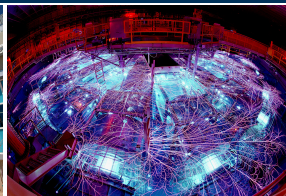


*Exceptional service in the national interest*



Sandia  
National  
Laboratories



# A Peridynamic Model of Degradation in Concrete

USNCCM 2021

Presenter: Jeremy Trageser

Collaborators: Reese Jones, Jessica Rimsza, Joshua Hogancamp



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND NO. SAND

# Outline

1. Motivation
2. Background
3. Model
4. Sensitivity analysis and uncertainty quantification
5. Future work
6. Conclusions and Acknowledgments



# 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.



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  $\sigma_c$ .
3. Shrinking: decrease of stress-free reference volume  $\alpha$ .
4. Increased permeability/diffusivity  $D$  of water.
5. Increased cement-water reactivity  $K$ .

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

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

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,  $\alpha$  is a shrinkage parameter,

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

and

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

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

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

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

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

where  $\kappa$  is a bond diffusion parameter.

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

## Mechanical model parameters:

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

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

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

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

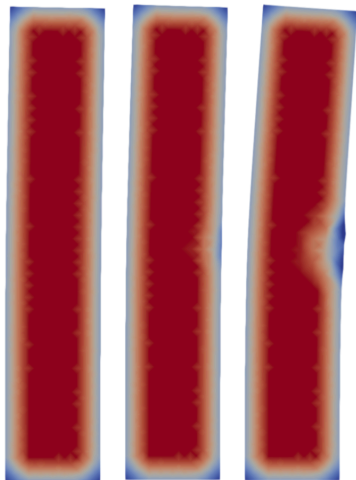
## Transport model parameters:

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

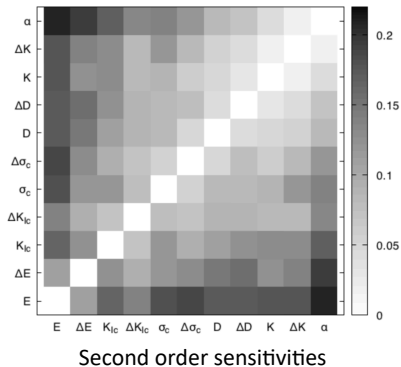
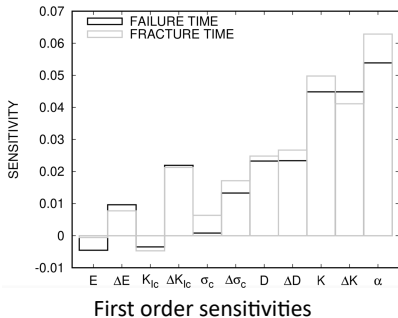
$$K = \bar{K} + \Delta K(1 - \underline{c}) \quad (\text{reaction rate})$$

# Simplified simulation of a bridge support

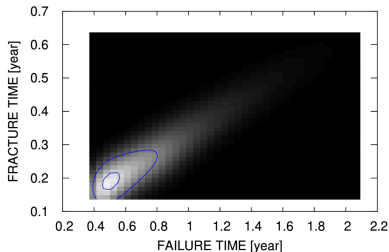
- A vertical 4 cm  $\times$  24 cm simply supported beam under static load that pre-compresses the beam to 10% of failure at nominal strain.
- The beam starts to buckle due to chemical attack at a point midway up on the right side due to a localized water source modeling a permeable flaw in the surface.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



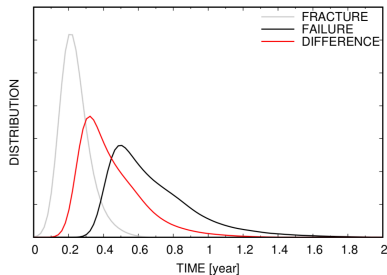
- We investigated first and second order Sobol sensitivities.
- Performed 240,000 independent simulations sampling uniform distributions for each parameter.
- Chemical and transport parameters were generally more influential than the mechanical parameters.



- 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

- 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

- 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

This work was fully supported by the Laboratory Directed Research and Development program of Sandia National Laboratories under Project 213007.