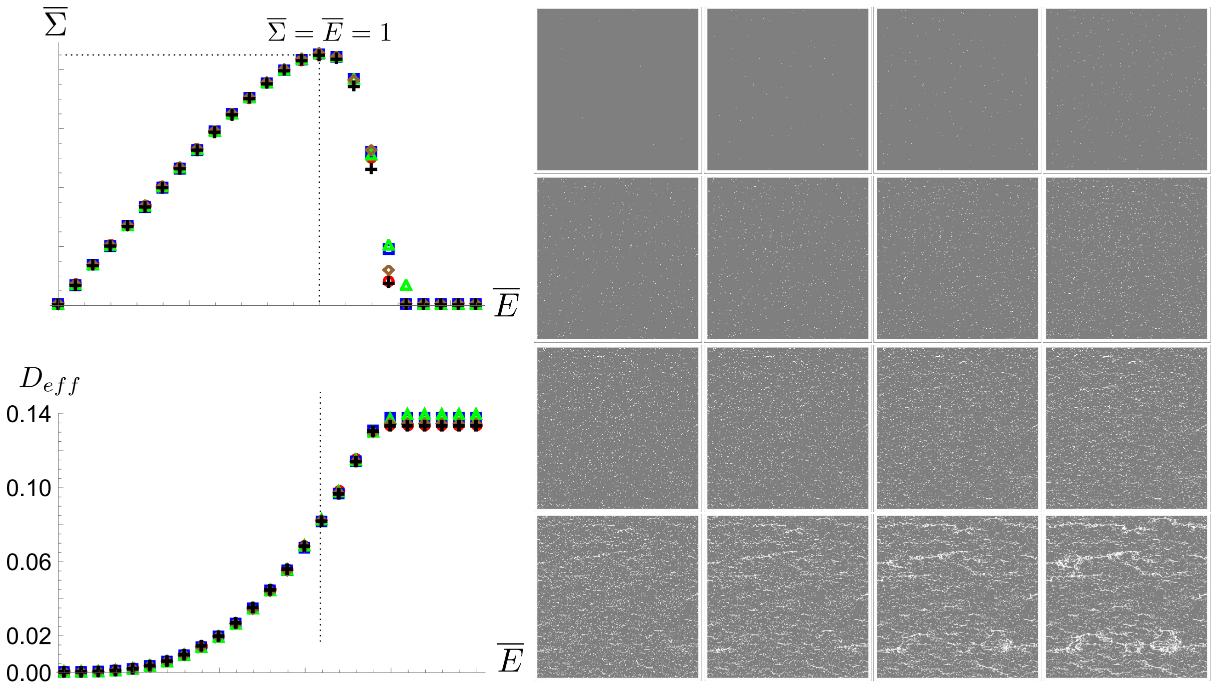

Figure 3. Pixel-Erosion simulation of material degradation and diffusion. Left-top: Macroscopic strength normalized stress vs macroscopic strength normalized strain for a specimen under uniaxial tension. Left - bottom: Evolution of the effective diffusivity of the material during material degradation (the colored symbols correspond to the 5 random realizations). Right: Evolution of microcracking in the specimen subject to tension upto localization.

investigated by characterizing the material at the microscale using a heterogeneous strength distribution. This degradation mechanism and its influence on the overall diffusivity of the material has been simulated using Pixel-FE computations.

Acknowledgments

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