Coupled Mechanical-Reactive Transport Modeling of Damage of Cementitious Materials due to Accelerated Decalcification

SCHOOL OF ENGINEERING

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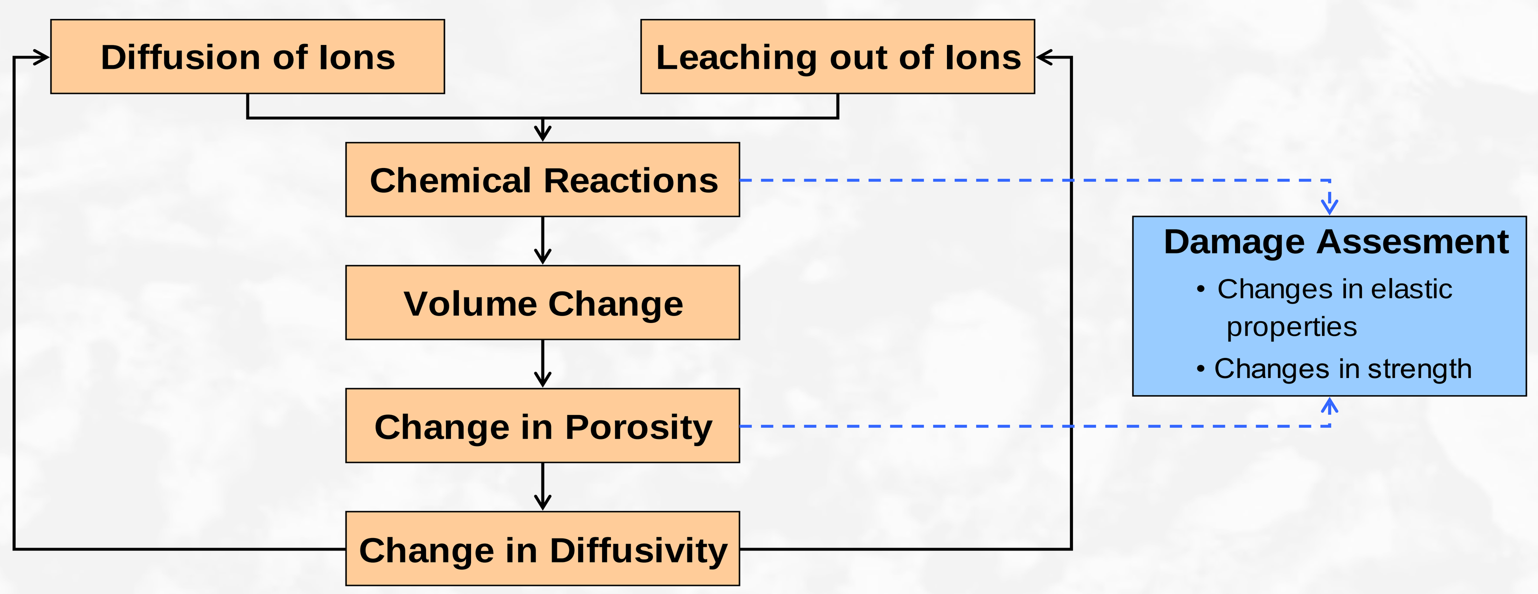
I. Motivation

- Cement-based materials are subjected to a variety of environmental weathering forces that cause internal chemical changes which result in an increase in localized stresses and a decrease in the mechanical properties
- Thorough understanding of the impact of degradation on the service life of cementitious materials is needed in order to design more sustainable structures
- Lab degradation tests can be lengthy in time and require a large number of samples, therefore a model which can couple the chemo-mechanical processes of cementitious materials exposed to aggressive environments is needed

II. Objectives

- Develop a numerical simulation framework capable of coupling the chemical reactions due to exposure to aggressive environments with changes in the mechanical properties of the material
- Simulate the influence of accelerated decalcification on the physical and mechanical properties of a Portland cement paste

III. Modeling Framework



- **Mineral Set Initialization**
  - Use of geochemical speciation code and pH dependent test data to generate a typical mineral set for a Type I/II Portland cement

III. Modeling Framework, cont'd.

- **Diffusion of Ions**
  - Use of diffusion equation in saturated porous media under isothermal conditions

$$\frac{\partial(\varphi c)}{\partial t} = div\left[\frac{D^0\varphi}{\tau\left(grad(c)\right)}\right]$$

c = concentration of an ion
D^0 = free solution diffusivity of an ion
φ = porosity
τ = tortuosity

- **Chemical Reactions**
  - Use of ORCHESTRA, a geochemical speciation and transport code, to calculate the equilibrium phases of the major material constituents
- **Changes in Porosity**
  - Use of changes in volume relationship to account for solid phase dissolution/precipitation in the matrix pores

$$\varphi = \varphi_0 - \frac{\Delta V_S}{V}$$

φ = current porosity
φ_0 = initial porosity
V = volume of the representative volume element
ΔV_S = change in the solid volume

- **Changes in Diffusivity**
  - Use of Sampson and Marchand's porosity/volume relationship[1] to account for changes in porosity

$$D = D^0 \frac{e^{\frac{4.3\varphi}{V_p}}}{e^{\frac{4.3\varphi_0}{V_p}}}$$

V_p = volume of the paste

- **Damage Assessment**
  - Determine homogenized stiffness matrix (elastic moduli)
    - Four homogenization stages
      - **Stage I:** C-S-H
      - **Stage II:** cement paste (homogenized C-S-H from Stage I, Portlandite, ettringite, gypsum, etc.)
      - **Stage III:** cement mortar (sand particles/capillary pores in a homogenized cement paste from Stage II)
      - **Stage IV:** concrete (coarse aggregate in a homogenized cement mortar from stage III)
    - Two homogenization schemes
      - Self-consistent approach (Stages I and II)
      - Mori-Tanaka approach (Stages III and IV)
  - Determine homogenized Young's modulus

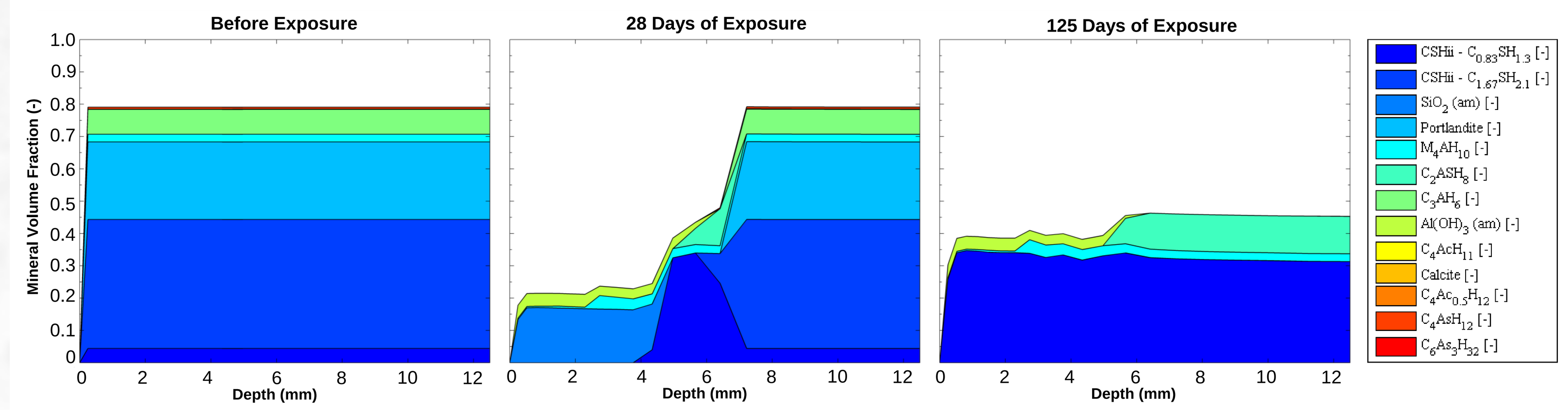
$$\bar{E} = \frac{9\bar{k}\bar{\mu}}{3\bar{k}+\bar{\mu}}$$

$\bar{k}$ = bulk modulus
$\bar{\mu}$ = shear modulus

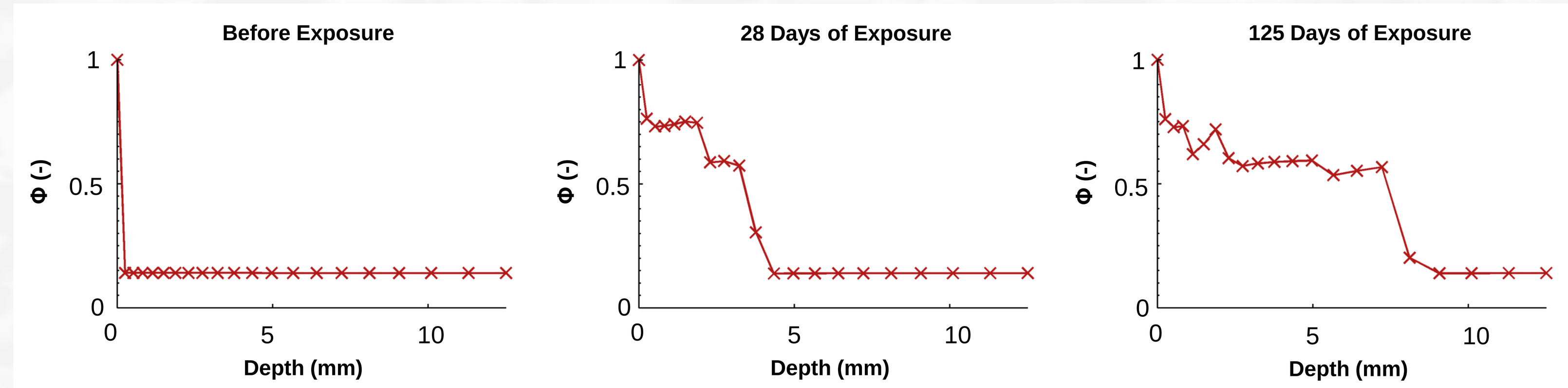
[1] Samson, E. and Marchand, J. Modeling the transport of ions in unsaturated cement-based materials. Computers & Structures, 2007. **85**(23-24). p. 1740-1756.

IV. Results

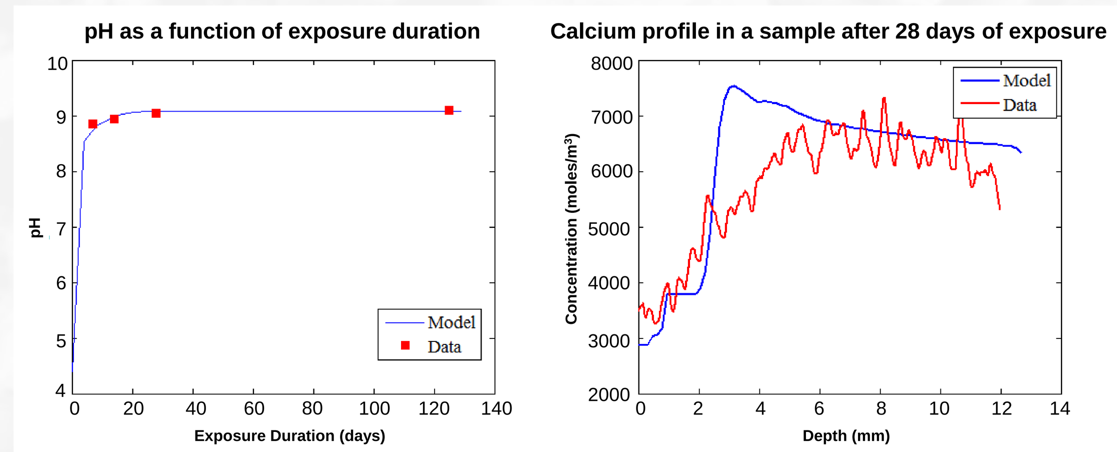
- **Case Study**
  - Portland cement paste (Type I/II)
  - Prismatic samples exposed to 6M ammonium nitrate solution for 7, 14, 28, and 125 days
  - For simulations, prismatic sample idealized as an 80 element one-dimensional structure
- **Mineral Volume Fractions**



- **Porosity**



- **Comparison with Experimental Data**



V. Future Modifications

- **Modifications to Accommodate Inclusions**
  - Dual regime model
    - Diffusion through immobile zone
    - Advection through mobile zone
    - Exchange between zones through diffusion