SPE • AAPG • SEG CCUS CARBON CAPTURE, UTILIZATION, AND STORAGE

THE INDUSTRY'S LEADING EVENT FOR CCUS MANAGEMENT AND DEVELOPMENT

3–5 MARCH 2025 HOUSTON, TEXAS

Microstructural Modeling of Cement Mechanical Properties under Carbonation Reactions and Its Implications to Wellbore Integrity

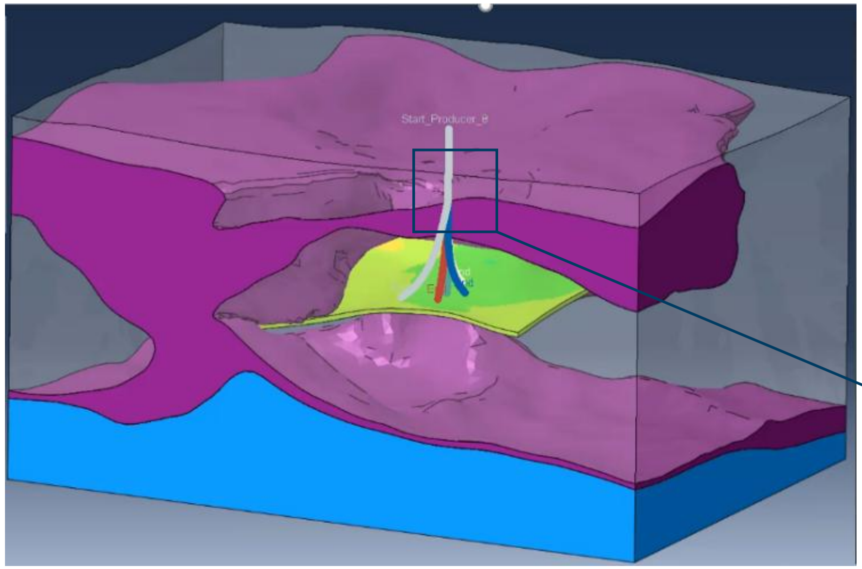
Zhuang Sun, Rafael Salazar-Tio, Andrew Fager, Bernd Crouse

Dassault Systèmes, USA

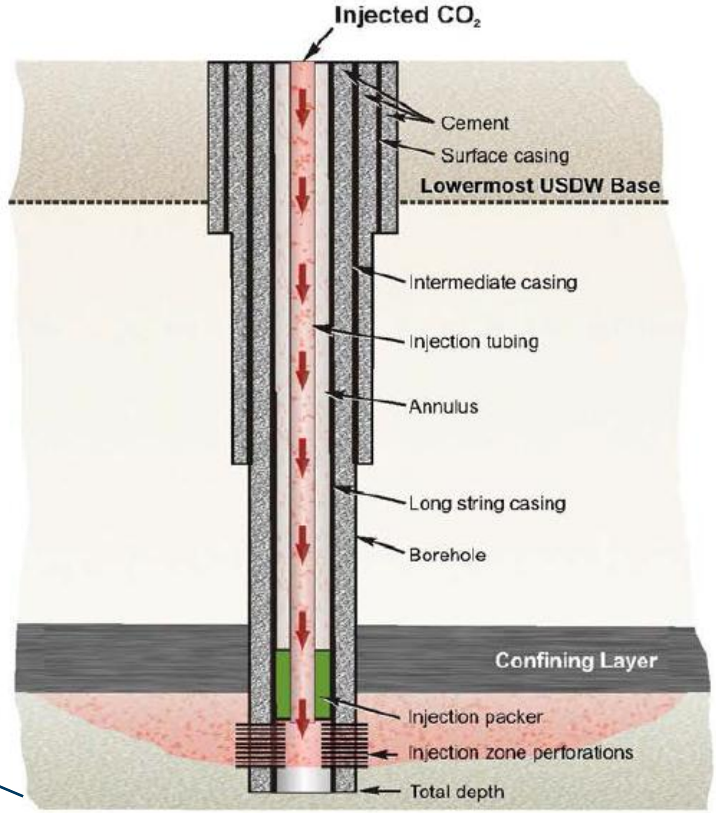
DASSAULT SYSTEMES

Industry Challenges

- Cementing is critical to ensure well stability and zonal isolation
- CO_2-cement interactions can pose challenges to long-term CO_2 storage



Wellbore trajectory



Schematic of injection well

Source: U.S. Environmental Protection Agency (EPA)

Chemistry of CO_2–induced Alteration: Carbonation & Bicarbonation

‘1’: Original Cement (White)

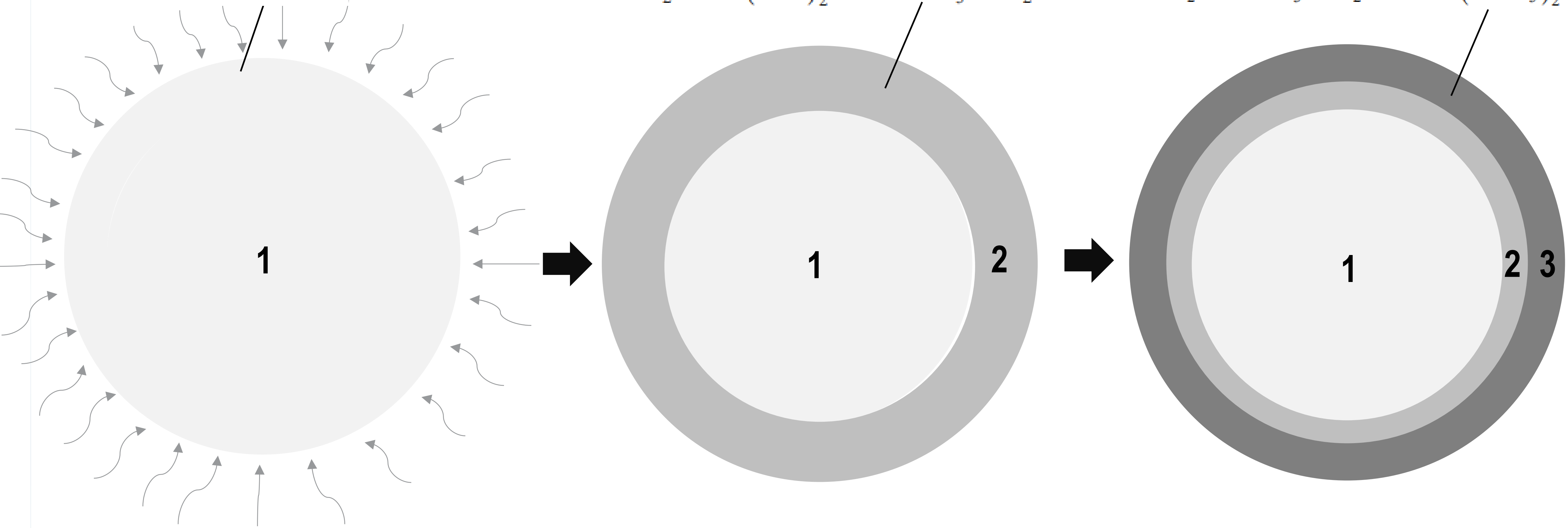
$Ca(OH)_2$

‘2’ : Carbonate (Light Gray)

$CO_2 + Ca(OH)_2 \rightarrow CaCO_3 + H_2O$

‘3’: Bicarbonate (Dark Gray)

$CO_2 + CaCO_3 + H_2O \rightarrow Ca(HCO_3)_2$



Plug is submerged in CO_2 saturated brine – CO_2 is diffusing into the cement through its circumference.

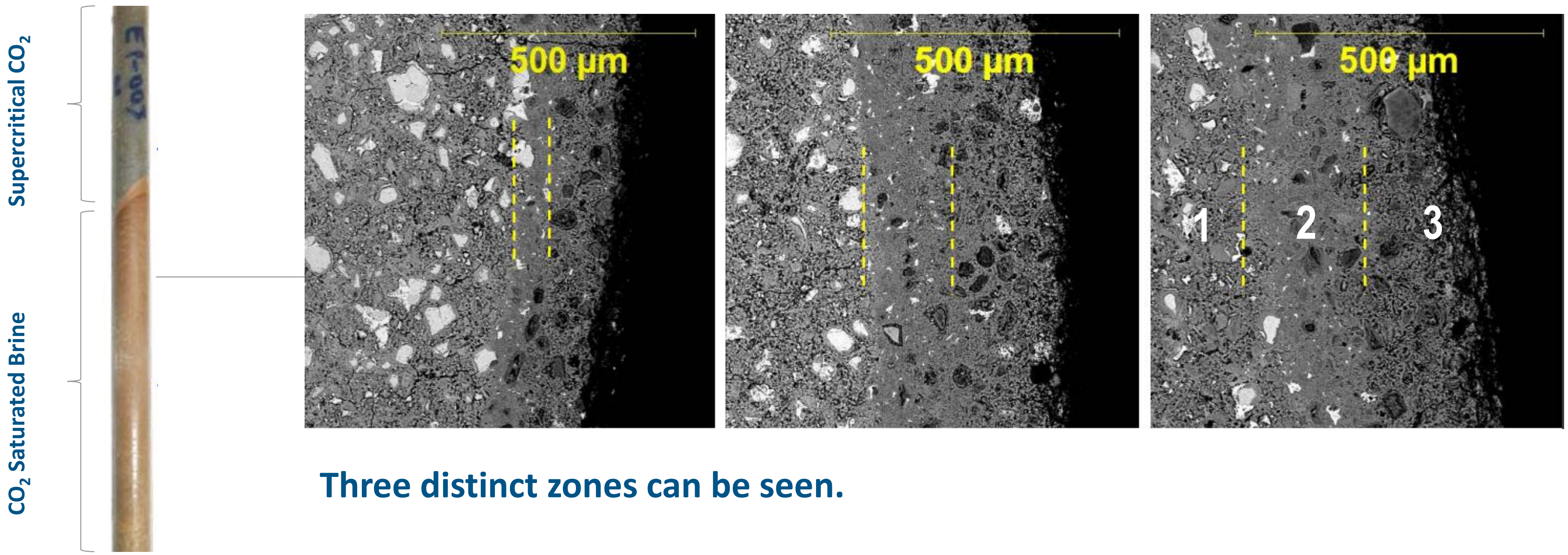
CO_2 reacts with hydroxide ($Ca(OH)_2$) in cement and forms carbonate.

Carbonate reacts with water to form bicarbonate.

Carbonation Depth – Experimental Observation

Exposure to CO_2 Saturated Brine

9 Days | **90 Days** | **365 Days**



Three distinct zones can be seen.

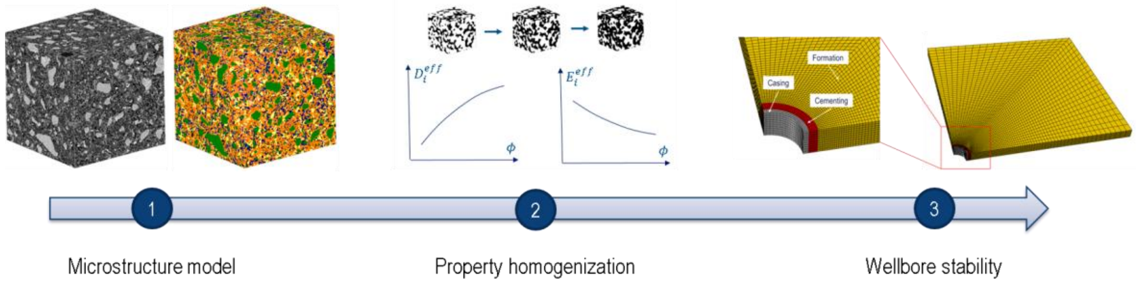
- Zone 1 is pristine cement (hardness reading 64 HV)
- Zone 2 is carbonated zone – has smaller permeability and higher strength (127 HV)
- Zone 3 (Bicarbonated) – has higher permeability and lower strength (27 HV)

Source: *Environ. Sci. Technol.* 2007, 41, 13, 4787–4792 (U.S. Department of Energy)

Benefits Of CO_2-Cement Interaction Multiscale Modeling

Improve accuracy in capturing cement properties by adding microstructure scale

Evaluation of carbonation reactions effect on cement properties

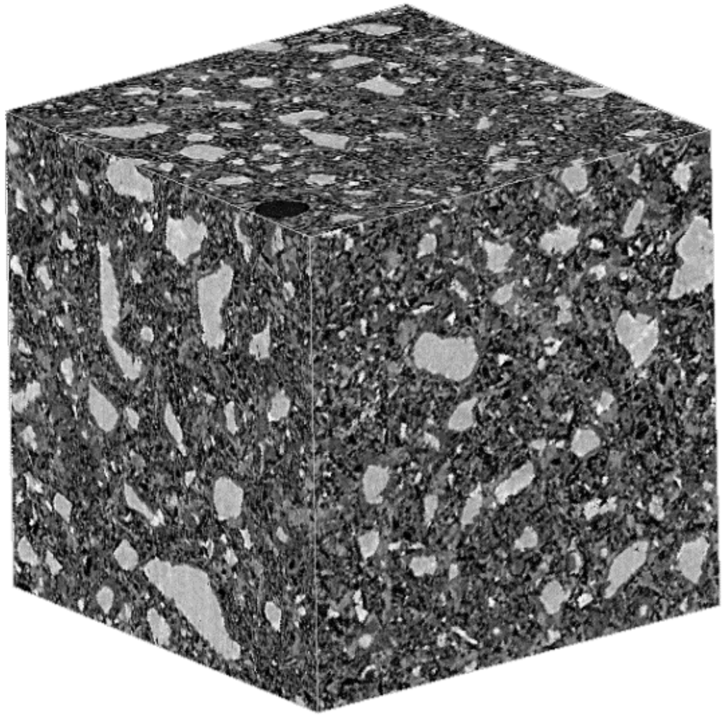


Large-scale evaluation of well integrity

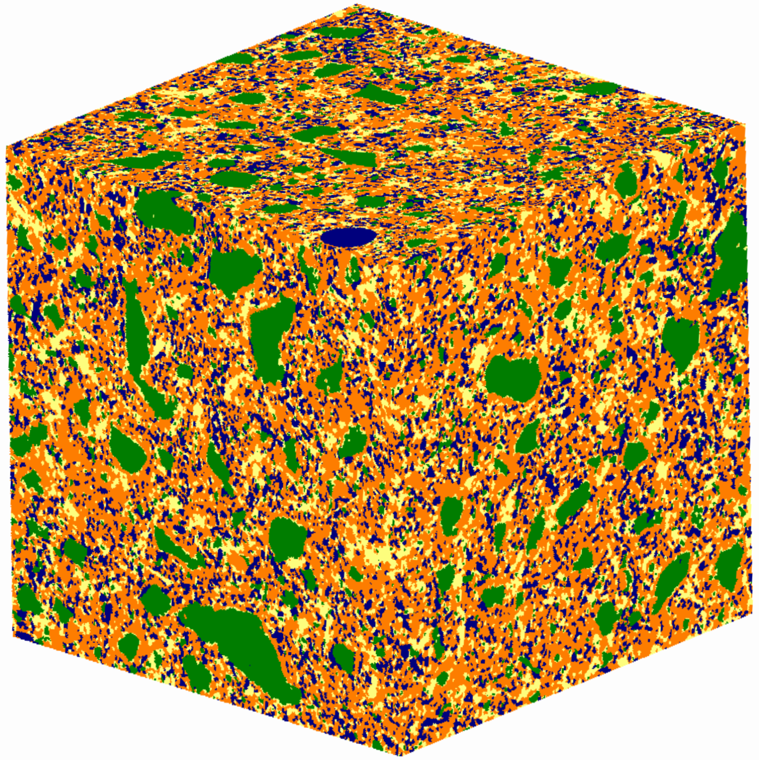
Image Segmentation

- Micro-CT image from NIST Visual Cement Data Set (Bentz et al., 2002), image resolution is 0.95 µm
- Water/Cement mass ratio is 0.45, curing time is 7 days
- Unique image processing capability that permits a more accurate N-phase segmentation

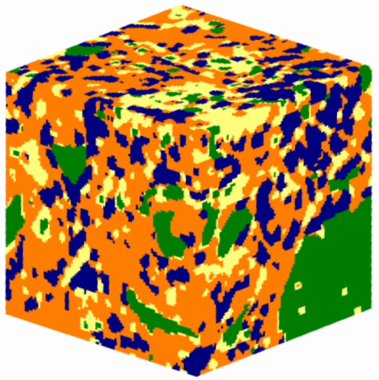
B600 grey scale image



B600 segmented cement image



B100 example



Unhydrated phase

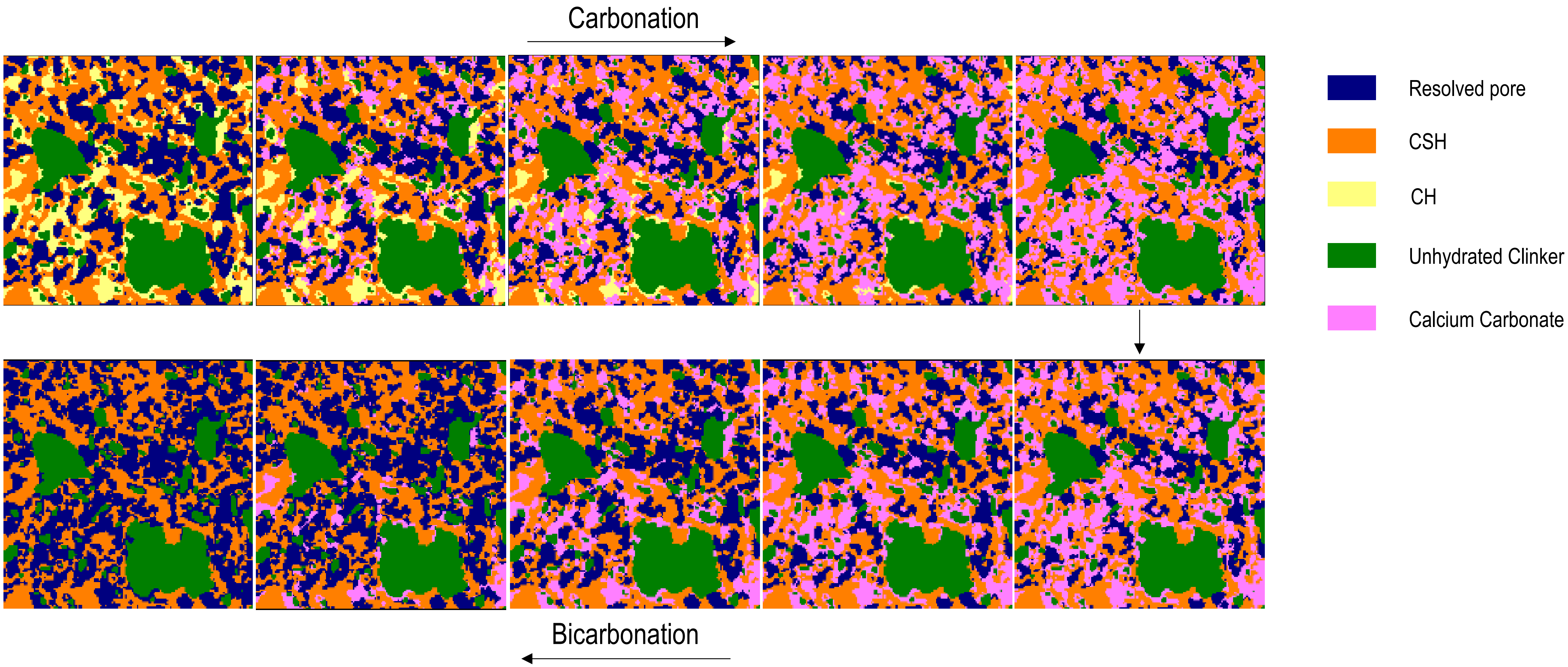
Resolved pore

CSH

CH

Assumptions for Carbonation And Bicarbonation

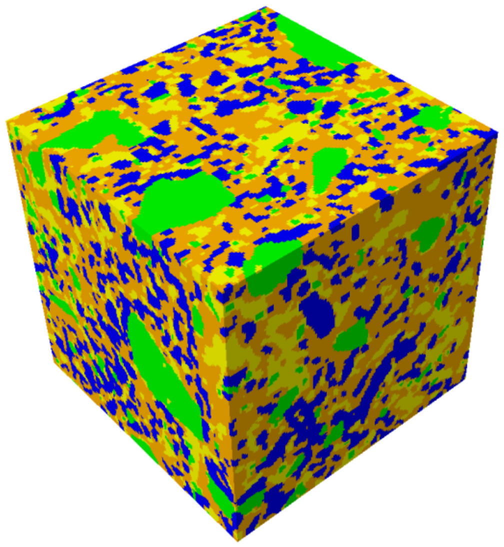
- Carbonation assumption: 100% of CH converts to $CaCO_3$ $$CO_2 + Ca(OH)_2 \rightarrow CaCO_3 + H_2O$$
- Bicarbonation assumption: $CaCO_3$ dissolved and converted to pore $$CO_2 + CaCO_3 + H_2O \rightarrow Ca(HCO_3)_2$$
- Image processing to mimic the carbonation and bicarbonation processes



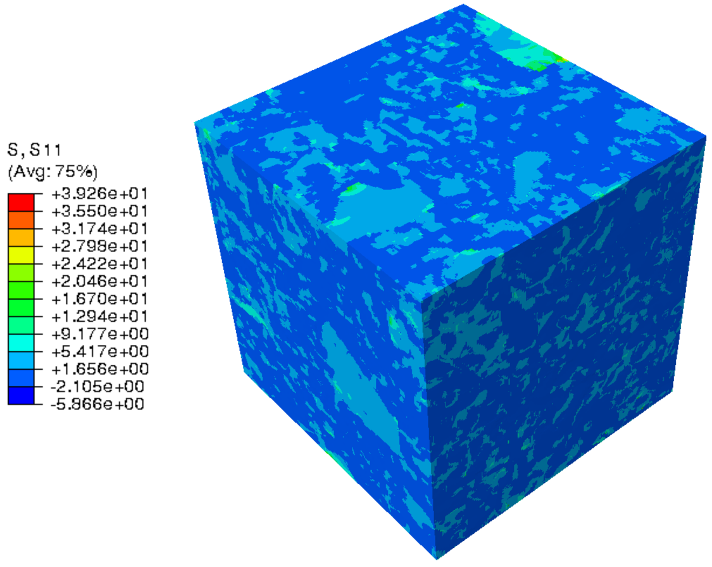
Baseline Simulation

- B150 is selected as the REV
- Apply deformation to measure the elastic modulus of cement sample

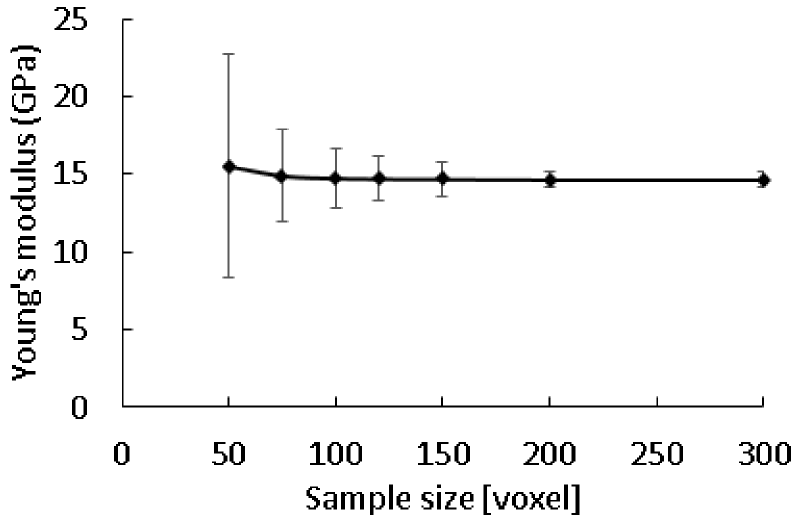
Image imported to Abaqus



Stress distribution



REV analysis



Unhydrated phase

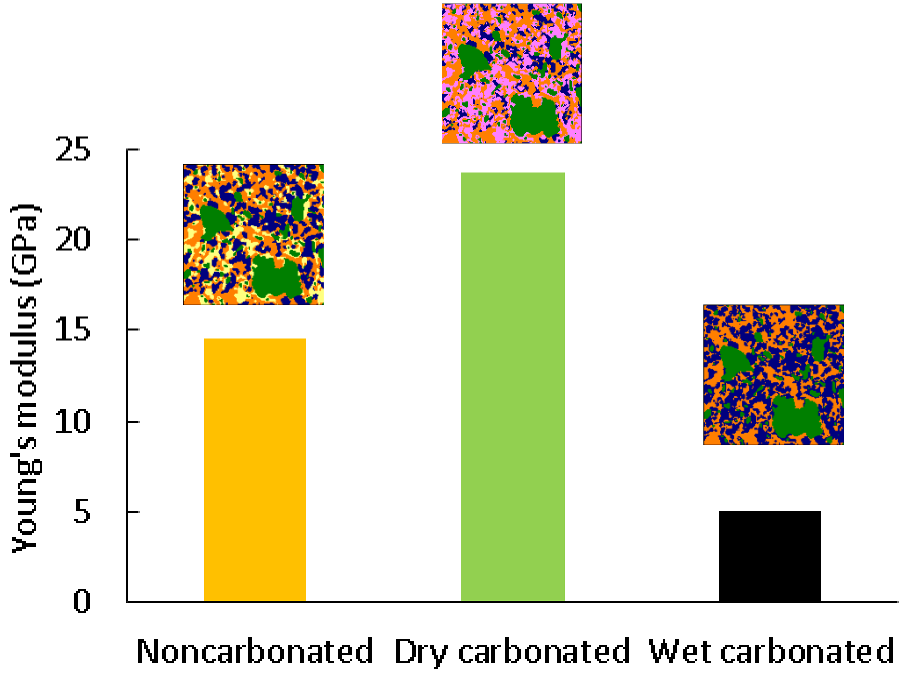
CSH

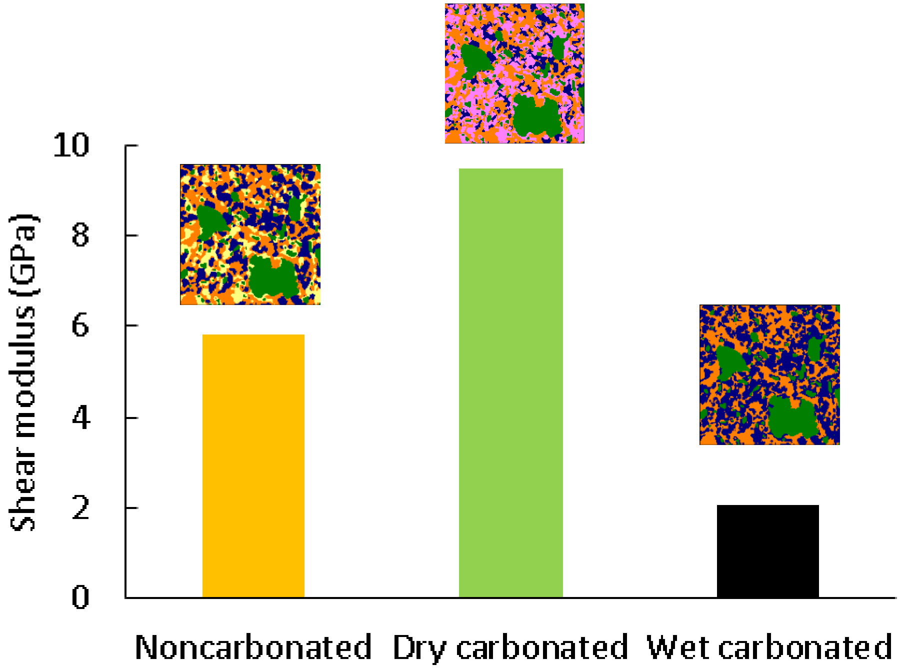
Resolved pore

CH

Change In Mechanical Property Due To Reactions

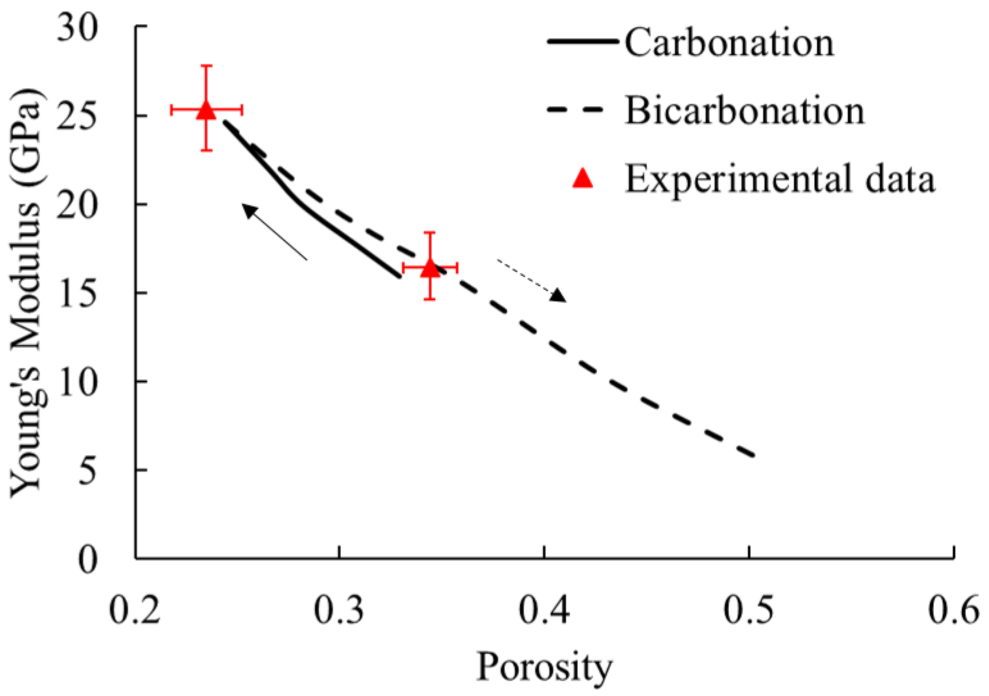
- Image processing to mimic the carbonation and bicarbonation processes
- Perform numerical simulations based on updated cement images
- Carbonation: $CO_2 + Ca(OH)_2 \rightarrow CaCO_3 + H_2O$
- Bicarbonation: $CO_2 + CaCO_3 + H_2O \rightarrow Ca(HCO_3)_2$

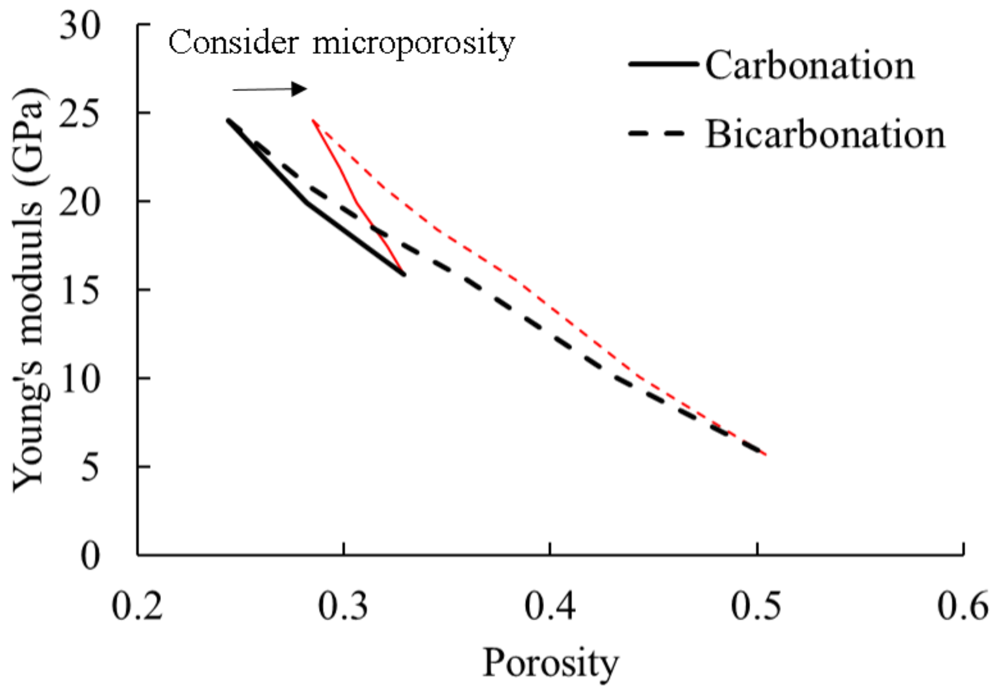




Validation with Experimental Data

- Experimental data from Zhang et al. 2020
- The sample was carbonated and their mechanical behavior was measured
- Small hysteresis is observed when plotting Young's modulus against porosity
- Inclusion of the $CaCO_3$ microporosity is critical to manifest the hysteresis

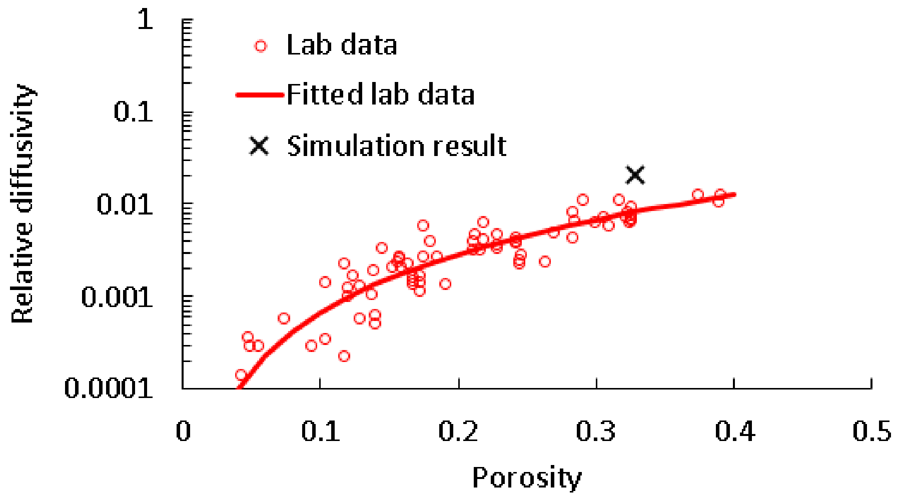




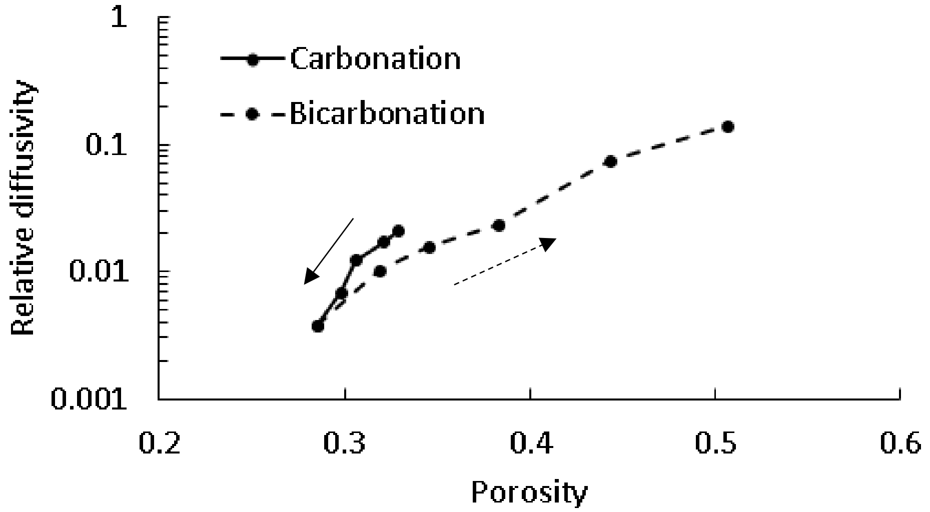
Diffusivity of Cement

- Lab data from steady state migration tests of chloride, iodide, and tritiated water (Limtong et al. 2023)
- Random walk code is used to evaluate the relative diffusivity
- Hysteresis is observed between carbonation and bicarbonation reactions

Validation with lab data for noncarbonated cement

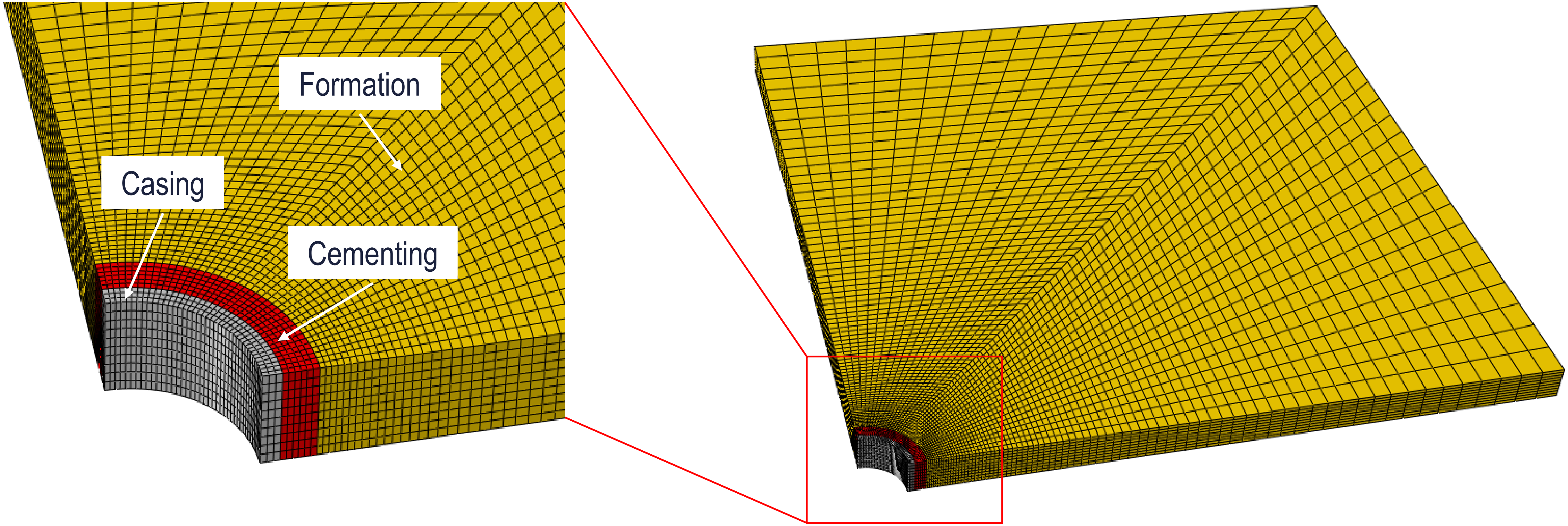


Hysteresis due to carbonation and bicarbonation reactions



Wellbore Model Geometry

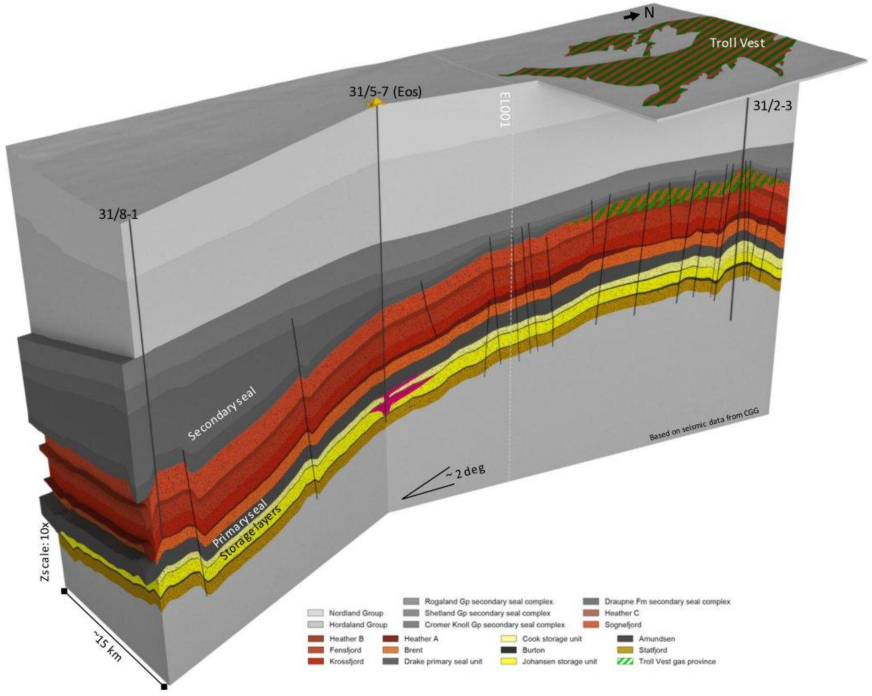
- Domain size: 2 m x 2 m x 0.1 m
- Cement outer radius : 0.1556 m
- Casing outer radius: 0.1254 m, casing inner radius: 0.1084 m



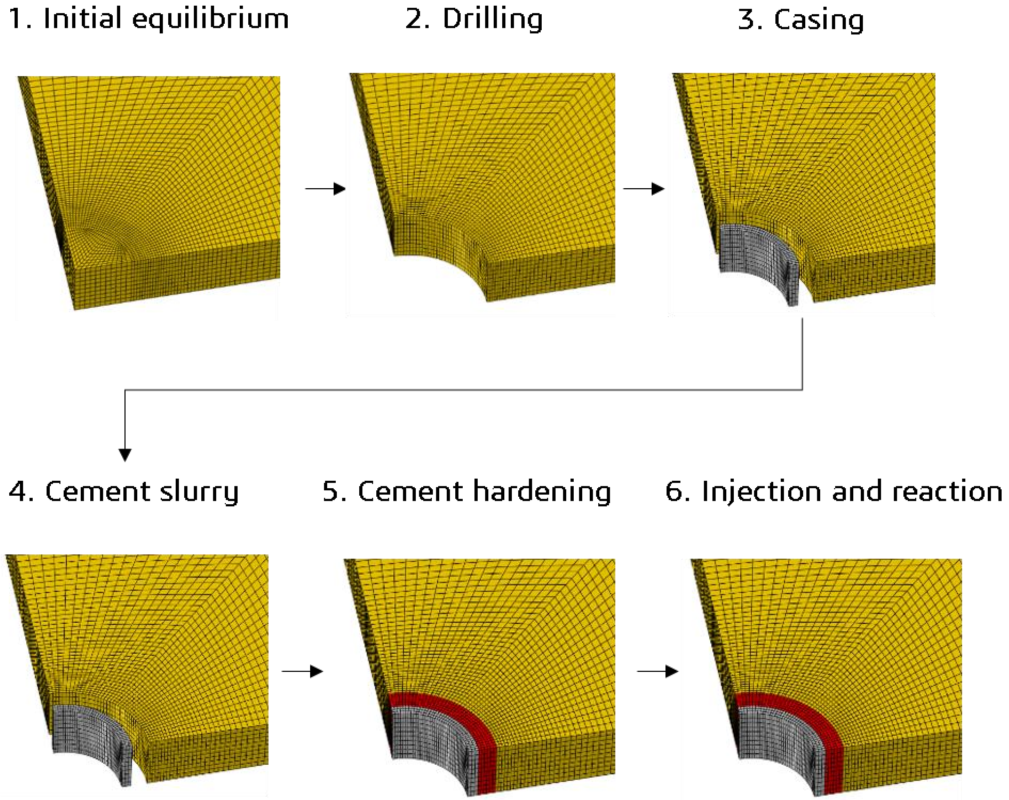
Multistage Finite Element Model

- Northern Lights project is part of the Norwegian full-scale CCUS project “Longship”
- Multistage model, which can quantify the stress condition and state variables in each well stage and permit us to capture the initial stress and strain state before modeling a certain stage
- Carbonation reactions occur during the injection stage

Schematic of subsurface



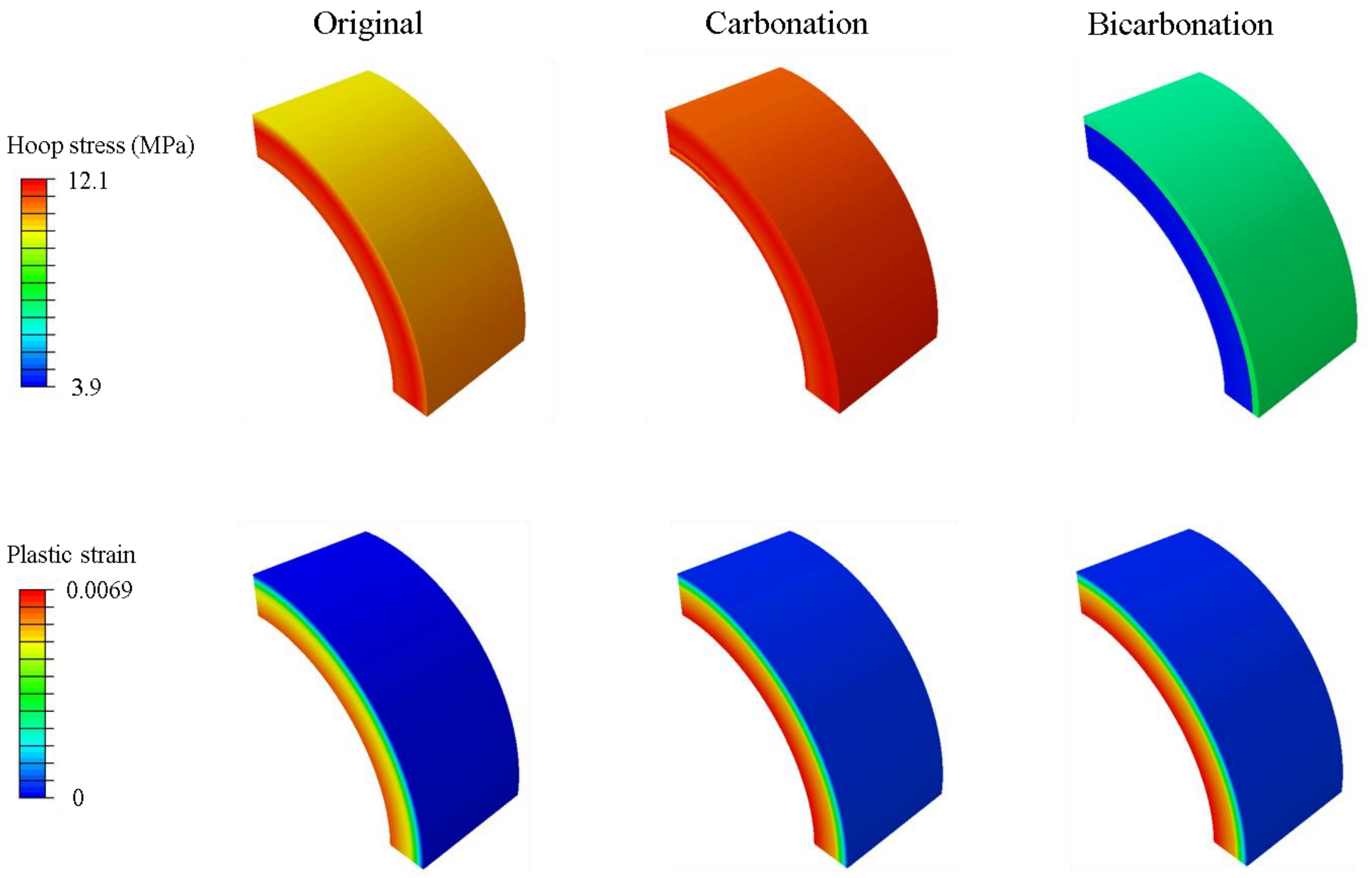
Multistage model



Source: the northern lights dataset was made publicly available by Equinor ASA

Implication to Wellbore Stability

- Thermal contraction caused by the cold injected CO_2 will induce tensile hoop stress and plastic strain in the cement annulus
- Carbonation process will further increase the hoop stress as well as the plastic strain
- Bicarbonation process will mitigate the hoop stress and induce no more plastic strain



Conclusions

- The changes on the cement 3D microstructure due to the carbonation reactions can be modeled by a rule-based process, when the Damkohler number is small.
- The microstructural simulation offers a unique opportunity to investigate the chemo-mechanical effects of carbonation reactions and the simulation results indicate that the bicarbonation process may lead to a non-trivial evolution of the constitutive relationship.
- The inclusion of the microporosity of $CaCO_3$ is critical to manifest the hysteresis behavior.
- The carbonation process could increase the cement modulus and impose an adverse impact on the well stability as it may induce tensile failure and damage to the cement.
- Although the bicarbonation process can reduce the stress level in the cement sheath, it tends to increase the porosity and permeability of cement as well as the apertures of pre-existing fractures, which may induce leakage of CO_2.