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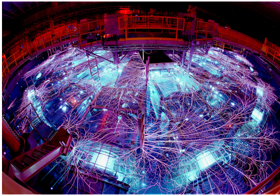

Modeling of concrete degradation with peridynamics

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U.S. DEPARTMENT OF ENERGY

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Outline

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Motivation

- Ordinary Portland cement is commonly a primary component in infrastructure such as buildings, bridges, and dams.

- Environmental conditions such as exposure to water can weaken concrete structures.

- A model that couples chemistry and fracture is crucial for safe infrastructure design as well as for ensuring long-term reliability.

Background

- The mechanisms of cement degradation are complex.
- We focus on one aspect of cement degradation: decalcification due to Portlandite dissolution.
- Decalcification degrades the mechanical properties of the cement.
- In this presentation we explore a chemo-mechanical model employing the peridynamics framework to describe cement degradation and fracture.
- We adopt a minimally complex model in two dimensions to facilitate uncertainty quantification.

Model

Five fundamental aspects of degradation in ordinary Portland cement included in the model are

1. Softening: decrease of elastic modulus E.
2. Weakening: decrease of fracture toughness K_{Ic} and compressive strength σ_c.
3. Shrinking: decrease of stress-free reference volume α.
4. Increased permeability/diffusivity D of water.
5. Increased cement-water reactivity K.

Model (mechanical)

The mechanics portion of our model is an adaptation of the well-known prototype microelastic brittle model:

$$0 = \int_{\mathcal{H}_{\mathbf{x}}} k\, s(\boldsymbol{\xi}, \boldsymbol{\eta}) \mu(t, \boldsymbol{\xi}) \frac{\boldsymbol{\eta} + \boldsymbol{\xi}}{\|\boldsymbol{\eta} + \boldsymbol{\xi}\|} d\mathbf{x}' + \mathbf{b}(\mathbf{x}, t), \qquad (1)$$

where k is the bond stiffness constant, $\mathbf{x}$ is a material point, $\mathbf{u}$ is the displacement field, $\boldsymbol{\xi} = \mathbf{x}' - \mathbf{x}$, $\boldsymbol{\eta} = \mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t)$, $\mathcal{H}_{\mathbf{x}}$ is the neighborhood of $\mathbf{x}$, $\mathbf{b}$ describes the body forces, α is a shrinkage parameter,

$$s(\boldsymbol{\xi}, \boldsymbol{\eta}) = \frac{\|\boldsymbol{\eta} + \boldsymbol{\xi}\| - (1 + \alpha)\|\boldsymbol{\xi}\|}{(1 + \alpha)\|\boldsymbol{\xi}\|}, \qquad (2)$$

and

$$\mu(t, \boldsymbol{\xi}) = \begin{cases} 1, & s_{\text{min}} < s(t', \boldsymbol{\xi}) < s_{\text{max}} \quad \text{for all} \quad 0 \leqslant t' \leqslant t, \\ 0, & \text{otherwise} \end{cases} \qquad (3)$$

Model (chemistry)

We employ a non-dimensional degradation parameter $\underline{c}$ correlated with the C/S ratio such that $\underline{c} = 1$ in pristine material and $\underline{c} = 0$ in fully degraded material. This parameter is described by

$$\dot{\underline{c}} = -Kv(c)\underline{c}, \tag{4}$$

where c is the concentration, v is a step function, and K is the reaction rate. The concentration is described through a nonlocal transport model:

$$\dot{c}(\mathbf{x}, t) = \int_{\Omega} \kappa \frac{c(\mathbf{x}, t) - c(\mathbf{x}', t)}{\|\xi\|} d\mathbf{x}', \tag{5}$$

where κ is a bond diffusion parameter.

Chemical degradation of parameters

We adopt a linear model for the degradation of the parameters:

Mechanical model parameters:

$$k = \bar{k} + \Delta k(1 - \underline{c}) \qquad \text{(bond stiffness)}$$

$$s_{\text{min}} = \bar{s}_{\text{min}} + \Delta s_{\text{min}}(1 - \underline{c}) \qquad \text{(crit stretch lower bound)}$$

$$s_{\text{max}} = \bar{s}_{\text{max}} + \Delta s_{\text{max}}(1 - \underline{c}) \qquad \text{(crit stretch upper bound)}$$

$$\alpha = \Delta \alpha(1 - \underline{c}) \qquad \text{(shrinkage parameter)}$$

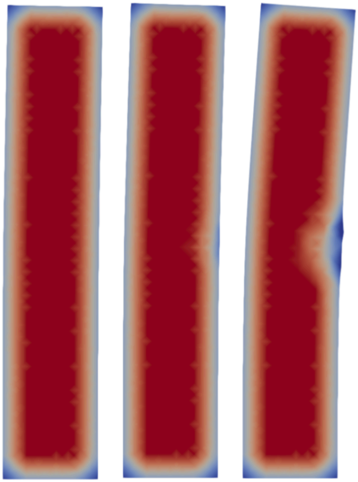
Transport model parameters:

$$\kappa = \bar{\kappa} + \Delta \kappa(1 - \underline{c}) \qquad \text{(bond diffusion)}$$

$$K = \bar{K} + \Delta K(1 - \underline{c}) \qquad \text{(reaction rate)}$$

Simplified simulation of a bridge support

- A veritical 4 cm $\times$ 24 cm simply supported beam under static load that pre-compresses the beam to 10% of failure at nominal strain.
- The beam starts to buckle due to chemical attack at a point midway up on the right side due to a localized water source modeling a permeable flaw in the surface.
- The support is colored by the damage field.



Sensitivities

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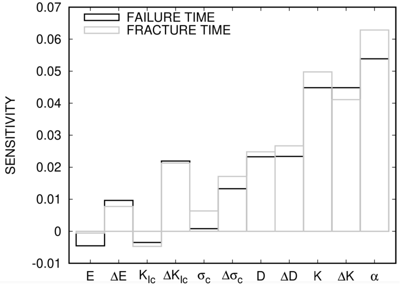
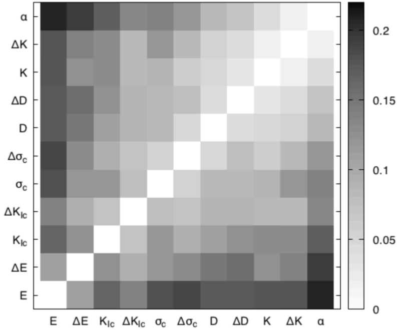
- We investigated first and second order Sobol sensitivities.
- Performed 240,000 independent simulations sampling uniform distributions for each parameter.
- Chemical and transport parameters were generally more influential than the mechanical parameters.



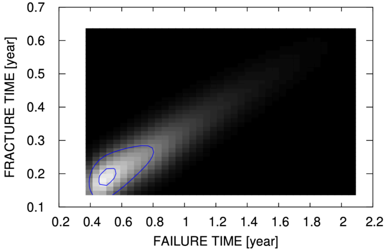
First order sensitivities



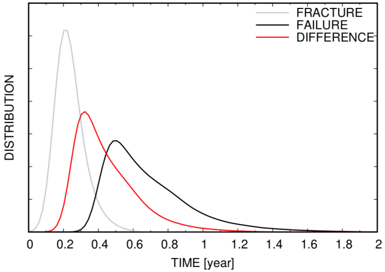
Second order sensitivities

Uncertainty Quantification

- Performed 20,000 independent simulations drawing parameter values using Latin hypercube sampling.
- The joint distribution indicates the time-to-fracture and time-to-failure are strongly correlated and that there is significant variance in the outcomes.
- The marginal distributions resemble log-normal distributions and shows a steep onset for both the time-to-fracture and the time-to-failure, and particularly long tail to time-to-failure distribution.



Joint Distribution



Marginal Distribution

Future Work

- Implement a three-dimensional degradation model into the open-source software Peridigm.
- Implement an aggregate model for degradation.
- Extend the model to the multiple reactions that describe complete degradation.
- Model validations with truly long term “natural” experiments.

Conclusions and Acknowledgments

Conclusions

- Developed a peridynamic chemo-mechanical model of the main phenomenological effects of water induced degradation of ordinary Portland cement.
- Calibrated the model to experimental data from the initial state of cement degradation, dissolution of Portlandite.
- Conducted sensitivity analysis and uncertainty quantification with eleven distinct parameters and their cross terms.

Acknowledgments

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