Fully coupled CTHM simulations of cement-based materials from early-age to hardened state

Coupling MFront and FEniCS

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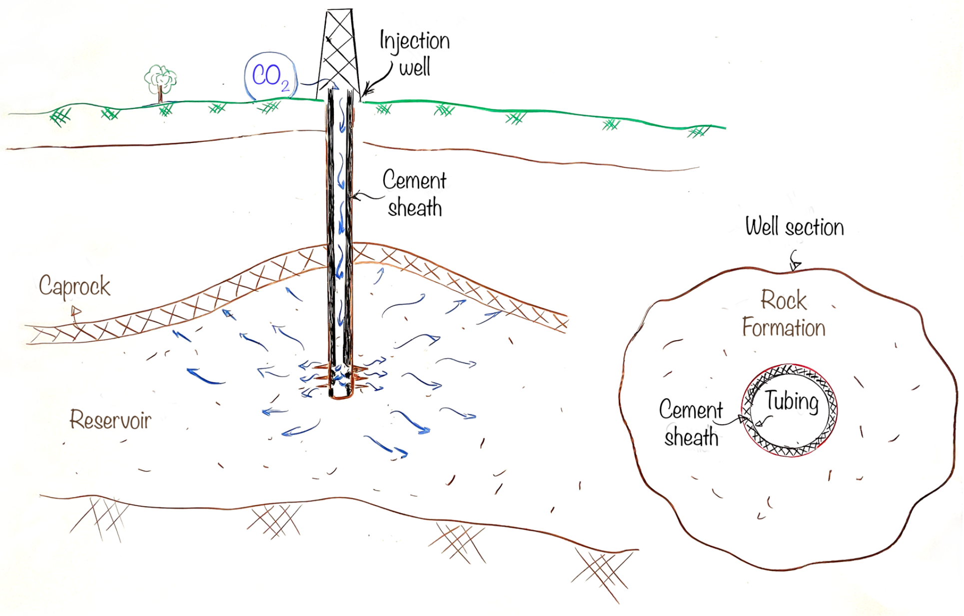
11th MFront User Day

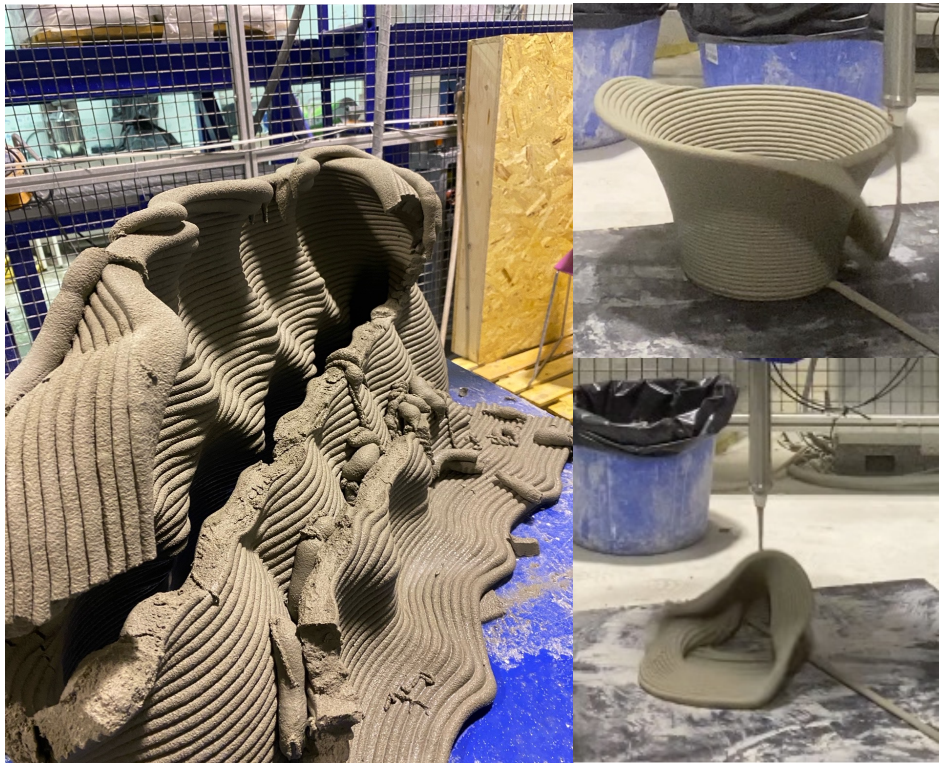
EDF Lab Saclay - November 20, 2025

Context

Many applications require understanding and modelling cement-based materials at the early-age :

- Cementing of **deep wells** (CO_2 sequestration, H_2 storage, deep geothermal systems ...)
- **Additive manufacturing** (extrusion 3D printing, shotcrete ...)





Need for coupled simulations taking into account :

- **Mechanics** (elasticity, viscosity & plasticity) with their evolution with cement hydration
- **Hydraulics** (water retention, transport and consumption)
- **Thermals** (heat capacity, transfer and generation)
- **Chemistry** (cement hydration reaction kinetics)

Some equations ...

Mechanical $\quad \mathrm{d}\underline{\underline{\sigma}} = \mathbb{C}(\xi) : \mathrm{d}\underline{\underline{\varepsilon}}^{el} - b(\xi) S_l \underline{\underline{1}} \mathrm{d}p_l - 3\kappa(\xi) \underline{\underline{1}} \mathrm{d}T$

Hydraulic $\quad \mathrm{d}\phi = b(\xi) \underline{\underline{1}} : \mathrm{d}\underline{\underline{\varepsilon}}^{el} + \dfrac{b(\xi) - \phi_0(\xi)}{K_s(\xi)} S_l \mathrm{d}p_l - 3\alpha_s (b(\xi) - \phi_0(\xi)) \mathrm{d}T - \Delta \overline{V}_s \mathrm{d}\xi$

Thermal $\quad \mathrm{d}S_s = 3\kappa(\xi) \underline{\underline{1}} : \mathrm{d}\underline{\underline{\varepsilon}}^{el} - 3\alpha_s (b(\xi) - \phi_0(\xi)) S_l \mathrm{d}p_l + \dfrac{1 - \phi_0(\xi)}{T} C_{\sigma_s} \mathrm{d}T$

Mechanical Hydraulic Thermal Chemical

+ Retention curve: $S_l = F(p_l, \xi_i)$

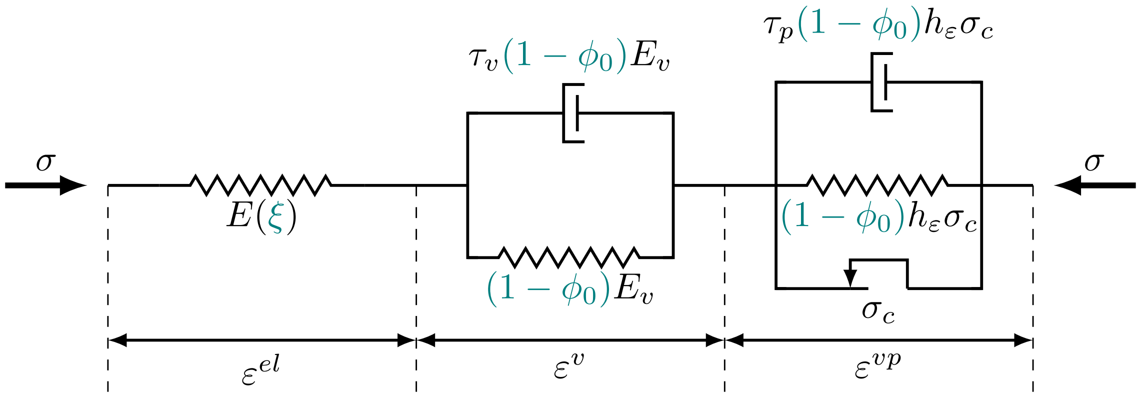
+ Hydration kinetics: $\dot{\xi} = A(\xi) \cdot \exp\left(-\dfrac{E_a}{RT}\right)$

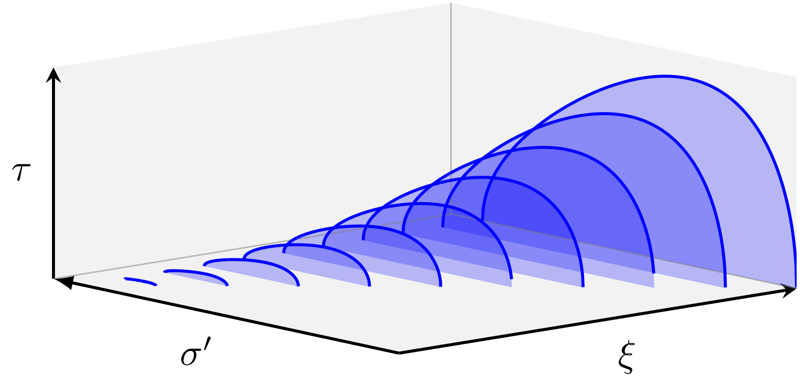
+ Darcy's law: $\underline{M}_w = -\rho_w(p_l, T) \dfrac{k_l(S_l, e)}{\eta_w} \underline{\nabla p_l}$

+Fourier's law: $\underline{q} = -k_T \underline{\nabla T}$

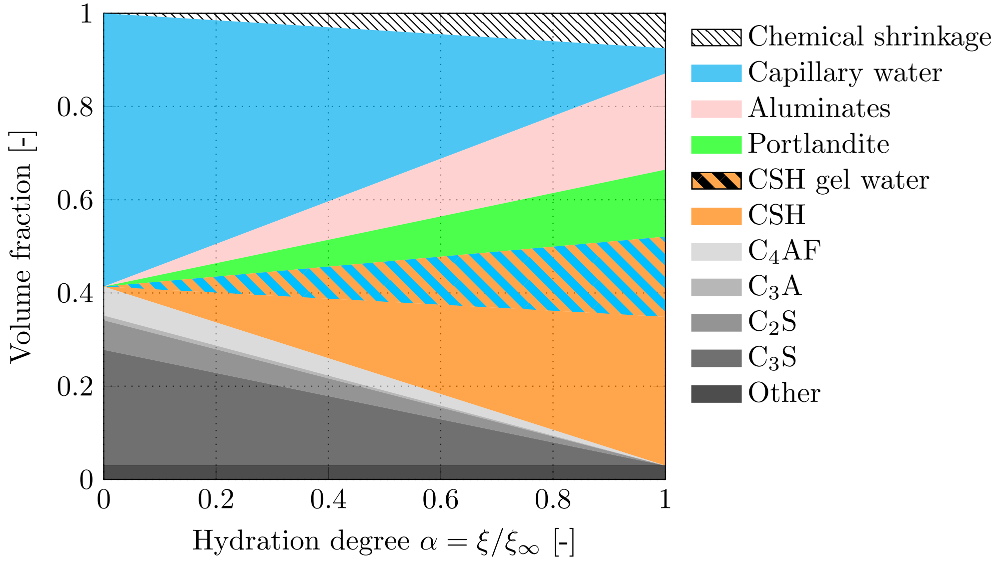
Mechanical model

Rheological model :

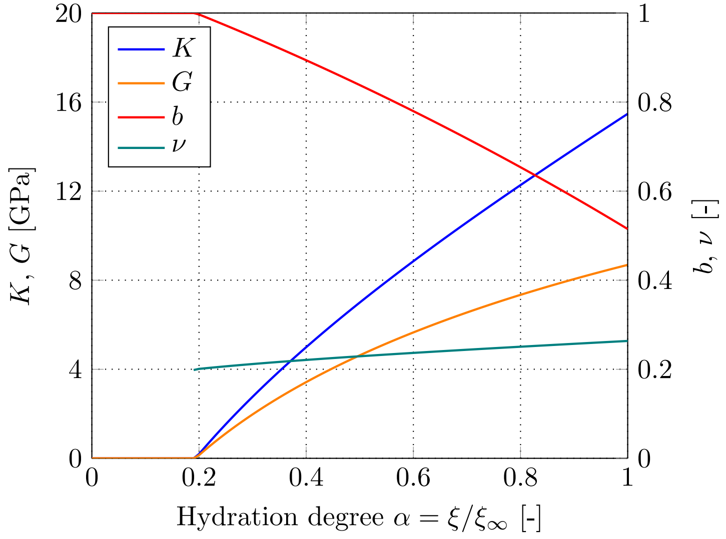




Yield surface



Self-consistent homogenisation



- For now, properties variations are input in MFront through regression expressions... Probably a better way is possible?

Hard/Heavy to implement models

- 3 external state variables (displacement, pore pressure, temperature) with full coupling
- 2 gradients (pore pressure, temperature)
- MANY model components :
  - Water retention curve
  - …
- MANY internal state variables :
  - Cement hydration
  - Porosity
  - Pore saturation degree
  - Relative permeability
  - All tangent thermo-poromechanical coefficients

- ~20 tangent operator blocks

The good stuff MFront provides

Main MFront file

Initialize internal variables

Cement hydration
Parameters depending on hydration…

Integrator

Solve for viscoelasticity and viscoplasticity

Integrator

Update fluxes (stress, porosity, entropy, heat and fluid fluxes)

Tangent operator

All needed blocks to pass to the FEM solver

MaterialLaw files

Model components

Cement hydration
Water Retention Curve
Parameters depending on hydration…
Water properties (p,T)

Partial derivatives components

Tangent water properties
WRC derivative
…

Thank god for Unicode support

```
∂σ⁄∂Δp_l   =  - b · (S_l + ∂S_l⁄∂Δp_l·Δp_l) · I₂ ;
∂σ⁄∂ΔT     =  - κ · I₂ ;

const real ∂φ⁄∂Δp_l = (b - φ₀)/ K_s · (S_l + ∂S_l⁄∂Δp_l·Δp_l) - ΔV_s · ∂ξ⁄∂Δp_l;
∂mf⁄∂Δp_l =  ∂ρ_f⁄∂Δp_l · S_l · φ + ρ_f · ∂S_l⁄∂Δp_l · φ + ρ_f · S_l · ∂φ⁄∂Δp_l;
const real ∂φ⁄∂ΔT = - 3 · α · (b - φ₀) - ΔV_s · ∂ξ⁄∂ΔT;
∂mf⁄∂ΔT    =  ρ_f · S_l · ∂φ⁄∂ΔT + ∂ρ_f⁄∂ΔT · S_l · φ;

∂S⁄∂ΔT     =  (1-φ₀_0) · Cₑ / Tref + sf · ∂mf⁄∂ΔT + ∂sf⁄∂ΔT · mf - (L / Tref) · ∂ξ⁄∂ΔT;
∂S⁄∂Δp_l   =  - 3 · α · (b - φ₀) · (S_l + ∂S_l⁄∂Δp_l·Δp_l) + sf · ∂mf⁄∂Δp_l + ∂sf⁄∂Δp_l · mf - (L / Tref) · ∂ξ


∂w⁄∂Δp_l   = - ( ∂ρ_f⁄∂Δp_l · k_eff + ρ_f · ∂k_eff⁄∂S_l · ∂S_l⁄∂Δp_l ) / η_f · (∇p_l + Δ∇p_l) ;
∂w⁄∂ΔT   = -  ∂ρ_f⁄∂ΔT · k_eff  / η_f · (∇p_l + Δ∇p_l) ;
∂w⁄∂Δ∇p_l =  - ρ_f · k_eff / η_f · tmatrix<N, N, real>::Id();

∂j⁄∂Δ∇T    =  - k_T · tmatrix<N, N, real>::Id();

StiffnessTensor De;
De = λ · (I₂ ⊗ I₂) + 2 · μ · I₄;
∂fε_el⁄∂Δεᵗᵒ = - I₄ ;
Stensor4 ∂Δε_el⁄∂Δεᵗᵒ ;
getIntegrationVariablesDerivatives_εᵗᵒ(∂Δε_el⁄∂Δεᵗᵒ);    // /!\ Overload à plusieurs variables dans l'ordre d
∂σ⁄∂Δεᵗᵒ = De · ∂Δε_el⁄∂Δεᵗᵒ;
∂mf⁄∂Δεᵗᵒ =  ρ_f · S_l · ( (b-β) · I₂ · ∂Δε_el⁄∂Δεᵗᵒ + β · I₂);
∂S⁄∂Δεᵗᵒ =  κ · I₂ · ∂Δε_el⁄∂Δεᵗᵒ + sf · ∂mf⁄∂Δεᵗᵒ ;
```

LABORATOIRE NAVIER

Material point level simulation

- mtest is a great tool:
  - Don't want to use a full FEM solver when only one material point is needed
  - **But**: No way to to control by fluxes (except stress) out of the box

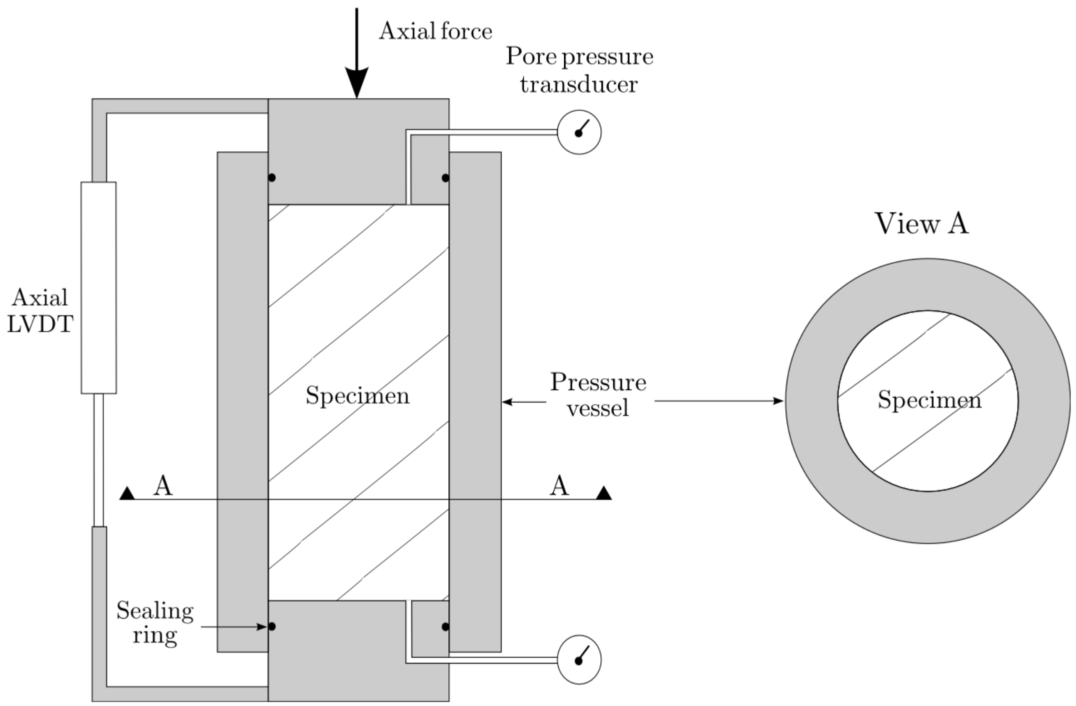
- The kind of conservation equations we want to use:

$$\frac{\mathrm{d}m_w}{\mathrm{d}t} = -\underline{\nabla} \cdot \underline{\boldsymbol{M}}_w + \nu_w \mathcal{M}_w \frac{\mathrm{d}\xi}{\mathrm{d}t}$$

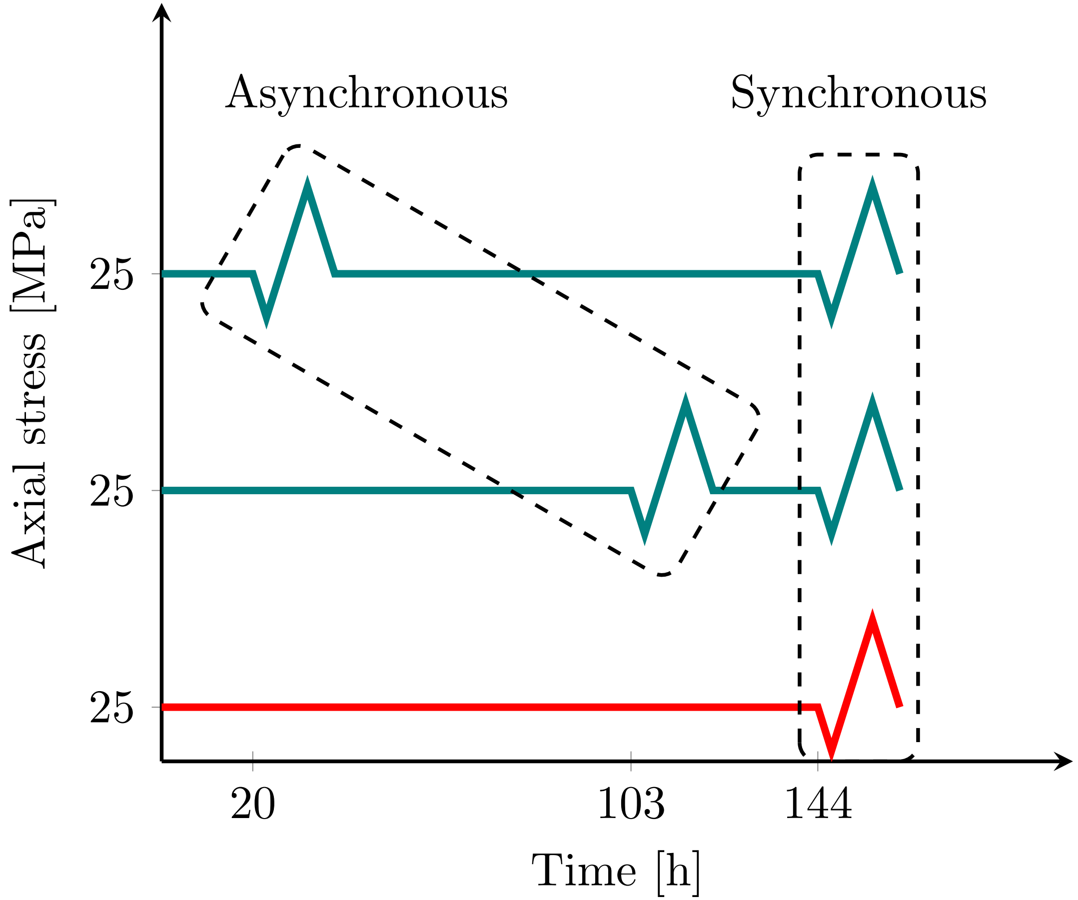
- Implementation of a « mtest multiphysics » solver using the python bindings:
  - Allows for flux control (Undrained/Adiabatic simulations) with mtest through a small newton solver

Model validation at material scale

- Oedometric tests on fresh class G cement paste

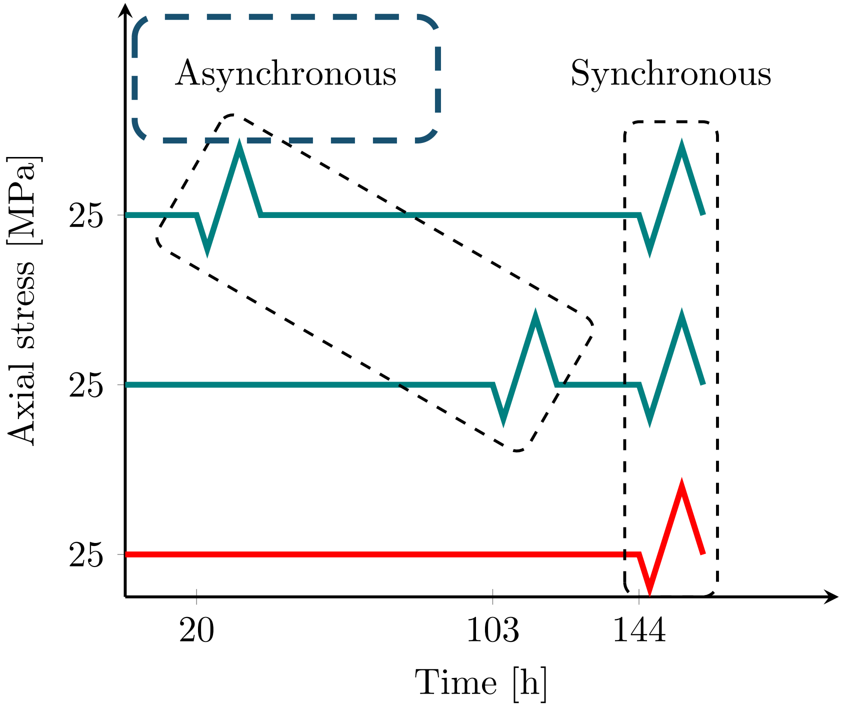


Oedometric cell used in Agofack et al. (2019)

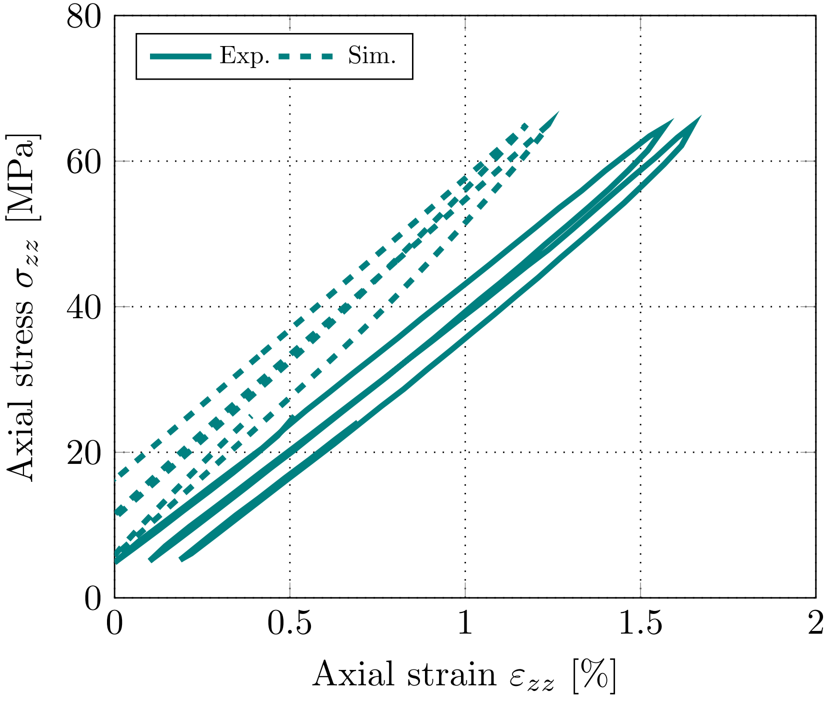


Loading history effect

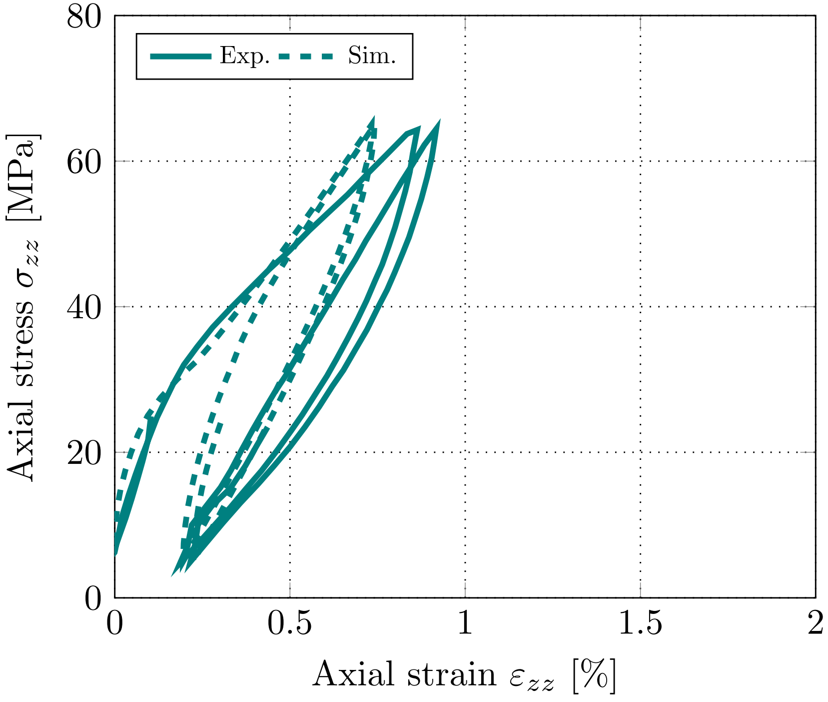
➢ First virgin loading at 20h or 103h, followed by reloading at 144h



Virgin loading at 20h



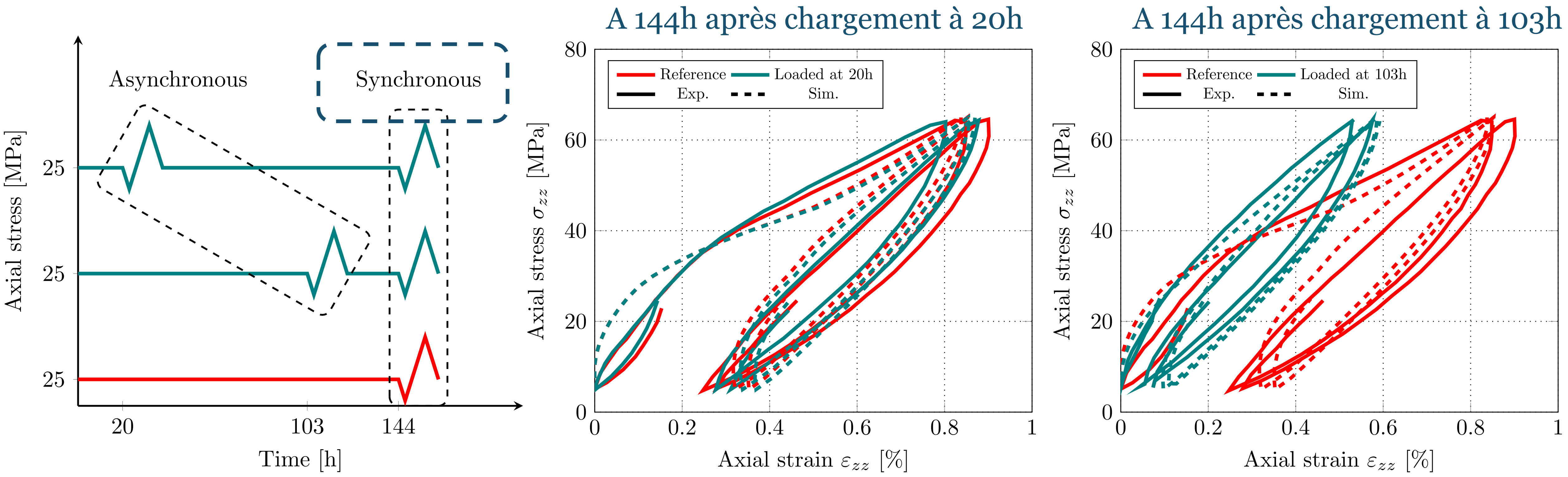
Virgin loading at 103h



➢ **Fluid-solid transition well captured by the model**

Loading history effect

➢ First virgin loading at 20h or 103h, followed by reloading at 144h



➢ **Complex hardening mechanisms captured by the model**

3D concrete printing

Modelling sequential material deposition

Printpath data

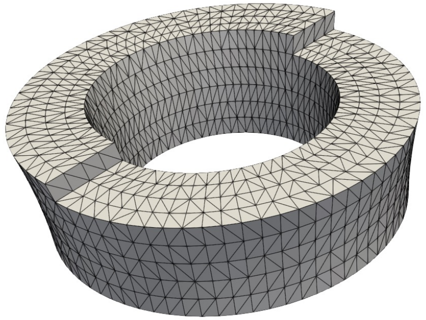
Full mesh

Extracted submesh

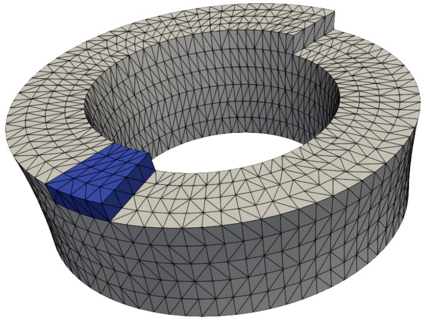
Linear geometric Elasto-plastic problem

Nonlinear geometric Elastic problem

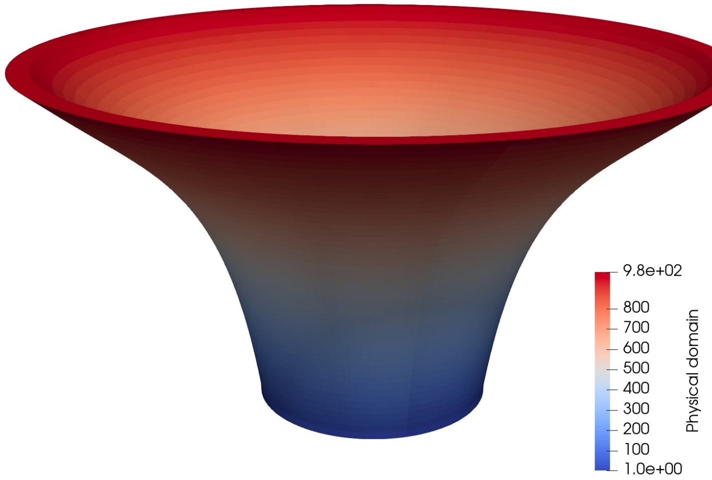
Pass to next step



Mesh at step n

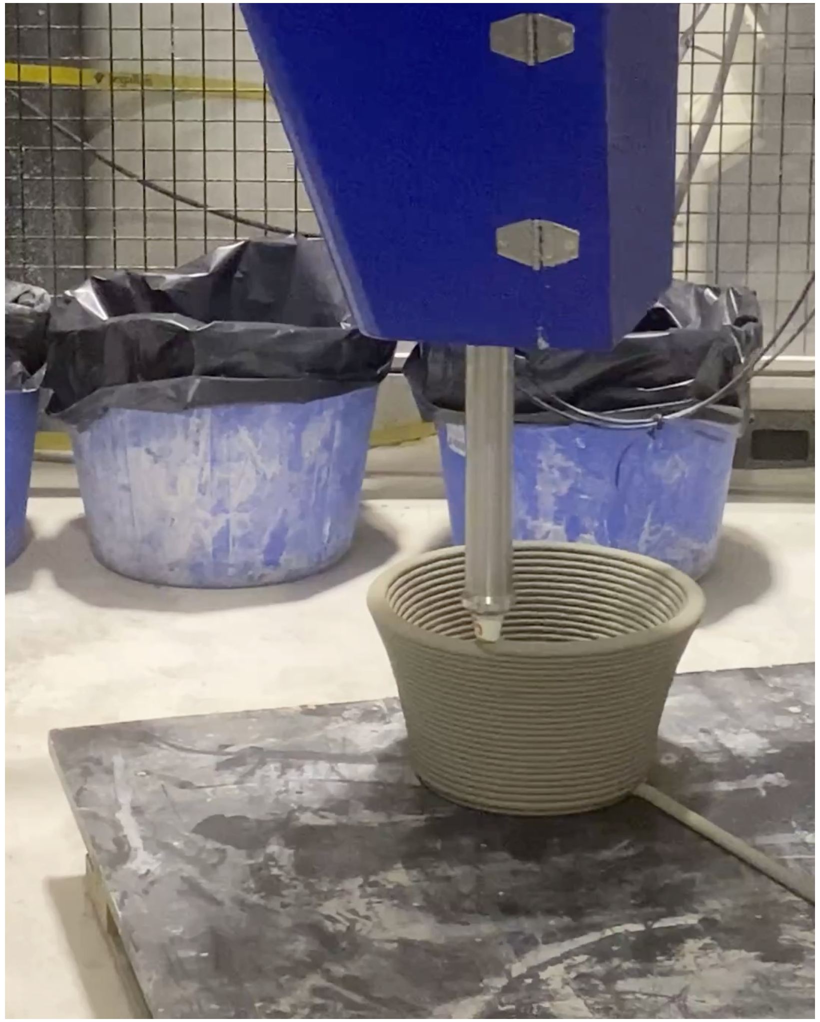


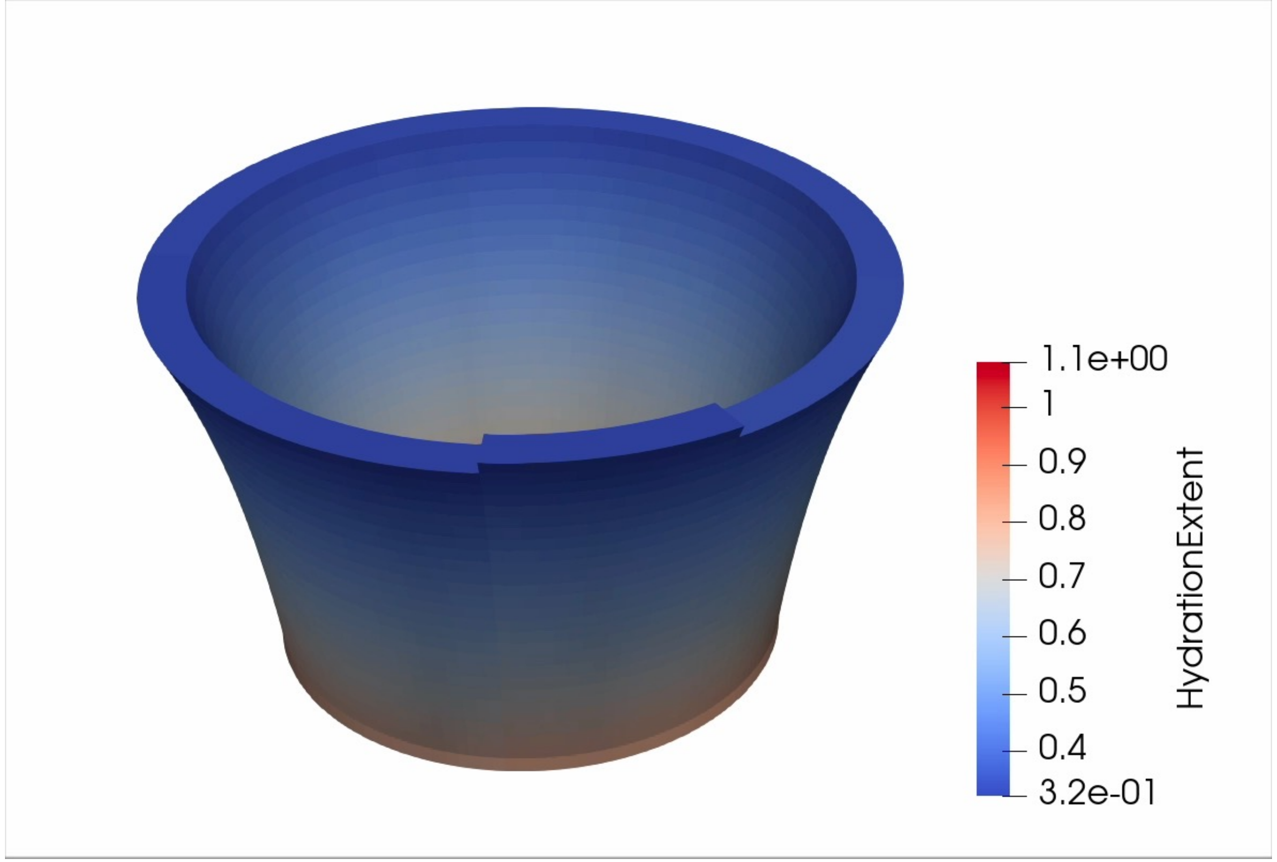
Mesh at step n+1
Blue part is the newly added mesh section



Mesh with 20 subdivisions per layer prepared with GMSH

Digital printing

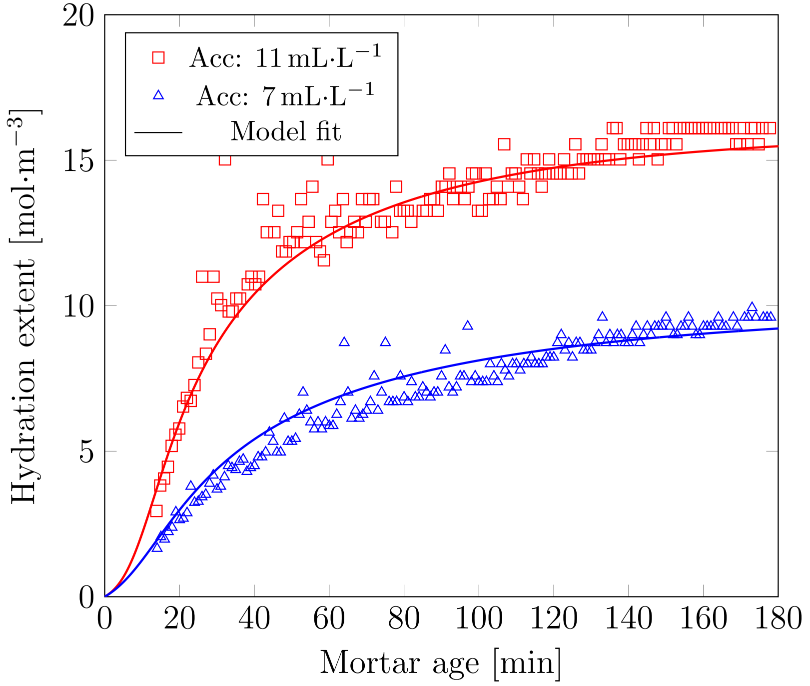




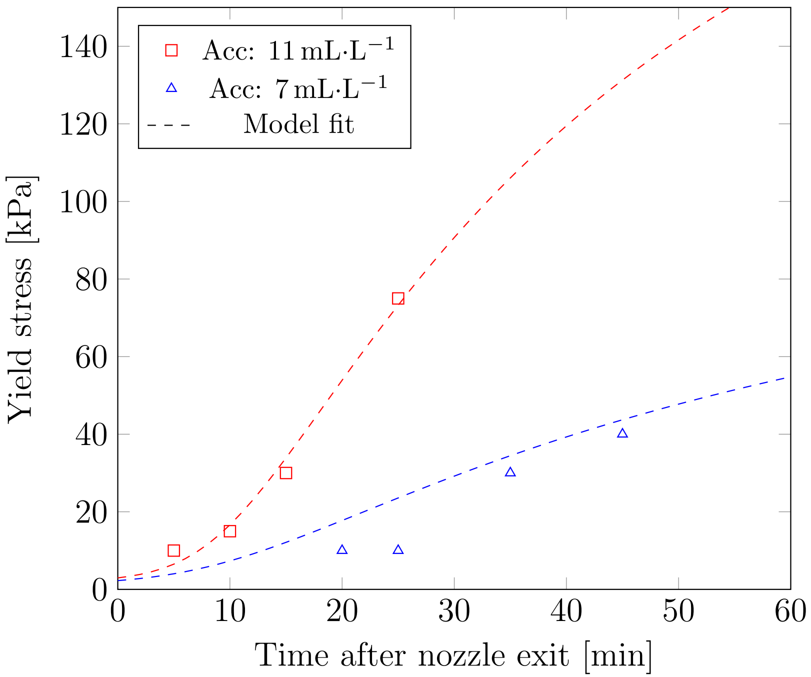
Fitting and predictive capability

- Model fitting on data with 11 mL/L accelerator (red)
- Model prediction for 7 mL/L

$$\frac{\mathrm{d}\xi}{\mathrm{d}t} = \frac{k_\xi}{\eta_\xi^0}\left(\frac{\mathcal{A}_\xi^0}{k_\xi \xi_\infty} + \xi\right)(\xi_\infty - \xi)\cdot \exp\left(-\bar{\eta}\frac{\xi}{\xi_\infty}\right)\cdot \exp\left(-\frac{E_a}{RT}\right)\cdot \beta_{Rh}$$



Hydration kinetics from p-wave velocity measurements

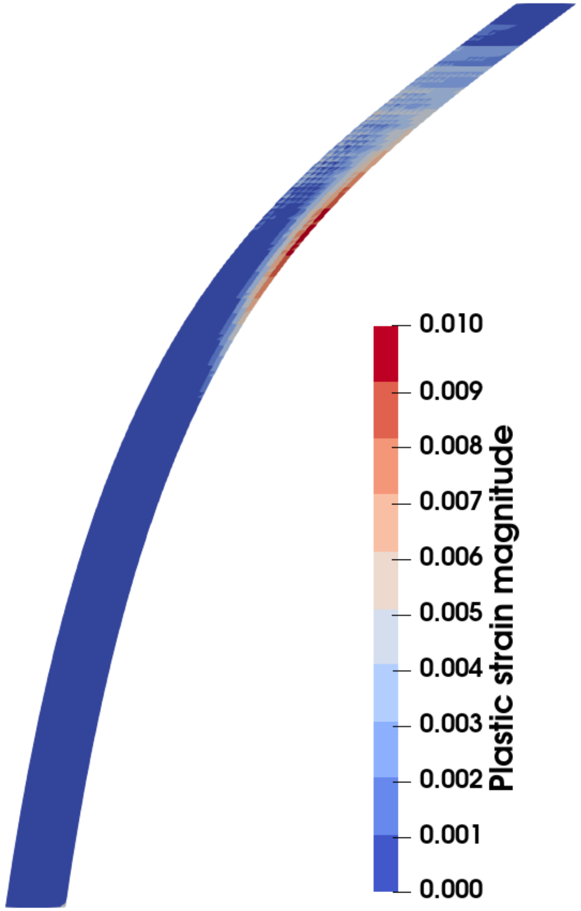


Yield stress measurements from hand shear vane

- **Ability to capture changes in accelerator dosage with a single parameter set**

Experimental comparison

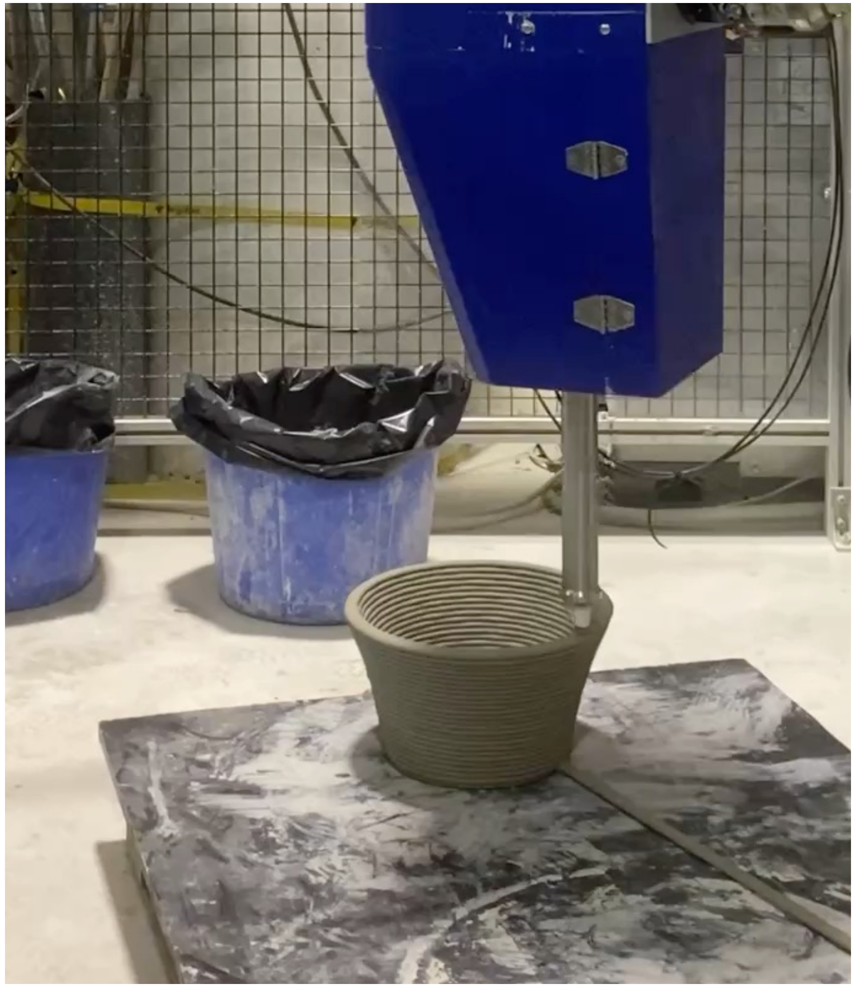
- ➢ Accelerator: 11 mL/L
- ➢ Printing speed: 13 cm/s

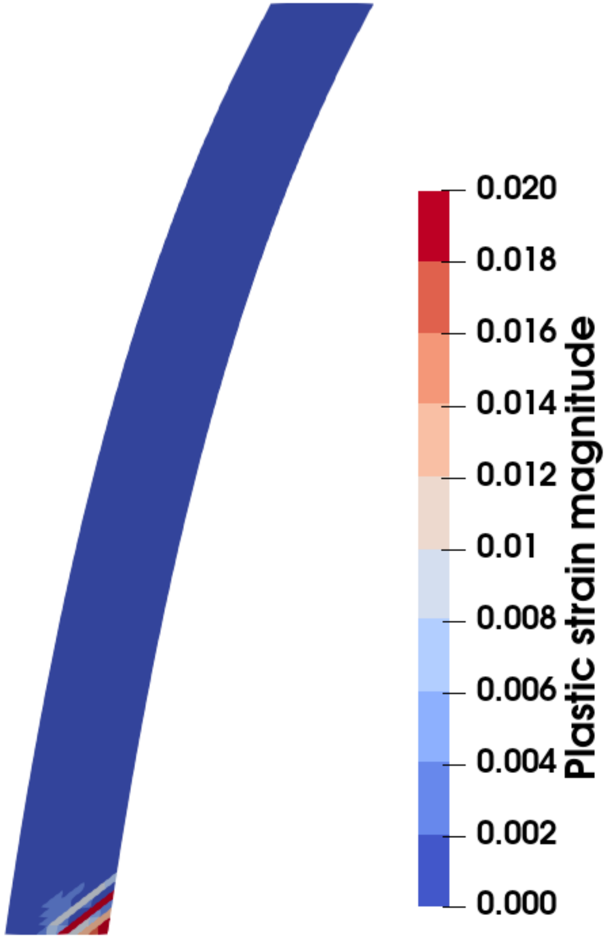


➢ **Plastic collapse does not necessarily initiate from the bottom layer**

Experimental comparison

- Accelerator: 7 mL/L
- Printing speed: 20 cm/s

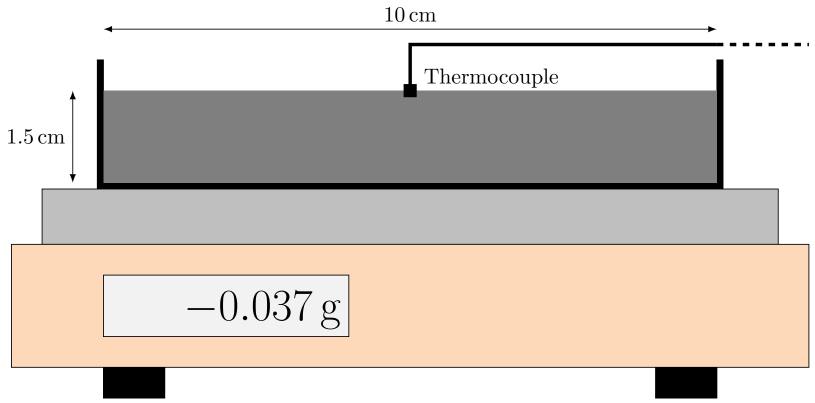




- **But sometimes it does initiate from the bottom layer**

Concrete drying/hydration couplings

Evaporation test and simulation setup



Experimental setup to measure surface temperature and water mass loss

- Identical mix to 3D printing with accelerating admixture
- Left to dry in air-conditioned room for two weeks
- Ambient $R_h \simeq 50\%$

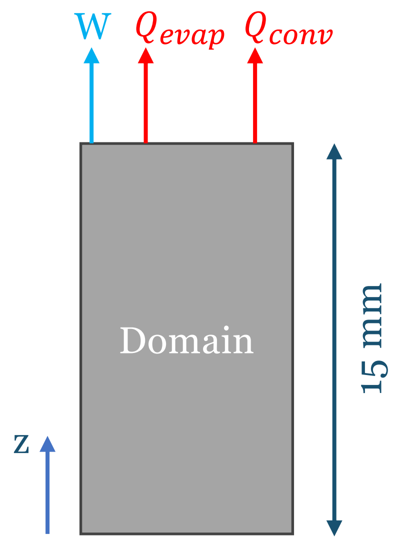
- Liquid evaporation boundary condition (Uno 1998):

$$\underbrace{W[\mathrm{kg{\cdot}m^{-2}{\cdot}s^{-1}}]}_{\text{mass flux}} = \underbrace{\left(\frac{1 + v_{wind}/v_0}{v_1}\right)}_{\text{wind speed}} \cdot \underbrace{(p_{v,int} - p_{v,ext})}_{\text{vapour pressure}}$$

- Thermal boundary conditions

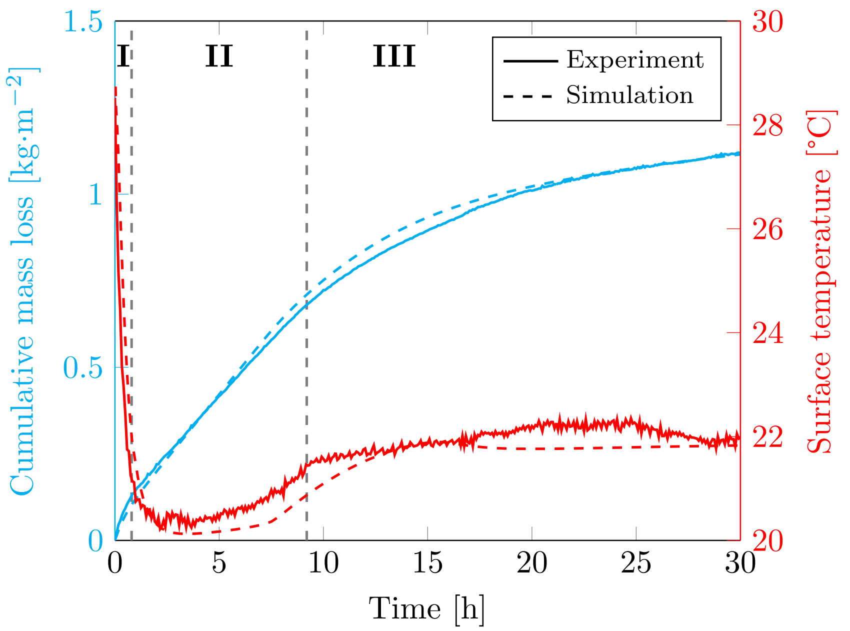
Evaporative: $$Q_{evap} = \frac{\Delta H_{vap}}{\mathcal{M}_{\mathrm{H}}} W$$

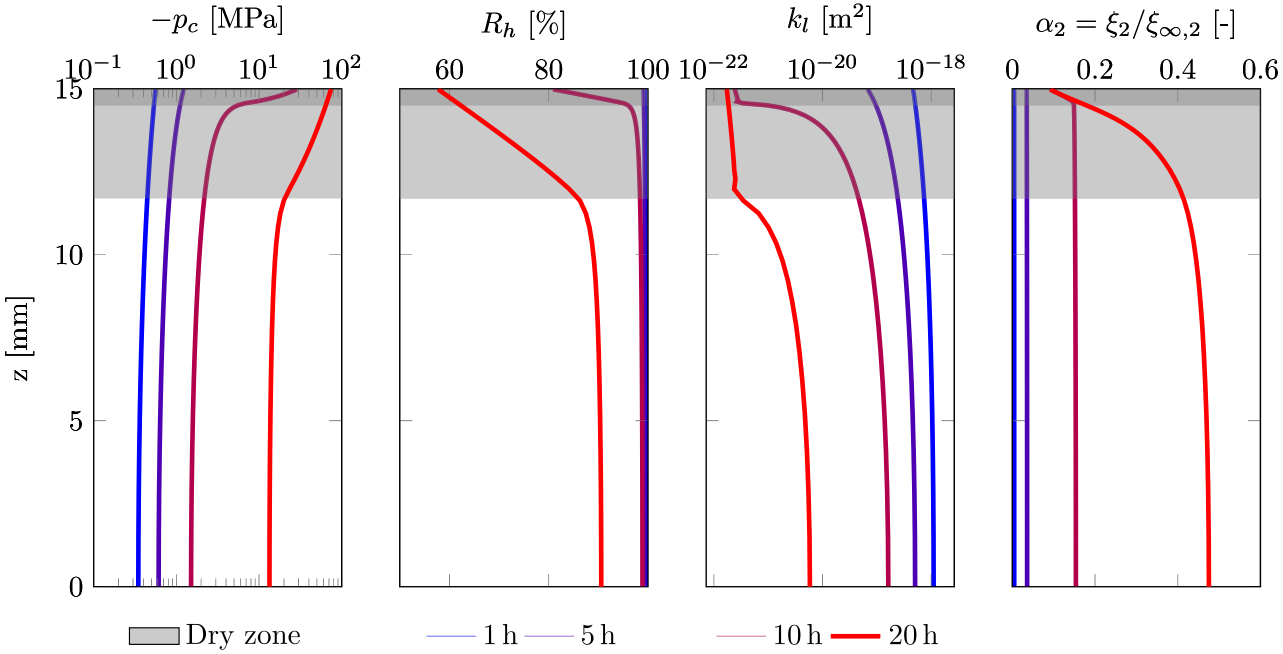
Convective: $$Q_{conv} = h_{conv}(T_{int} - T_{ext})$$



Simulation domain and boundary conditions

Model validation





- 5h: Slight permeability decrease near surface
- 10h: Dry front initiation
- 10h+: Dry zone progresses inside the material

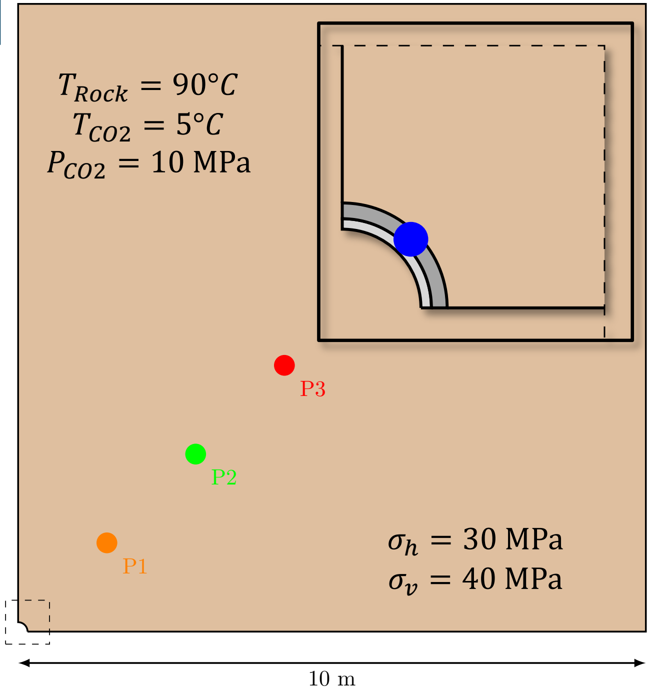
Simulated variables profile in the slab's thickness
(evaporation surface on top)

- **Consistent results with experiment and knowledge on drying of porous media**

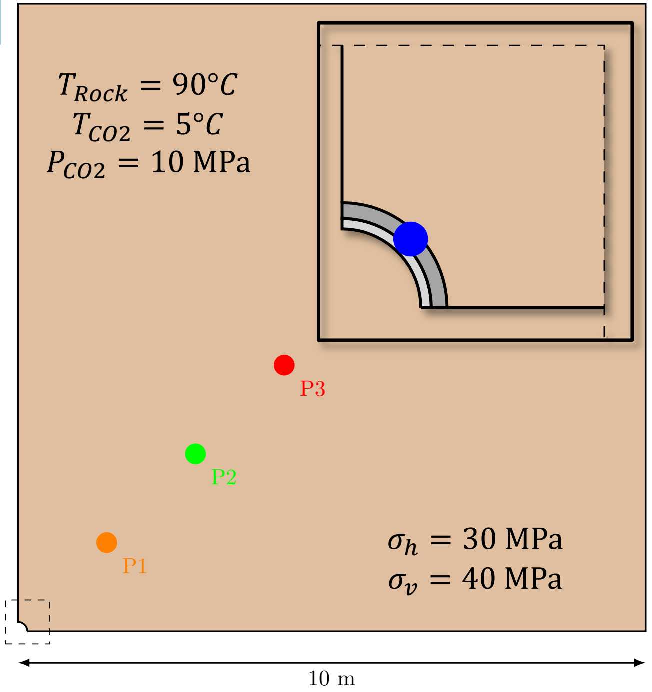
CO_2 injection in deep wells

Multi-material coupled THM

THM multimaterial simulation for deep CO2 injection



THM multimaterial simulation for deep CO2 injection



Thank you for your attention