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Chemo-Hydro-Mechanical variational phase-field fracture model in cementitious systems

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We present a fully coupled chemo-hydro-mechanical variational phase field model for simulating fracture initiation and propagation, including chemical reactions in cementitious systems. In a staggered approach, we coupled three subprocesses: (i) fluid flow in porous media, (ii) reactive transport, and (iii) mechanical deformation of fractured porous media using the variational phase field.

We use the geochemical package PHREEQC [1] coupled in an operator-splitting approach with a finite element transport solver to calculate chemical reactions in thermodynamic equilibrium (dissolution or precipitation) while taking into account changes in porosity. We couple mechanical deformation and fluid flow using the fixed-stress splitting approach. For chemical damage, we introduce a variable to a constitutive relation that represents a degree of chemical damage ranging from zero (intact) to one (damaged material). The chemical damage variable represents changes in porosity caused by chemical reactions independently from the phase field variable that represents the mechanical damage [2]. Additionally, as effective diffusion and hydraulic conductivity increase in the presence of fracture and changes in porosity, phase field variable, and chemical damage should impact the hydraulic conductivity [3] and the diffusion coefficient [2, 4, 5].

We conducted different benchmarks to demonstrate the model's capabilities and properties to capture the fracture initiation and propagation due to chemical reactions. The proposed model was implemented in the open-source finite element framework OpenGeoSys [6, 7]. The research work has been conducted in the frame of the EURAD project (in particular in the WP MAGIC).

Participation

In-Person

References

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