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MODELING ELECTROLYTE DIFFUSION IN CRACKED CEMENTITIOUS MATERIALS USING CASCADE CONTINUUM MICROMECHANICS AND PHASE-FIELD MODELS

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Abstract. Electrolyte transport in fracturing porous materials such as concrete is strongly influenced by the complex and random topological structure of the pore space, the state of distributed micro-cracks inevitably caused by autogenous and drying shrinkage of concrete and finally by propagating cracks caused by various loading conditions. Information on macroscopic diffusion properties of the intact concrete requires up-scaling of transport processes within nano- and micro-pores over several spatial scales. The macroscopic transport coefficients are computed using a cascade continuum micromechanics model. The cascade continuum micromechanics model recursively embeds shape information in the form of the ESHELBY matrix-inclusion problem to obtain the homogenized effective diffusivity as a function of a perturbation index and the porosity. The effects of the micro-structure on the transport properties are characterized by porosity dependent short range and long range inter-phase interactions. To take into consideration the effects of oriented, diffusely distributed micro-cracks on electrolyte diffusion properties, the homogenization scheme for electrolyte diffusion in intact concrete is enhanced by representing micro-cracks as additional ellipsoidal inclusions within the aforementioned homogenized porous matrix. Finally, the effect of propagating macro-cracks on the diffusion process is taken into consideration by weakly coupling the diffusion model and a fracture energy based staggered phase-field model to simulate brittle fracture.

1 INTRODUCTION

Three major topological factors influence transport processes in fracturing cementitious materials: the micro-structure of the pore-space, the effect of diffuse micro-cracks and finally, localized fracture zones. In general, transport properties are accounted for on the macroscopic scale using an equivalent diffusivity that takes into account the aforementioned effects in an averaged sense. However, in such a classical approach, the relation between the microstructure and the observed macroscopic behavior is lost. Considering that the transport mechanisms act at different scales and are of a hierarchical nature clearly warrants a multi-scale approach to model the corresponding effects. Investigations into the diffusivity of porous materials suggests an existence of a percolation threshold and thus a strong influence of the micro-structure on diffusion for porosities up to 60-70 % beyond which the pore space is no more tortuous. In the proposed model, continuum micromechanics is used as the major modeling strategy to account for the tortuosity of the pore-space and the effect of diffuse micro-cracks on the transport behavior of cementitious materials. Classical micromechanics methods for homogenization are not suitable as they either cannot predict a percolation threshold (MORI-TANAKA, Differential, and Dilute) or predict non-physical values for a particular range of porosities (self-consistent) [4]. The above drawbacks of the classical schemes motivates us to rethink the way in which the physics of the problem could be correctly translated into a micro-mechanical model while retaining the simplicity of an analytical model. The cascade model [4] considers the interaction of the micro-structure hierarchically through a cascade of ESHELBY matrix-inclusion problems. The model is characterized by a micro-structure characterizing variable in addition to the porosity to predict the constitutive behavior of the material with regard to transport. This allows for modeling percolation thresholds. Micro-cracks enhance diffusion and thus these effects can be accounted for by embedding ellipsoidal inclusions which represent micro-cracks in the previously homogenized porous material. With regard to macroscopic cracks, brittle fracture is considered as an energy minimization problem [1] wherein the crack surface is approximated by a phase-field [2] which in turn is coupled to the diffusion problem. The phase-field which characterizes the crack path is used to compute the orientation and the micro-crack volume fraction which are functions of the constitutive equation for the diffusion problem.

2 EFFECT OF POROUS MICROSTRUCTURE

Intact porous materials are characterized by an isotropic distribution of pore-channels. The pore-space is characterized by a pore-size distribution and the tortuosity. The tortuosity is a phenomenological artifact which takes into account the effects of constrictivity, the connectivity, and dead end pores on diffusion processes. The microstructure effect is modeled using the cascade continuum micromechanics method. We consider an REV^{uc} which is isotropic w.r.t. the pore-channel distribution. Initially we model a spherical fluid-filled pore embedded in a matrix which has zero microstructure information. This state is characterized by a state variable n. Localization tensors are computed for this matrix-inclusion problem. The obtained homogenized diffusivity is now the new matrix material. The matrix material is updated from the solution of the previous homogenization problem. Thus the interactions of the pores are taken into account hierarchically. This allows us to model percolation thresholds which are micro-structure dependent. An explicit equation for the diffusivity of intact porous materials is finally obtained in terms of the cascade index n and the porosity ϕ. See [3, 4] for details. The model counterpart of the phenomenological tortuosity is the inverse of the localization tensor A_f. The diffusivity of the porous material is given by,

$$D^{uc} = \phi A_f (n) D_f. \qquad (1)$$

3 EFFECT OF MICRO-CRACKS

Mechanical stresses due to external forces or localized chemical reactions such as ASR (Alkali-silica reaction) in concrete give rise to nucleation of micro-cracks. Micro-cracks tend to enhance the connectivity of the pore-space and thus considerably affect the diffusion process. As a result, the enhanced pathways are no longer isotropic, and a suitable model must consider the effect of oriented cracks.

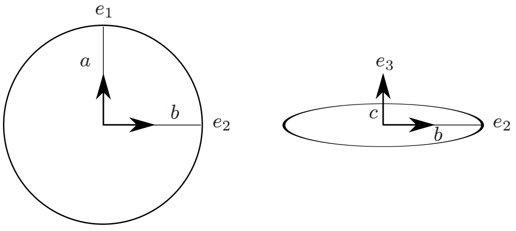

Figure 1: Geometry of an ellipsoidal approximation of a micro-crack

We consider an REV^c with oriented micro-cracks. REV^c is modeled with penny-shaped ellipsoids (see Fig.1) representing micro-cracks embedded in the already homogenized porous matrix as described in the previous section. The homogenized diffusivity thus obtained is anisotropic. The model automatically takes into consideration the effect of the interaction between the surrounding porous matrix and the micro-cracks [3] through an anisotropic interaction tensor $\boldsymbol{\Upsilon}$. In Fig.2, the normalized macroscopic diffusivity is plotted against the micro-crack volume fraction φ_c and the porosity ϕ for the crack aspect ratio 0.001.

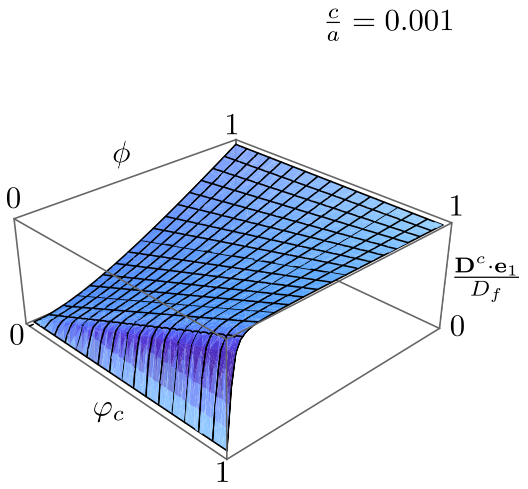

Figure 2: Effect of micro-crack volume fraction on diffusivity for a micro-crack aspect ratio 0.001

4 EFFECT OF A PROPAGATING MACRO-CRACK

Localized cracks have a major influence on the transport properties of structures made of cementitious materials such as concrete, since they provide transport channels with high permeability through the material. With regard to propagating macro-cracks, energy minimization [1] is used to simulate brittle fracture. To regularize the crack surface, a phase field is introduced [2] which in turn is used to compute the vectors parallel to the crack. The intensity of the phase field which varies from 0 for the fully damaged situation and 1 for the intact situation together with the vectors parallel to the crack is used compute the anisotropic diffusivity $\mathbf{D}^c$.

$$\mathbf{D}^c = D_f\left(1 - c_r\left(\mathbf{x}\right)\right)\cdot\boldsymbol{\Upsilon}\left(\nabla c_r\right) + D^{uc}\mathbf{I}. \quad (2)$$

D_f is the diffusivity in the pore solution, c_r is the crack volume fraction field which is obtained by minimizing the following potential:

$$\begin{aligned}\Pi_m &= -\int_\Omega W_\varepsilon\left(\boldsymbol{\varepsilon}\left(\mathbf{x}\right), c_r\left(\mathbf{x}\right)\right)\\ &\quad -\int_\Omega W_{c_r}\left(c_r\left(\mathbf{x}\right)\right). \end{aligned} \quad (3)$$

As proposed in [2], the surface energy is approximated using the field c_r, a regularization length parameter l and the fracture energy $\mathcal{G}_c$ as follows:

$$\int_\Omega W_{c_r} = \int_\Omega \mathcal{G}_c\left(\frac{1}{4l}\left(c_r\left(\mathbf{x}\right) - 1\right)^2 + l\left(\nabla c_r\left(\mathbf{x}\right)\right)^2\right) \quad (4)$$

5 NUMERICAL EXPERIMENT

Consider a L-shaped concrete panel illustrated in Fig.3. It is subject to concentration DIRICHLET boundary conditions which imply a steady state situation. As the crack propagates due to the applied mechanical load, the steady state concentration increases along the crack path (the red, blue and the green curves in Fig.4 correspond to the concentration).

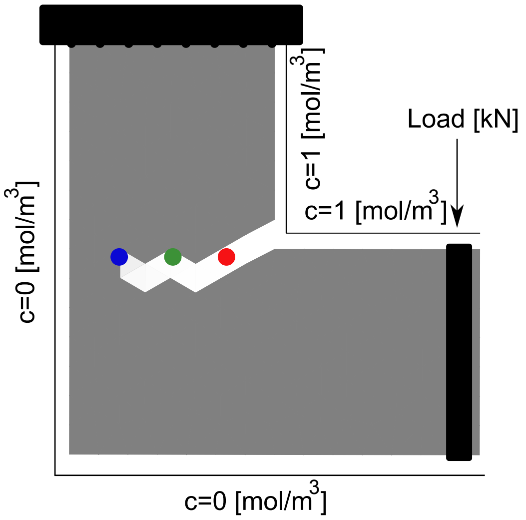

Figure 3: Prescribed concentration boundary conditions on the L-shaped panel

The post peak relaxation of the steady state concentration field in Fig.4 is attributed to the porous material around the macro-crack. After the crack opens, the species diffuses through the walls of the crack to achieve a steady state.

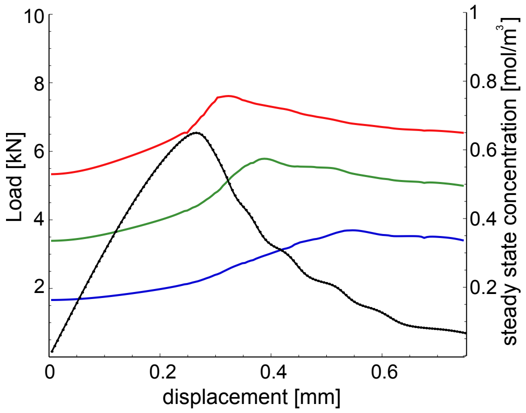

Figure 4: Change in concentration due to a propagating crack

6 CONCLUSIONS

A multiscale model to simulate transport processes in intact and cracked porous materials has been proposed. A novel Cascade Continuum Micromechanics model has been proposed to take into account the effect of the porous micro-structure, incorporating a variable (the cascade index), which directly reflects the degree of tortuosity. This model predicts a threshold value for the porosity below which no transport is possible due to lack of connected micropores. The Cascade continuum micro mechanics model for the intact porous material has been linked to a micromechanics model to incorporate distributed micro-cracks. This combined model is able to consider the interactions between these topological entities with regard to the transport behavior. For the consideration of the effect of propagating localized macro-cracks on transport processes, a phase-field model has been coupled to the homogenized diffusion problem on the continuum level. This crack model correctly predicts the effect of the highly anisotropic character of the diffusivity of porous cementitious materials in the presence of macro-cracks. Nucleation of cracks enhances the transport pathways leading to an increase in the concentration along the crack. The model finds application in prediction and prevention of leakage of nuclear waste materials, corrosion and failure of concrete structures in marine environments etc.

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