Microscale Lattice Discrete Particle Model for chemo-mechanical behavior

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Abstract:
Predicting the linear and nonlinear mechanical behavior of cementitious materials from early age can be a very delicate task, as a multitude of phenomena occur at the same time. To tackle this problem, accurate computational micro-scale modeling of cementitious materials microstructure that can encompass chemical and mechanical properties evolution is indispensable in order to obtain realistic and predictable material behavior over the long term.

This research presents a new model called μ-LDPM which makes use of the advantages of two state-of-the-art models used in modeling the behavior of cementitious materials at the microscale. Microscale chemical reactions will be modeled by using μic[1], which is a vector-based model that simulates the formation of reaction products around idealized spherical particles. The model is theoretically resolution-free, and is very versatile as it allows for defining a variety of: materials (reactive and inert), reaction rules, and particle compositions. Microstructural elastic and damage behavior is modeled by a variant of the Lattice Discrete Particle Model (LDPM)[2] known for its wide successes in modeling cementitious materials failure under multidirectional stress states and various loading and ambient conditions. μ-LDPM explicitly models cementitious material particles mechanical interaction using discrete mechanics like LDPM and updates their inter-particle constitutive laws based on chemical reactions evolution from μic. In this formulation, damage is postulated to occur only within the void space between the particles. This represents the microstructure with much less Degrees of Freedom (only 6 DOF at the particles centroids) as opposed to all currently available FE-based models and Lattice-based models which have to subdivide the cement core to very small elements to represent the microstructure reasonably.

To calibrate the model, the hydration process is calibrated by comparing different phase contents with data from literature, while the results from nano-indentation tests provide the averaged mechanical properties of each phase. The elastic analysis of the model is validated by comparing simulation results with multiple experimental datasets with various curing times and water-to-cement ratios. The model damage parameters are then calibrated and validated through simulating uniaxial compression, wedge splitting and cantilever beam tests. The presented results demonstrate that μ-LDPM can replicate the mechanical performance of cementitious materials at the micro scale with high efficiency and accuracy.

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[1] Bishnoi, S., & Scrivener, K. L. (2009). μic: A new platform for modelling the hydration of cements. Cement and concrete research, 39(4), 266-274.
[2] Cusatis, G., Pelessone, D., & Mencarelli, A. (2011). Lattice discrete particle model (LDPM) for failure behavior of concrete. I: Theory. Cement and Concrete Composites, 33(9), 881-890.