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Modeling of Soil Carbonation for sustainable soil subgrade stabilization.

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Motivation

- Collapse in subgrade soils due to Freeze-Thaw.
- Conventional stabilizing agents have a large carbon footprint (approximately 1 ton of carbon dioxide (CO_2) gas per ton of cement (UNEP-GEAS, 2010) or lime (Stork et al., 2014) production.
- One solution to increase strength and stiffness while reducing net CO_2 emissions is using carbonate binders, which consume CO_2 through carbonation.

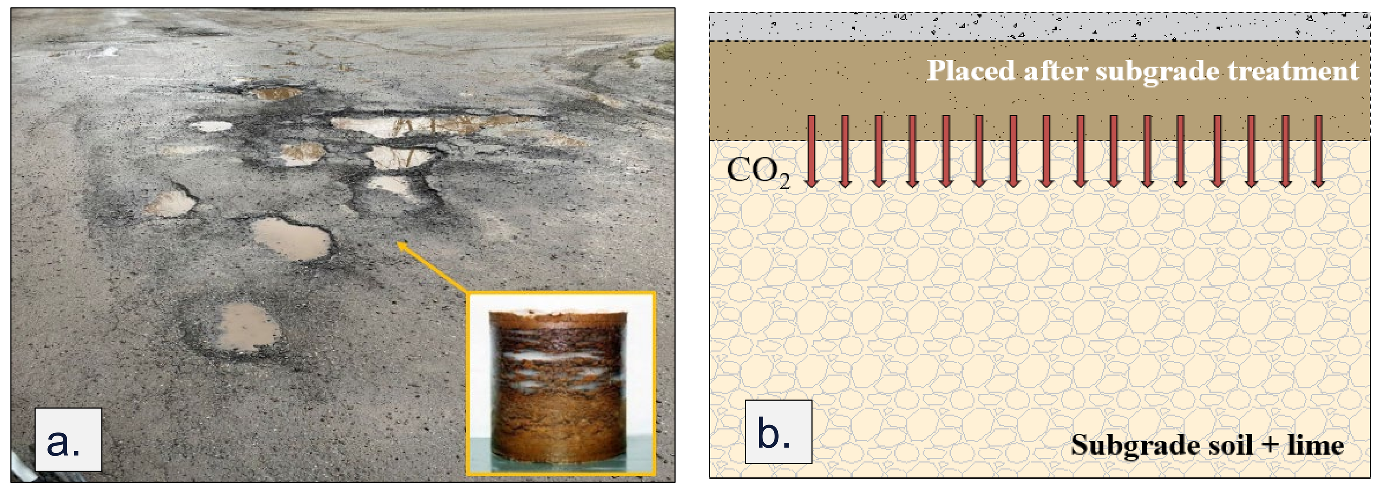

Fig. 1). a. Pavement damage due to soil frosting.
b. Potential solution with Soil Carbonation

How does it work?

- The CO_2 reacts with the lime (at controlled saturation conditions)
- This reaction creates stable carbonate minerals (binder) that attach the particles.
- Increase in the strength and stiffness of soil

$$\underbrace{Ca(OH)_2}_{\text{Lime}} + \underbrace{H_2O}_{\text{Water}} + \underbrace{CO_2}_{\text{Carbon dioxide}} \xrightarrow{\text{Heat}} \underbrace{CaCO_3}_{\text{Binder}} + 2H_2O$$

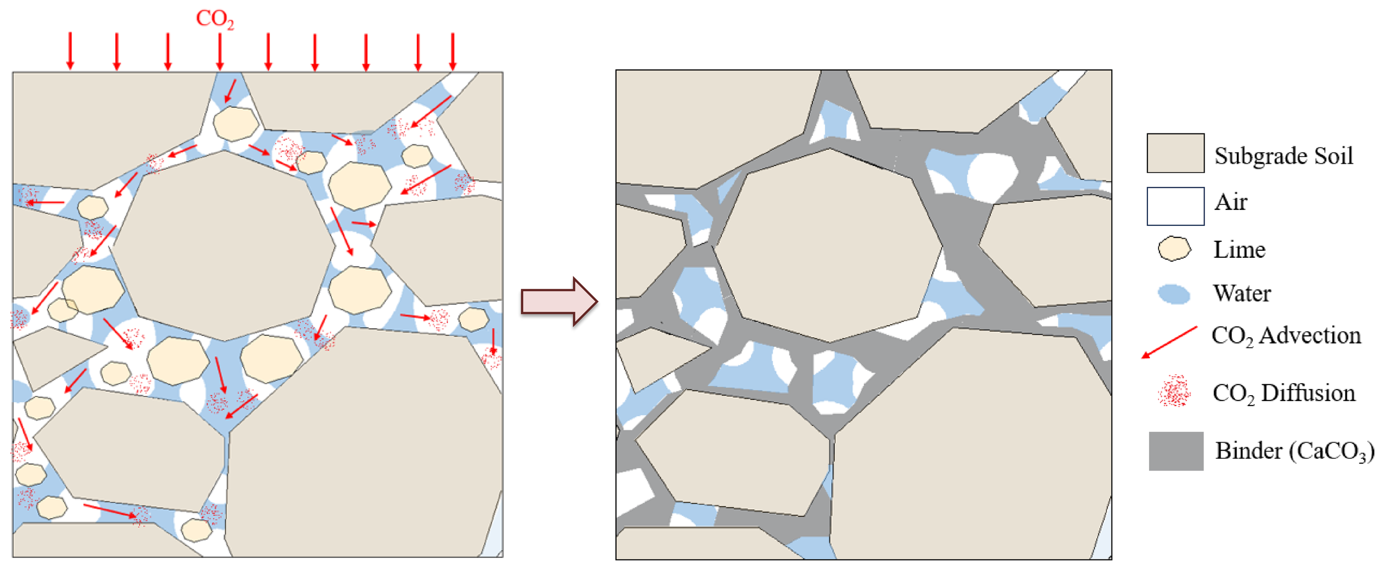

Fig. 2). Microstructure of the soil fabric during carbonation

Modeling Soil Carbonation

Step 1. Gas Transport in Porous Media (No reaction included)
Discretization using Finite Element Analysis (FEA) for multigas transport was done using Mass Conservation combined with Darcy's and Fick's law for advective and diffusive flow, respectively.

$$\underbrace{\mathbf{M}\left[\frac{\partial(\theta \vec{c^i})_k}{\partial t}\right]}_{\text{Change in Concentration}} = \underbrace{-\mathbf{K}^i_{ad}\left(\sum_{j=1}^{N} \vec{c^j_k}\right)}_{\text{Flow Advection}} \underbrace{-\mathbf{K}_{diff}\left(\sum_{j=1}^{N} D_{ij}\vec{c^j_k}\right)}_{\text{Flow Diffusion}} + \underbrace{\vec{q}}_{\text{Output/Input Flow}}$$

Model Validation: from Ogata and Banks (1961) analytical solutions

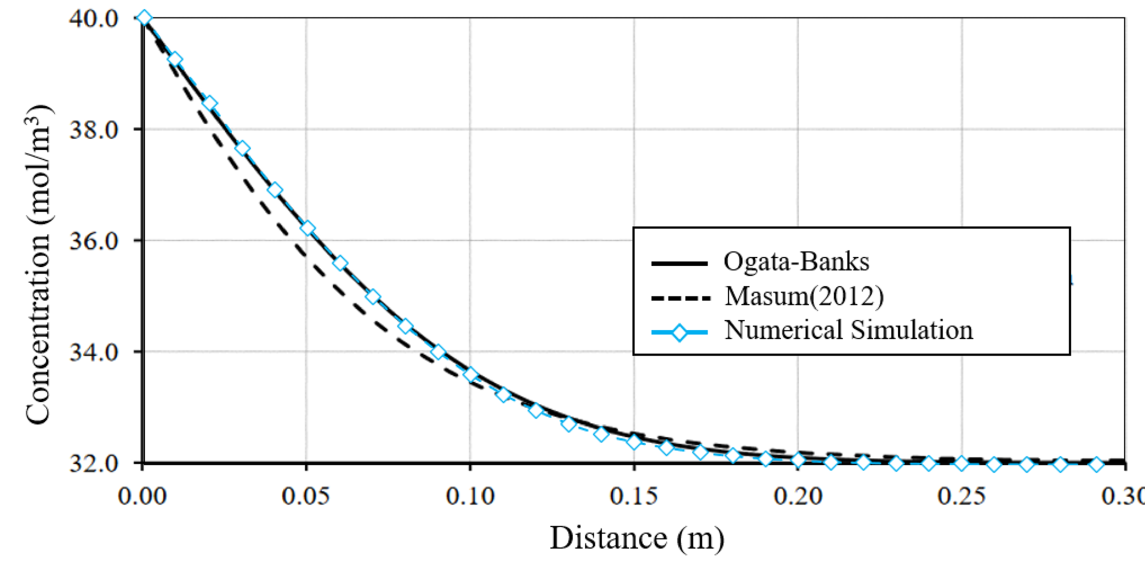

Fig 3). Comparison between Ogata-Banks(1961) analytical solution, Mason' (2012) numerical model, and the current numerical simulation for an advection-diffusion problem

Step 2. Including Carbonation Reaction :
Carbonation: Represents the consumption of CO_2 in the system because of the production of CaCO3 (Binder)

$$\mathbf{M}\left[\frac{\partial(\theta \vec{c^i})_k}{\partial t} + \underbrace{\frac{\partial(\theta_g \vec{S^i_g})_k}{\partial t}}_{\text{Carbonation / (Sink term)}}\right] = -\mathbf{K}^i_{ad}\left(\sum_{j=1}^{N} \vec{c^j_k}\right) - \mathbf{K}_{diff}\left(\sum_{j=1}^{N} D_{ij}\vec{c^j_k}\right) + \vec{q}$$

The rate of $CaCO_3$ production from the reaction of CO_2 with $Ca(OH)_2$ is based on Papadakis et al., 1991:

$$S_{CaCO_3} = \underbrace{K_i}_{[m^3/g*s]} \times \underbrace{[Ca(OH)_2]}_{[g/m^3]} \times \underbrace{[\theta_w]}_{[-]} \times \underbrace{[CO_2]}_{[g/m^3]}$$

K_i: Coefficient of the carbonation reaction; θ_w: Volumetric water content [-]

FEM features / preliminary results

GiD → MATLAB → ParaView

Geometry/mesh/ boundary conditions	Executes source code	Visualization

Simulation of a one-dimensional carbonation test:

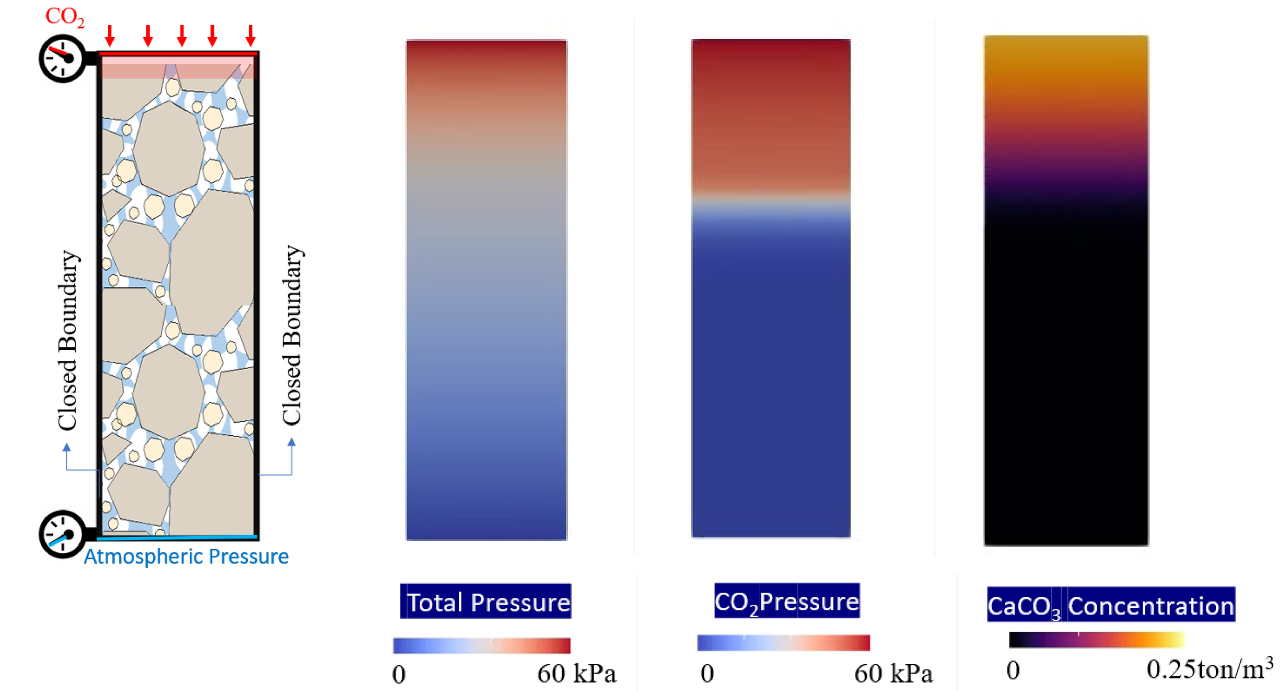

Fig 4). One-dimensional carbonation simulation

Laboratory work for calibration

Need to calibrate K_i (Coefficient of the carbonation) from laboratory results

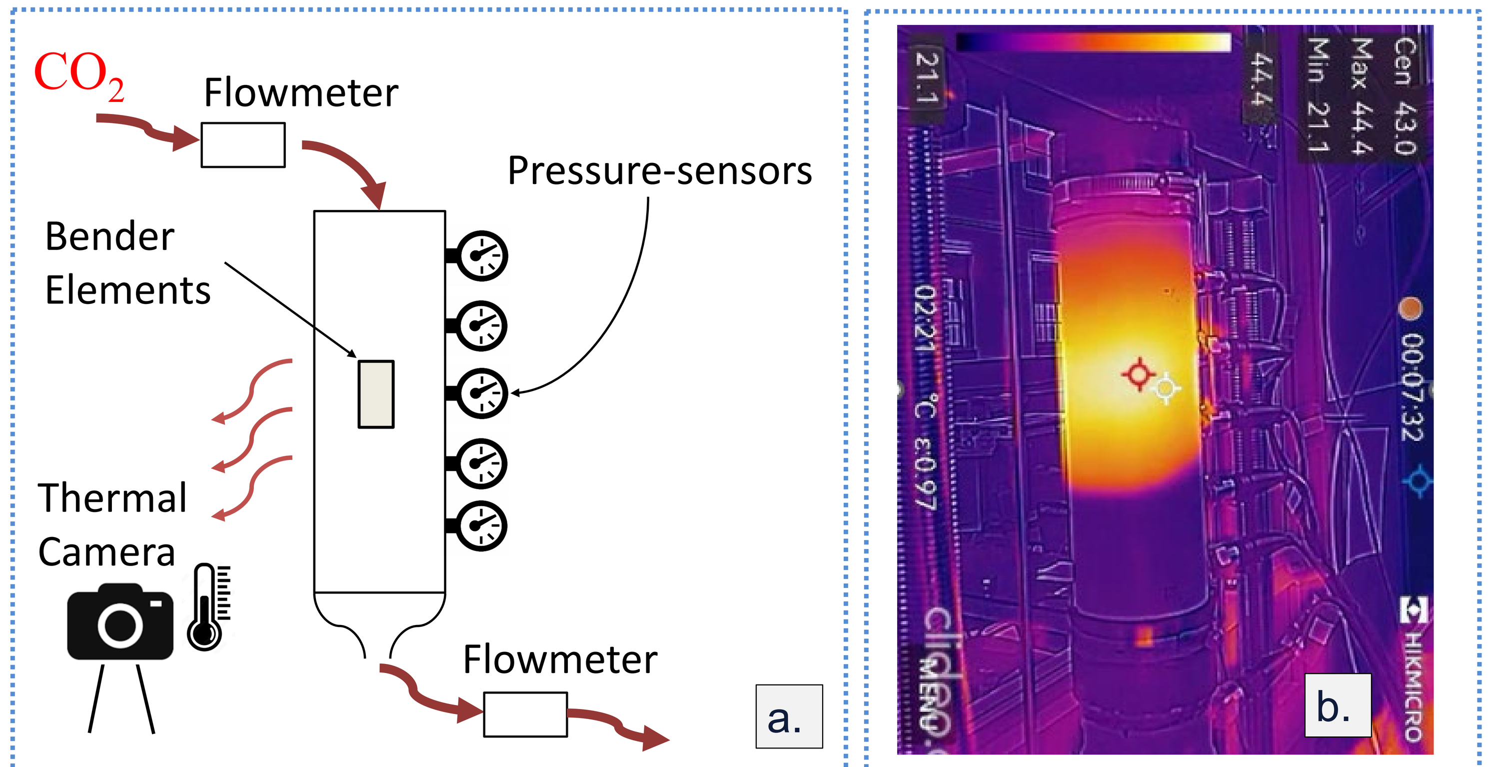

Fig 5). Laboratory setup – b. Thermal Camera capturing carbonation

Future work

- Parametric study for calibration of the carbonation reaction based on the laboratory results.