A PHASE FIELD MODEL FOR DAMAGE NUCLEATION IN GEOPOLYMER COMPOSITES

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Abstract
The structural integrity of geopolymer composites is analyzed by studying the microscopic cracks nucleating from preexisting pores in the matrix and the effect on their macroscopic fracture toughness using a computational framework of phase field (PF) modeling. To assess the effect of a random distribution of voids, the composite microstructure is modeled using a take and place algorithm and a plate under tension is simulated to study the damage initiation and propagation. The homogenized elastic properties of the composites are determined by Mori-Tanaka and Self-consistent homogenization schemes. The PF model investigates the damage in the composite due to initiation of cracks from the voids.

1. Introduction
The phase field model, built upon Griffith's crack theory, is one of the most accurate techniques to study localized failure and is a promising approach to simulate crack nucleation, onset of crack propagation, complex crack paths arising due to crack branching and interaction among multiple cracks. The present work aims at describing evolution of damage from already existing voids in geopolymer composite microstructure using the phase field approach.

1.1 Phase field fracture model
It is supposed that an arbitrary body $\Omega \subset R^d$ ($d \in \{1,2,3\}$) containing a crack represented by Γ. The crack is represented using a diffusive crack topology in the PF model by the introduction of a scalar viz., the phase field variable $\phi(x,t)$ [1] whose value varies from 0 to 1; 0 for intact domain and 1 for the fully cracked domain in Ω. As per Griffith's thermodynamics, brittle fracture is an energy minimization problem [2] where the total potential energy is the sum of the elastic strain energy density ψ and the fracture energy G_c as:

$$\mathscr{E}(u) = \int_\Omega \psi(\epsilon(u))dV + \int_\Gamma G_c dS \tag{1}$$

where u is the displacement field and $\epsilon = (\nabla u+\nabla u^T)/2$ denote the strain field. The minimization of the above functional gets restricted due to the intricacies related to tracing the fracture propagation surface Γ. This is where the PF variable ϕ comes into use; a degradation function $g(\phi) = (1- \phi^2)$ is used to simulate the reduction of stiffness with damage evolution such that the energy functional (Eq.1) is re-formulated as:

$$\mathscr{E}(u, \phi) = \int_\Omega [(1- \phi^2)\psi(\epsilon(u)) + G_c(\frac{\phi 2}{2l} + \frac{l}{2}|\nabla\phi|^2)]dV \tag{2}$$

where l is a length scale parameter which determines the size of the fracture process zone.

1.2 Overview of the work
A PF model based on the strain decomposition is implemented to study the damage occurring in geopolymer composites. Initially, using mean field homogenization approaches such as Mori-Tanaka (MT) method [4] and Self-consistent (SC) [5] scheme, the overall elastic properties of the composite is determined. A representative volume element (RVE) of composite microstructure containing matrix with randomly distributed of voids is generated by utilizing the take and place algorithm [3]. The RVE of the composite generated is later used to simulate a plate under tension. The phase field damage is executed on the model using the multi-field modeling software COMSOL Multiphysics. The damage nucleation and the path of crack progression from the preexisting pores is studied from the results obtained. The role of pre-defined pores on the crack trajectory is analysed.

2. Results

An RVE of the geopolymer microstructure with matrix and pore phases is generated with a random distribution of voids; the RVE size is determined by performing a trial and error procedure until convergence of the elastic properties is attained. The design mix and the distribution of pores are taken from the literature. The homogenized elastic properties of the RVE obtained as computed using MT and SC methods are given in Table 1. The microstructure generated in MATLAB is exported to COMSOL, meshed using quadrilateral plane strain elements and a vertical displacement is applied on top of the specimen. Figure 1 shows the geometry model of the plate containing randomly distributed pores and the different stages of crack evolution from the pores.

Table 1: Homogenized elastic properties of the geopolymer composite with matrix and pores

MFH Scheme	Young's modulus (GPa)	Poisson's ratio
Mori-Tanaka	6.2808	0.1509
Self-consistent	6.2804	0.1510

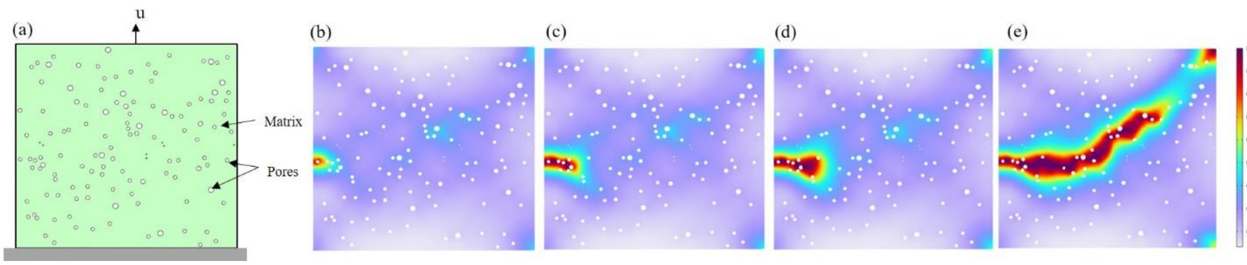

Figure 1: Composite microstructure subjected to tension: (a) Model setup for a plate of geopolymer matrix containing pores (b)-(e) Crack propagation from pores

3. Conclusion

The work focuses on the evolution of damage from randomly distributed defects in geopolymer composite. The effective elastic properties are predicted using MFH schemes. Further, a model of a plate under uniaxial tension is simulated using COMSOL and initiation of fracture from the defects is analyzed. The PF approach to investigate the fracture properties of geopolymer composites as part of their damage modeling is currently in progress.

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