Multiscale Modelling of Transport and Degradation Phenomena in Cement-based Materials

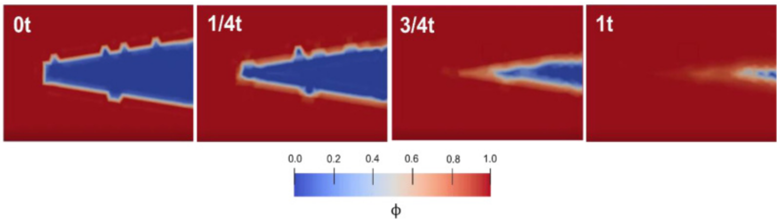

Figure 1: Simulation of a self-healing crack in cement-based material by using phase-field method (ϕ is the phase-field order parameter, where 0 represents a pore, and 1 is solid).

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Project Term
2019 - 2020

Clusters
Lichtenberg Cluster Darmstadt

Additional Software
MOOSEframework

Institute
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Introduction

This project aims to investigate the autogenous self-healing process of small cracks in concrete using the phase-field method in order to extend the service life of concrete, improve the durability of concrete, and improve the economic benefits of constructions.

Methods

The dissolution process of calcium hydroxide into solution and the precipitation process of calcium carbonate are controlled by a solute concentration field that is continuous at solid-liquid interface. Then, a model is developed by incorporating the chemical reaction kinetics, diffusion and thermodynamics, and numerically implemented by the finite element method (FEM) within the MOOSE framework. We further investigate the microscopic crack morphology by performing multiple simulations with the parameter informed from the experimental tests.
By using this method, the concrete healing interface can be easily tracked, and the geometry of the interface can be accurately described. This has important guiding significance for the implementation and optimization of self-healing technology in practice.
There are already several modelling approaches available for simulating the self-healing behaviour of concrete, but only a few models simulate the evolution of self-healing products from the perspective of the prevailing reaction mechanisms, thermodynamics and chemical kinetics. The phase field method has been applied to various phenomena in materials research, such as, solidification, solid-state phase transformation, recrystallization, grain growth, and fracture. The classical phase-field method is formulated based on the theory of thermodynamics and can be employed to solve morphological evolution processes, which are rather difficult to achieve through traditional sharp interface models. It is worth noting that, solidification and precipitation processes are quite similar to

many solute-solvent systems, like self-healing process in cement based composites actually are. There are various studies on self-healing mechanisms and microstructure evolution, which provide an overview of the use of phase-field methods.

Results

Concrete itself has an effective self-healing potential. In addition, the repaired concrete was subjected to bending and tensile tests and found that the strength of these concrete specimens had the same good strength as the original test block and even higher strength than before. And the ductility of concrete materials has also been greatly improved. The main component of the healing product is calcium carbonate. It can be found through the simulation that the growth of calcium carbonate grains on the fracture surface is an important factor to promote the healing of the fracture.
By using the chemical free energies and thermodynamic database, the space-time distribution of phase parameters and the ions can be accurately determined. Furthermore, the numerical results of the validation simulations are in very good agreement with the experimental data.

Discussion

The phase-field method is a powerful tool to simulate microscale material behaviour. As a connection between the calculation of chemical reactions, in which among others the free energies and surface energies are taken into account, and the macroscopic behaviour this method can give important conclusion about the material capabilities.
The important step of using the phase-field method to simulate the self-healing process in concrete is the determination of parameters. All parameters should have a clear physical meaning in the phase-field method. The phase mobility indicates the speed of the interface movement, which can be accurately obtained through the formula proposed in this project. Under the condition of the finite interface thickness, the phase-field results showed very good agreement with the analytical solution.

Outlook

In future research, the diffusion coefficient of ions in capillary pores will be considered in the model. Many factors can be affect it, such as the age of the concrete, the curvature of the capillary pores, the thickness of the healing products on the crack surface, etc. The interaction between these parameters will be discussed in the next step.

Reference

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Last Update: 2022-11-30 16:45