Modelling the durability of cementitious material at multi-scales

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14/03/2024 VTT – beyond the obvious

Contents

- Introduction of cementitious materials at multi-scales
- Thermo-chemo-cracking modelling -- ASR
- Poromechanical modelling -- sulfate attack
- Chemo-mechanical modelling -- drying-carbonation-corrosion
- Reactive-transport modelling -- Interaction with exposure solutions

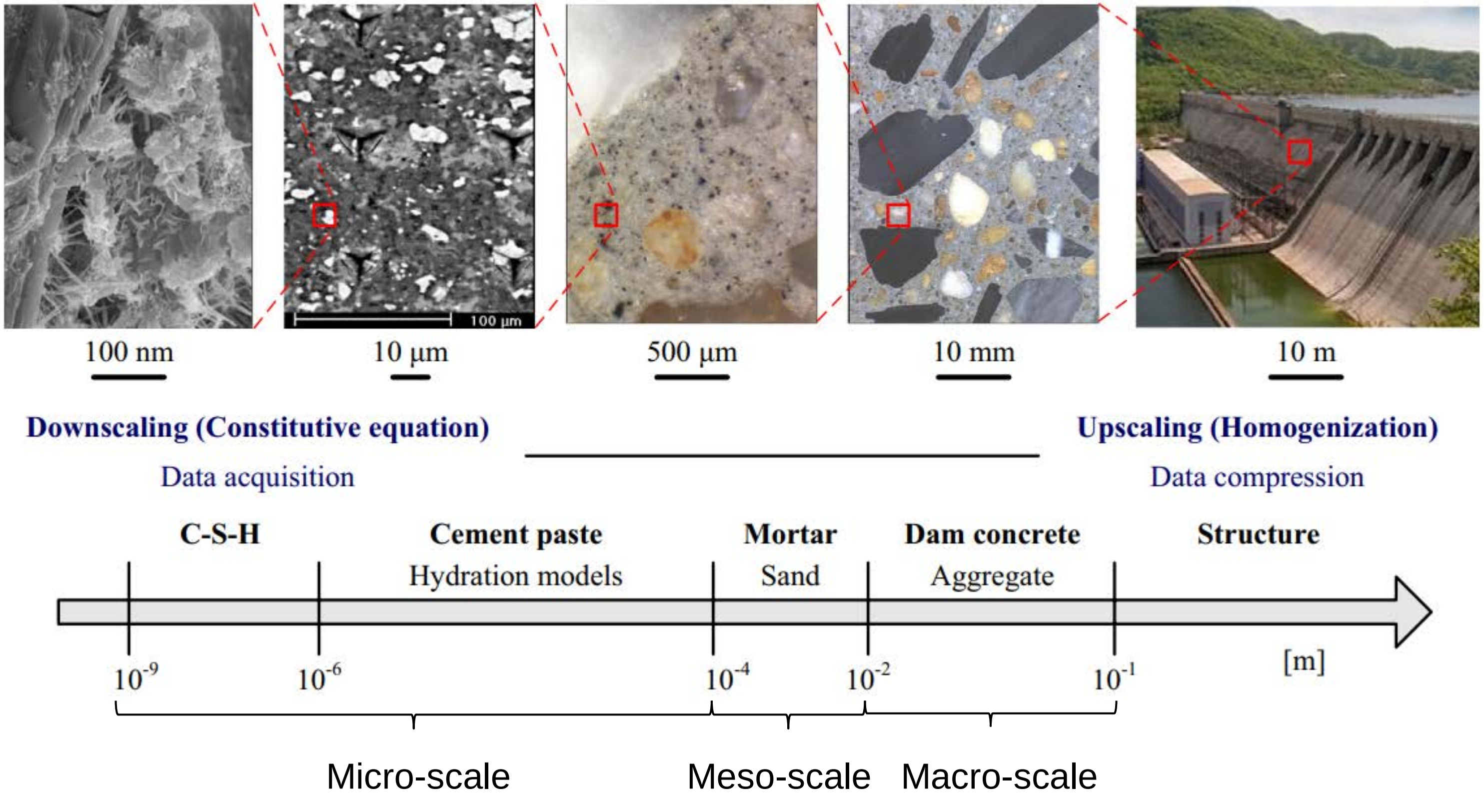
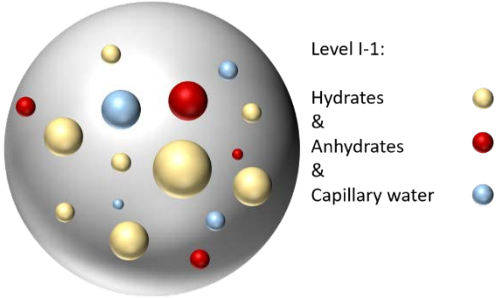
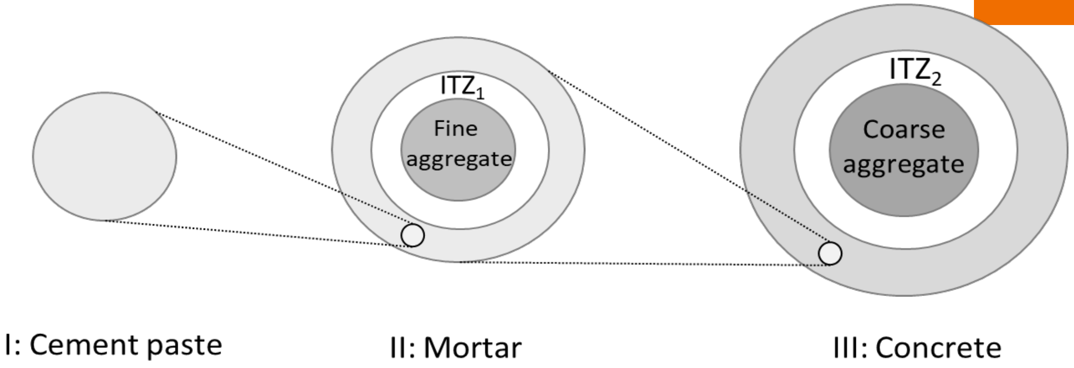


Fig. 1 Cementitious material represented at multi-scales (Su et al. 2018).

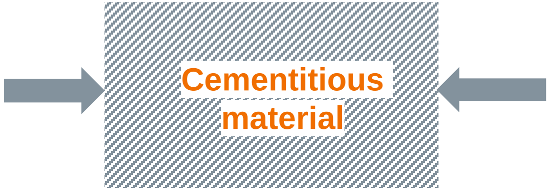
Su, H., Hu, J. and Li, H., 2018. Multi-scale performance simulation and effect analysis for hydraulic concrete submitted to leaching and frost. *Engineering with Computers*, *34*, pp.821-842.





(Gu et al. 2022)

Boundary Conditions



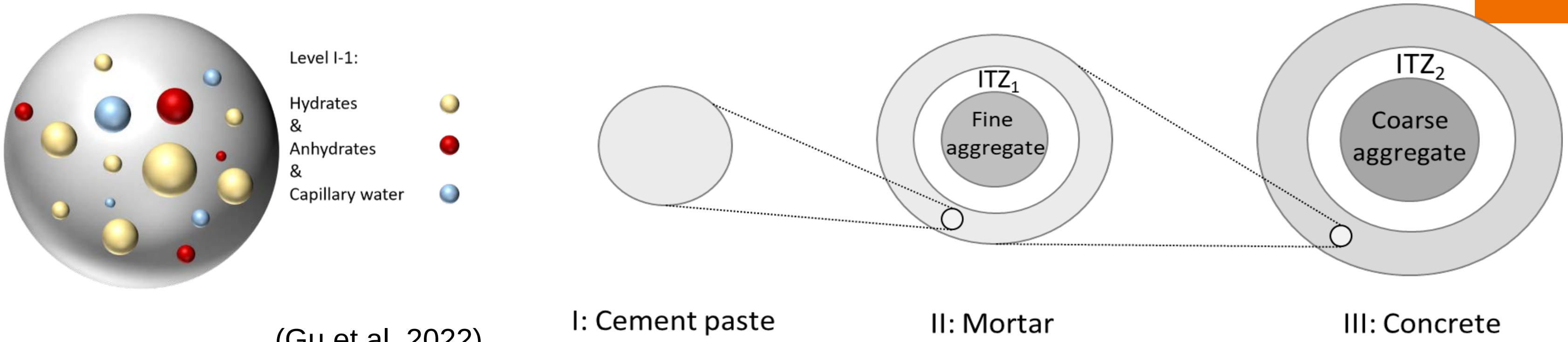
Degradation mechanism

- Carbonation
- Sulfate attack (SA)
- Alkali-silica reaction (ASR)
- Leaching
- Chloride ingress
- Etc.

Changes regarding

- Chemical phases
- Microstructure
- Mechanics

Gu, Y., Bary, B., Machner, A., De Weerdt, K., Bolte, G. and Haha, M.B., 2022. Multi-scale strategy to estimate the mechanical and diffusive properties of cementitious materials prepared with CEM II/CM. *Cement and Concrete Composites*, *131*, p.104537.



(Gu et al. 2022)

Boundary Conditions

Degradation mechanism

- Carbonation
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- Leaching
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Modelling methods

- Phenomenological modelling
- Thermodynamic modelling
- Poromechanical modelling
- Mechanical modelling
- Cracking / damage modelling
- Reactive-transport modelling
- Thermo-hydro-chemo model
- Etc.

Thermo-chemo-cracking modelling - ASR

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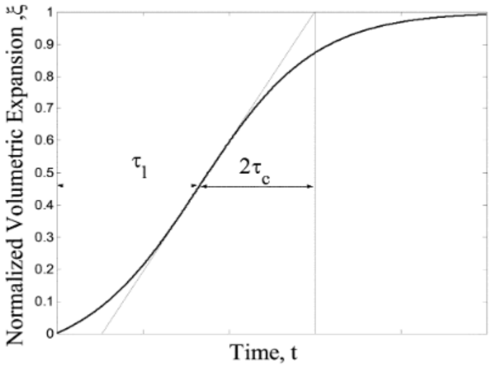
Input



τ_l: Latency time;

τ_c: Characteristic time;

ε^{∞}: Predicted maximum free volumetric expansion or target expansion.

Output

- Expansion curve replication

$$\dot{\varepsilon}_{vol}^{AAR}(t) = \Gamma_t(f_t', \sigma_1|COD) * \Gamma_c(\bar{\sigma}, f_c') * f(h) * \dot{\zeta}(t,\theta) * \varepsilon^{\infty}|_{\theta=\theta_0}$$

Γ_t: Reduction due to tensile cracking;

Γ_c: Reduction due to compressive stresses;

$\dot{\zeta}(t)$: Impact of temperature;

$f(h)$: Impact of RH.

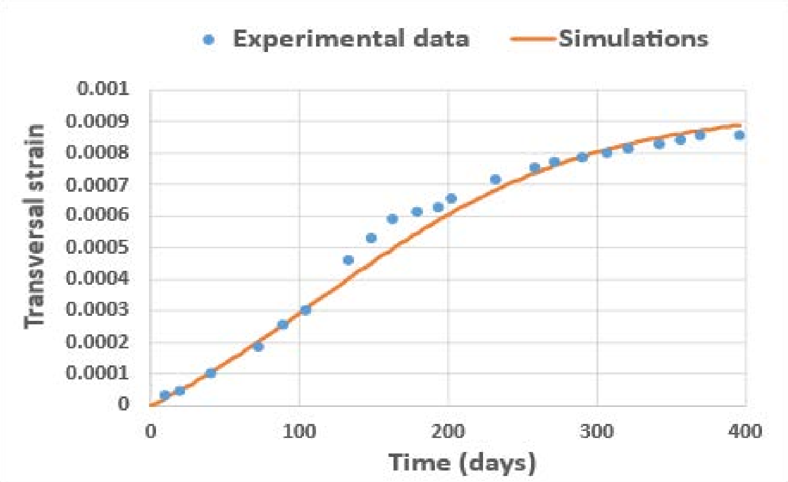


Fig. 2 Comparison of the simulated expansion curve to experimental data.

(SAFER-FN-CAMP) ıd the obvious

Poromechanical modelling of sulfate attack

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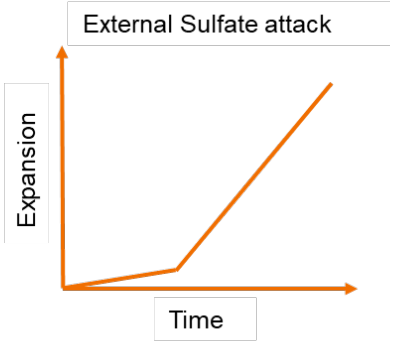
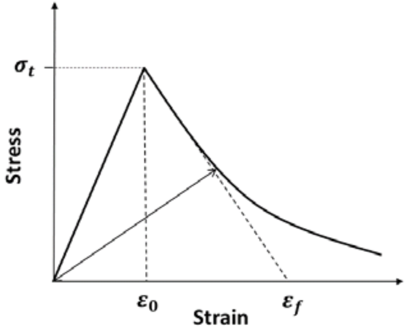
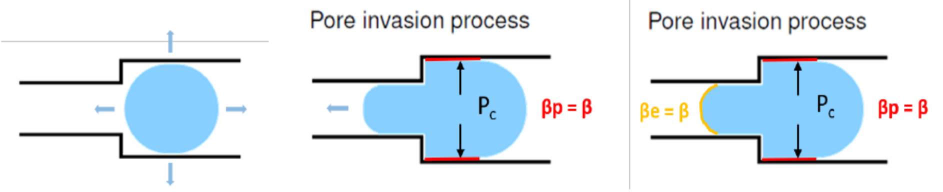




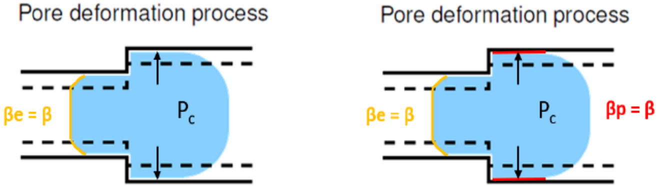


(a) Crystal growth in a supersaturated solution;

(b) Crystallization in the pore invasion process and crystals at the crystal-solid interface reaches equilibrium by exerting a crystallization pressure;

(c) Crystals in equilibrium at the crystal-solid and the crystal-liquid interfaces;

Poromechanics to predict the crystallization pressure → Expansive stress



(d) Crystallization in the pore deformation process without crystals in equilibrium at the crystal-solid interface;

(e) Crystallization in the pore deformation process with the crystal in equilibrium at the crystal-solid interface.

Input

- Main reactants
- Composition of pore solution
- Microstructure
- Boundary conditions

Output

- Expansion curve prediction
- Phase changes
- Porosity

(GU et al. 2022); Platform: BIL

Chemo-mechanical modelling – Drying-Carbonation-Corrosion

Input

- Main reactants
- Microstructure
- Boundary conditions

Output

- Phase changes
- pH value
- Carbonation depths
- Initiation of corrosion
- Damage propagation

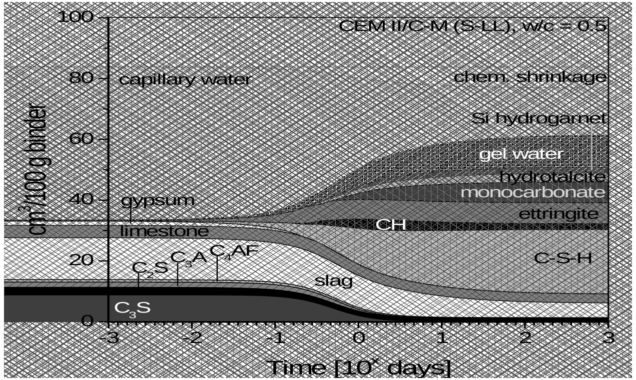
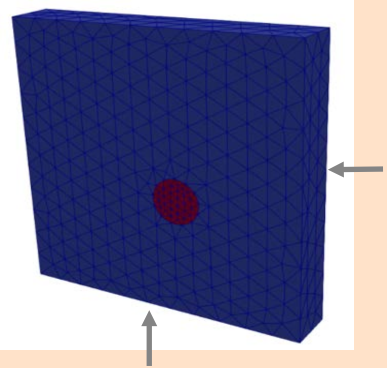


Fig. 3 Phase assemblage of hydrated cement paste calculated by thermodynamic modelling



Boundary conditions:

$C_{CO_2} = 1\%$;

RH=60%;

$C_{O_2} = 8.6\ \mathrm{mol/m^3}$

Assumption: Corrosion becomes active when carbonation reaches the steel surface.

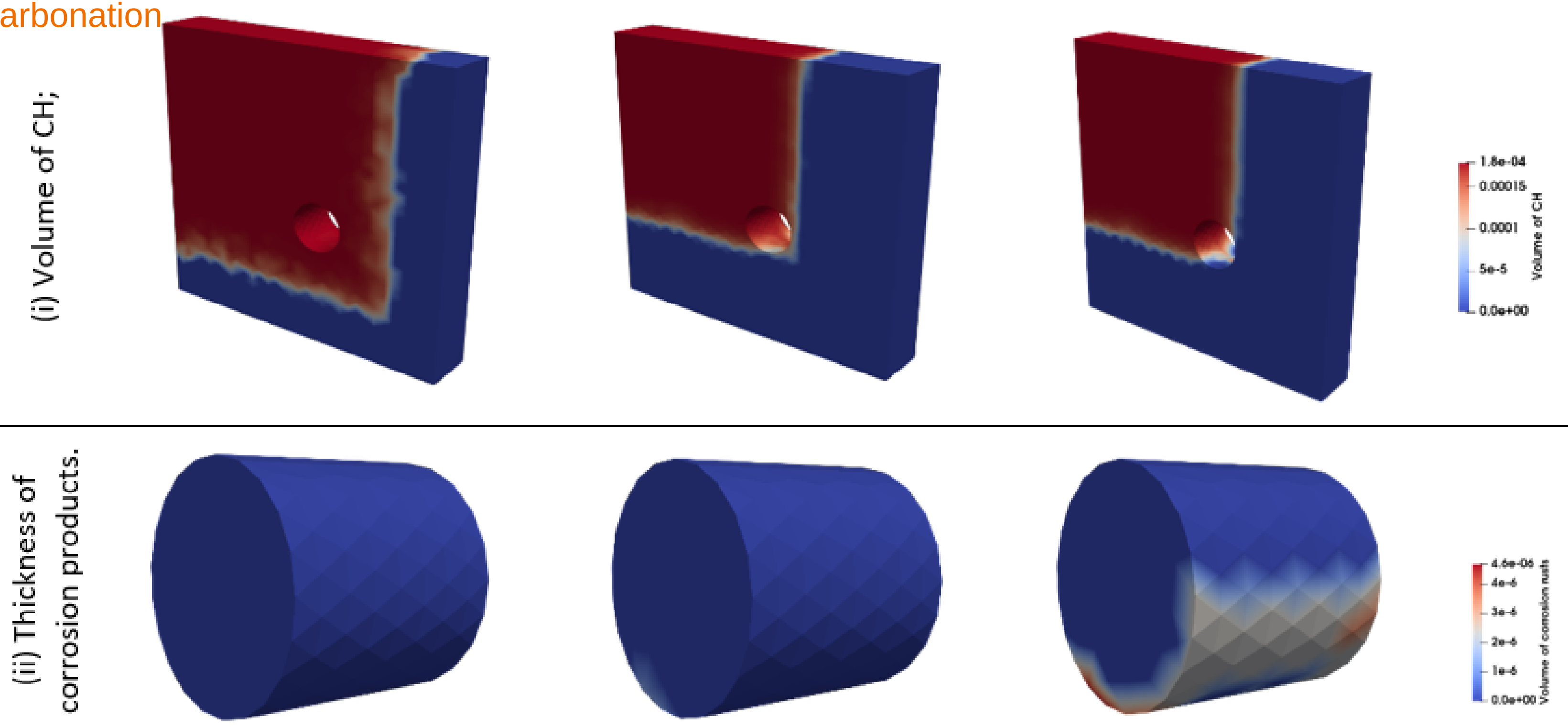
Mass balance equations regarding moisture, CO_2, O_2

Volume changes due to carbonation and corrosion

Coupled with a damage model

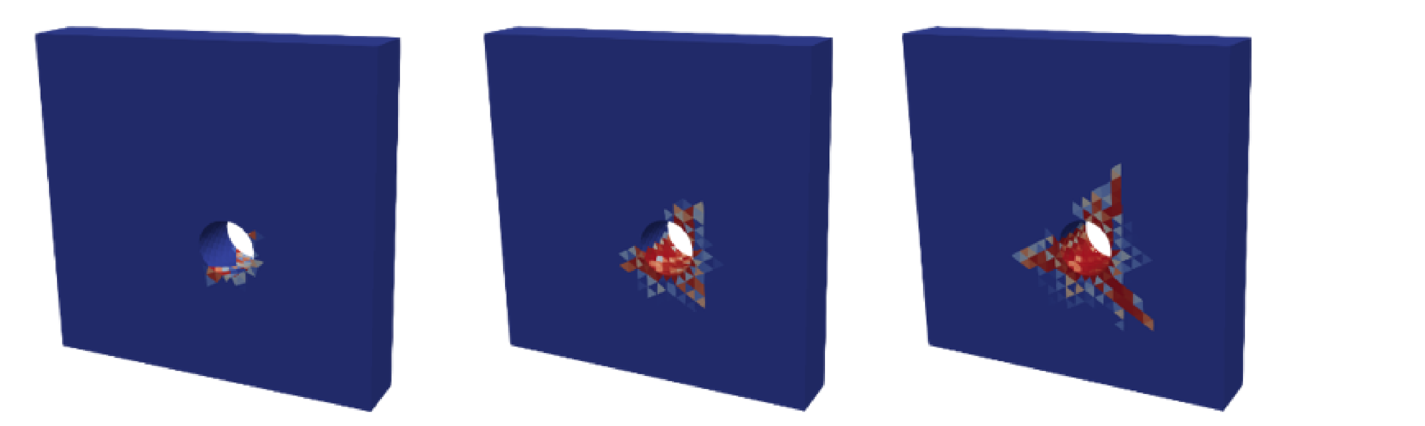
Software: Cast-3M

Carbonation

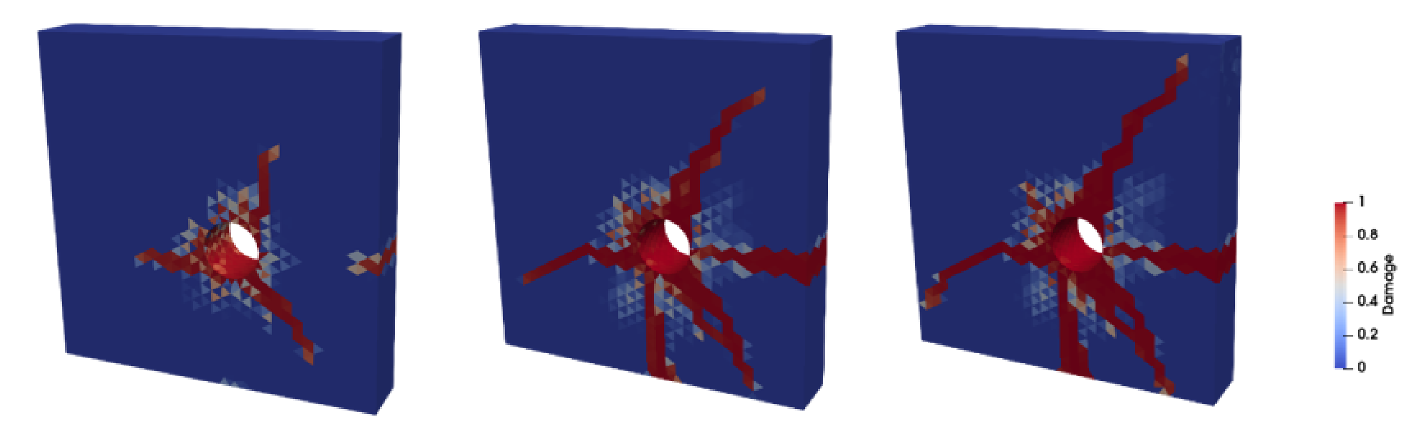


Corrosion (a) After 0.3 year; (b) After 0.9 year; (c) After 1 year.

Damage propagation

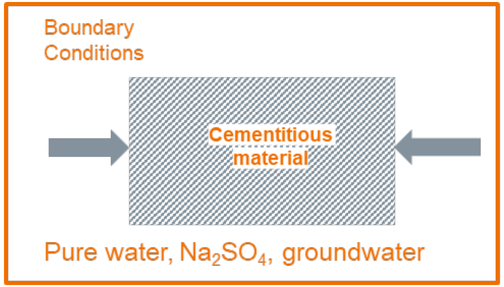


(a) After 1 year; (b) After 1.2 years; (c) After 1.5 years;



(d) After 1.7 years; (e) After 3 years; (f) After 5 years.

Reactive-transport modelling – Interaction with exposure solutions



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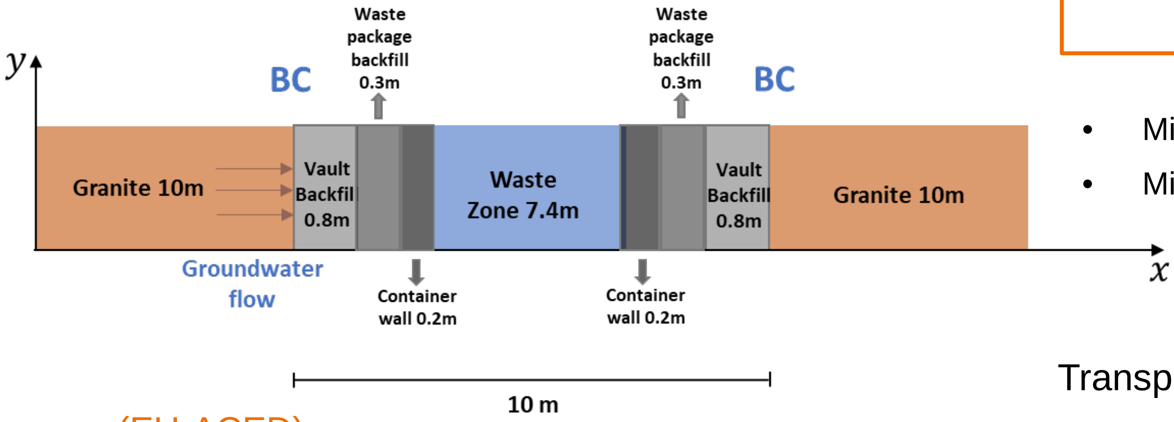


(EU-ACED)

Input

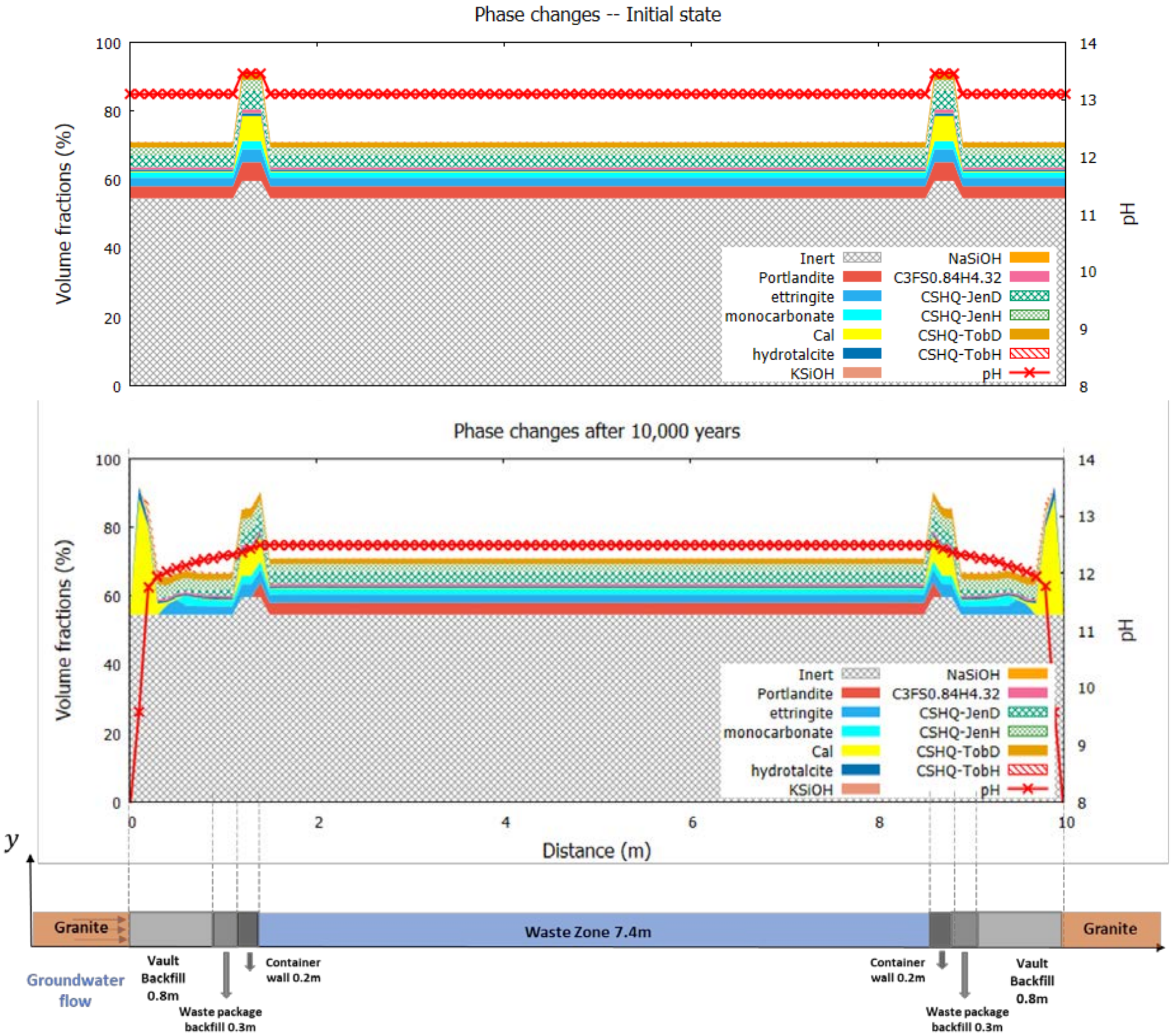
- Initial mineralogical phases
- Composition of concrete pore solution and exposure solutions
- Boundary conditions (including hydraulic pressure)

Output

- Mineralogical evolution / profiles
- Microstructural evolution / profiles

Transport simulation software: HYDRUS HP1.

- Simplified cement model with a thermodynamic database: CEMDATA v18 – PHREEQC version;
- Initial mineral phases present in the ILW disposal cell;
- Porosity = white space;
- Inert phase in cement-based materials is aggregate;
- pH value is shown on the secondary axis on the right;
- Chemical gradients are produced by the ingress of groundwater and the interfaces among materials;
- Interaction with granite is simplified to a constant advection-diffusion of groundwater on left and right boundaries with a hydraulic gradient.



Thanks for your attention!