Multiscale poromechanics of mature cement pastes: Expansion during isothermal re-wetting

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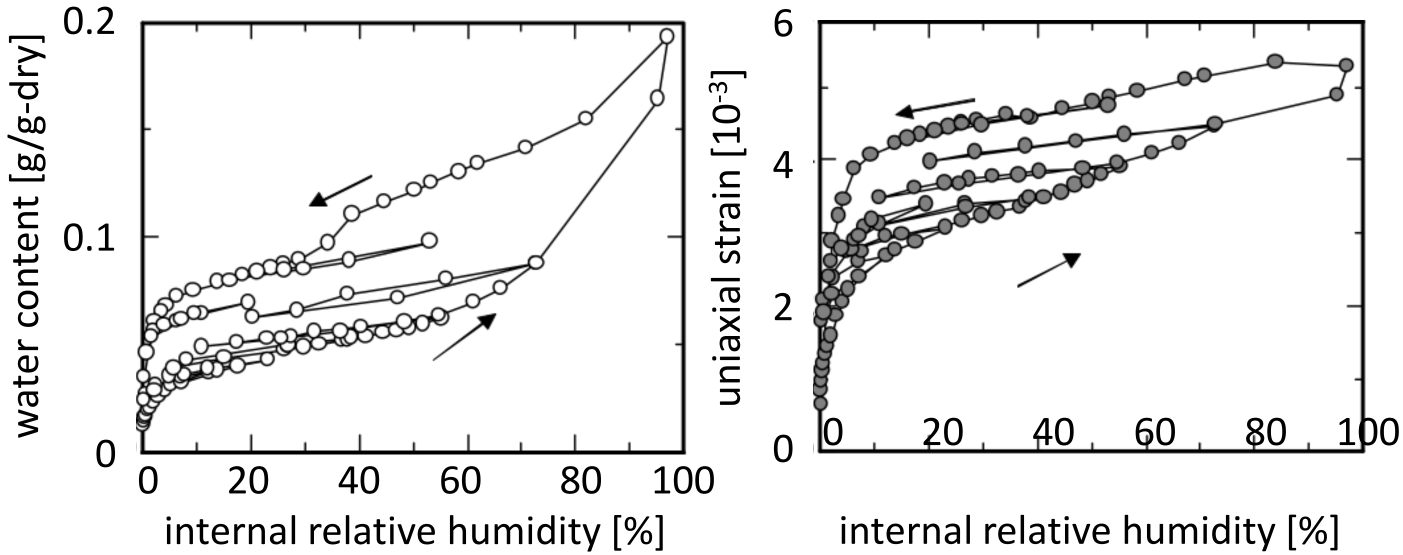
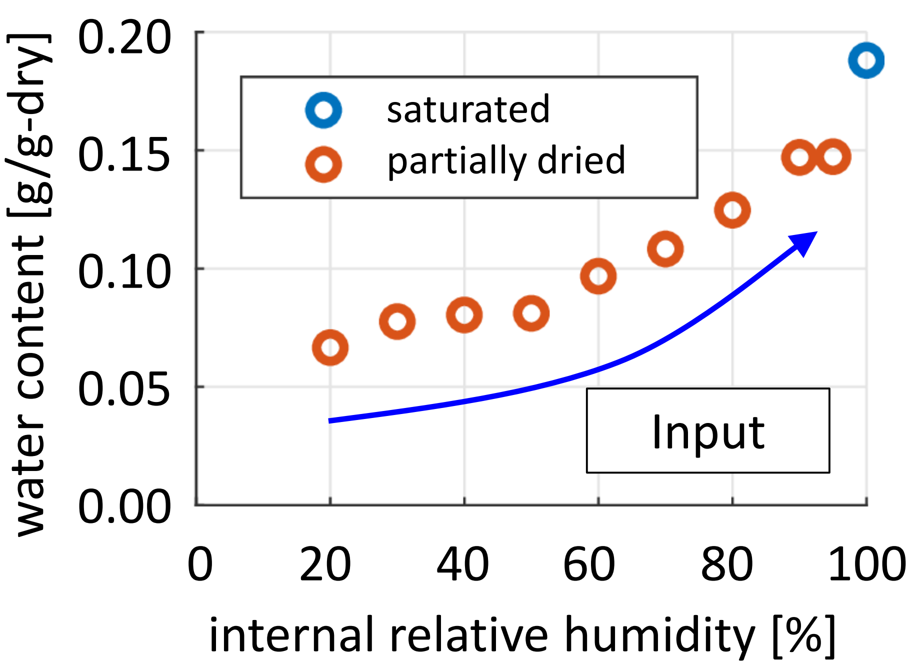
Motivation

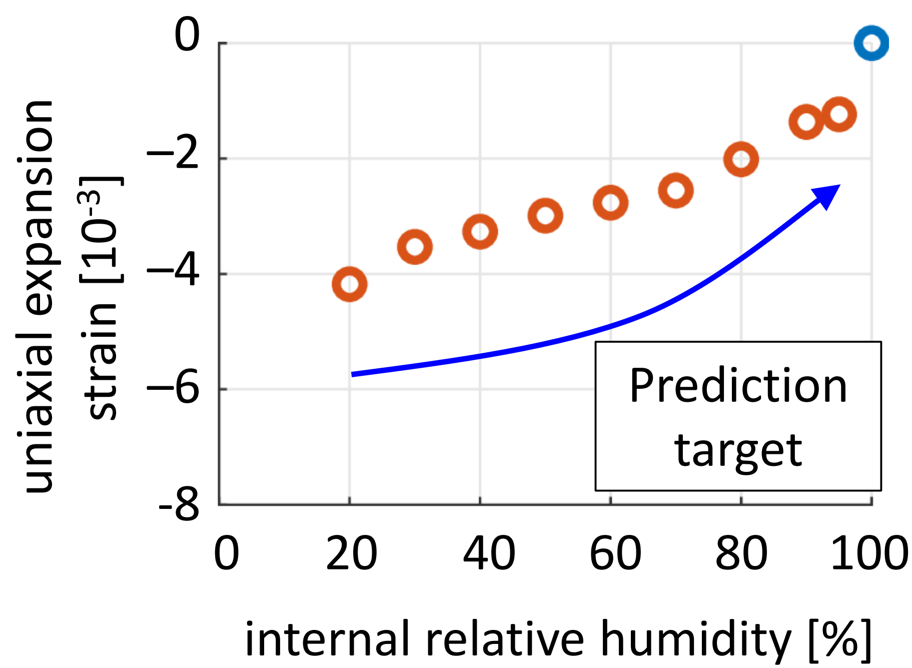
- Desorption/adsorption cycles result in hysteresis of water content and macroscopic volume changes



- Other constituents of concrete do not exhibit this behavior
- Internal stresses → Cracking

Experiments by Maruyama: data from first isothermal re-wetting



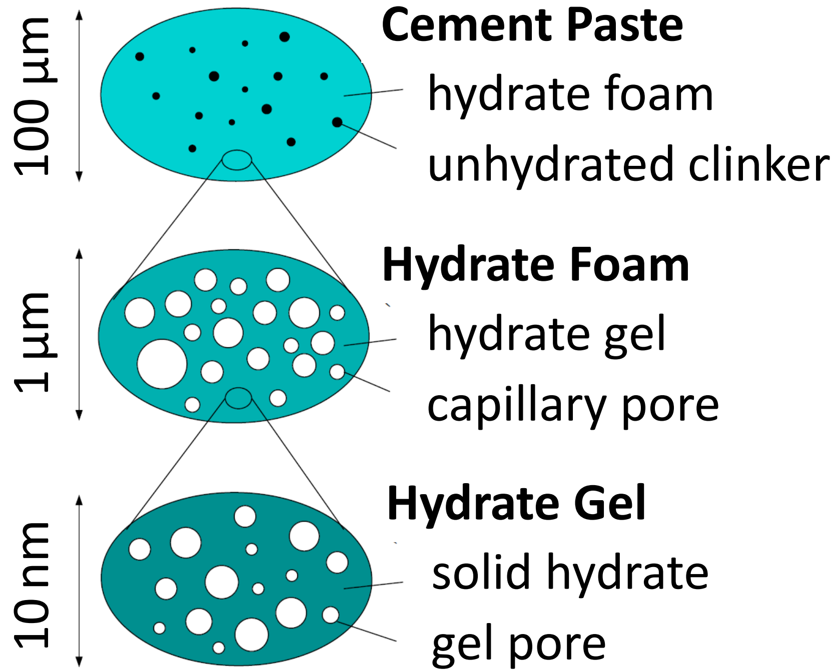


Aim: Development of multiscale hygro-poro-elastic model

- Input: water content as a function of relative humidity
- Aim: predicting expansion as a function of relative humidity

[Maruyama, Journal of Advanced Concrete Technology, 2010] http://doi.org/fjm3vx

Hierarchical organization of mature cement pastes + properties of solid constituents



Volume fractions

$$f_{hf}^{cp} = \frac{w/c + 0.32\,\xi}{w/c + 0.32}$$

$$f_{clin}^{cp} = \frac{0.32\,(1-\xi)}{w/c + 0.32}$$

$$f_{gel}^{hf} = \frac{0.68\,\xi}{w/c + 0.32\,\xi}$$

$$f_{cpor}^{hf} = \frac{w/c - 0.36\,\xi}{w/c + 0.32\,\xi}$$

$$f_{hyd}^{gel} = 0.72\,, \qquad f_{gpor}^{gel} = 0.28$$

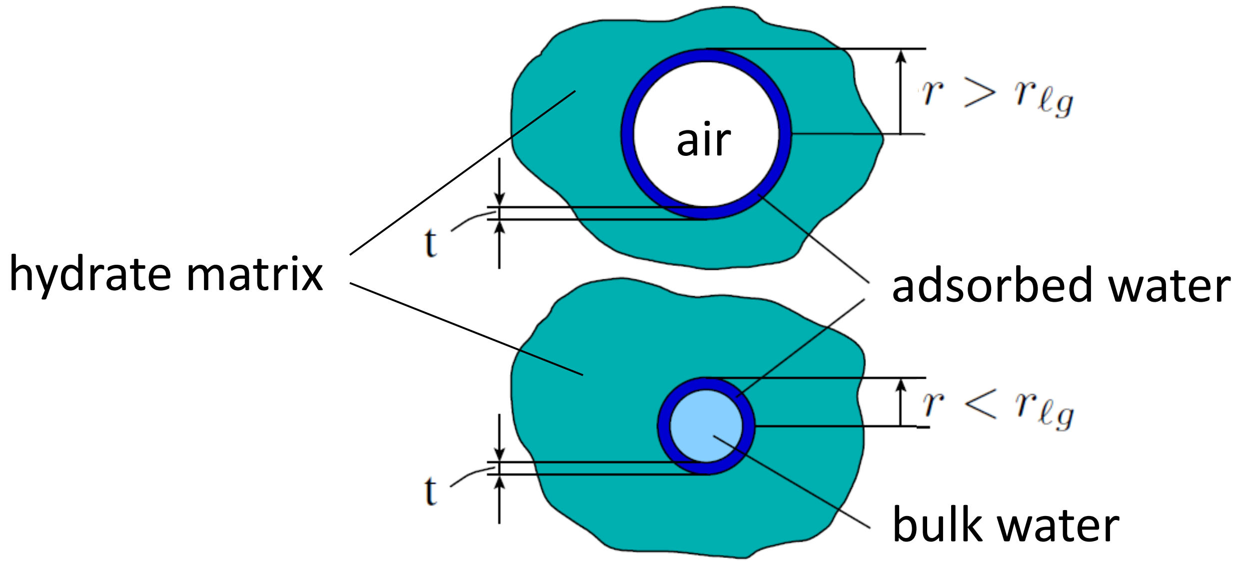
Elastic stiffness constants

$$\mathbb{C}_k = 3k_k \mathbb{I}_{vol} + 2\mu_k \mathbb{I}_{dev}\,, \qquad k \in \{clin, hyd\}$$

$$k_{clin} = 116.7\,\text{GPa}\,, \qquad \mu_{clin} = 53.8\,\text{GPa} \qquad k_{hyd} = 31.8\,\text{GPa}\,, \qquad \mu_{hyd} = 19.1\,\text{GPa}$$

[Wang et al., Cement & Concrete Research, 2018] http://doi.org/csgw

Status of pores under partial saturation



thickness of adsorbed water layer

$$t = 0.385\text{nm} - \ln[-\ln(RH)] \cdot 0.189\text{nm}$$

[Badmann et al., J. Colloid Interf. Sci., 1981]

radius distinguishing air-/water-filled pores

$$r_{lg} = -\frac{2\,\gamma^{lg} v_m \cos\theta}{\ln(RH)\;RT} + t$$

Kelvin-Cohan equation

[Wang et al., Cement & Concrete Research, 2018] http://doi.org/csgw

Effective pore pressures acting on solid skeleton

1) Effective pressure of individual pores:

$$p(r) = \begin{cases} p_\ell - \frac{2\,\gamma^{s\ell}}{r-t} & \cdots \quad r \le r_{\ell g} \\ p_g - \frac{2\,\gamma^{sg}}{r-t} & \cdots \quad r > r_{\ell g} \end{cases}$$

Combination with

- Kelvin-Laplace equation
  minimization of Gibbs free energy
  $$p_g - p_\ell = -\ln(RH)\frac{RT}{v_m}$$
- Young's equation
  equilibrium of forces
  $$\gamma^{\ell g}\,\cos\theta = \gamma^{sg} - \gamma^{s\ell}$$
- Berthelot's state equation
  energy of adhesion $W_{sl} = \sqrt{W_{ss}W_{ll}}$
  $$\gamma^{s\ell} = \gamma^{\ell g} + \gamma^{sg} - 2\sqrt{\gamma^{\ell g}\,\gamma^{sg}}$$

➢ Effective pressure of individual pores:

$$p(r) = \begin{cases} \ln(RH)\frac{RT}{\nu_m} & \cdots \quad r \le r_{\ell g} \\ -\frac{2\,\gamma^{\ell g}}{r-t} & \cdots \quad r > r_{\ell g} \end{cases}$$

2) Average effective pore pressure of gel and capillary pore families:

$$p_k = \int_0^\infty p(r)\,\phi_k^{pdf}(r)\,\mathrm{d}r\,, \quad k \in [\,gpor\,;\,cpor\,]$$

$\phi_k^{pdf}(r)$ … pore size distribution

[Wang et al., Cement & Concrete Research, 2018] http://doi.org/csgw

Identification of pore size distributions: adsorption porosimetry

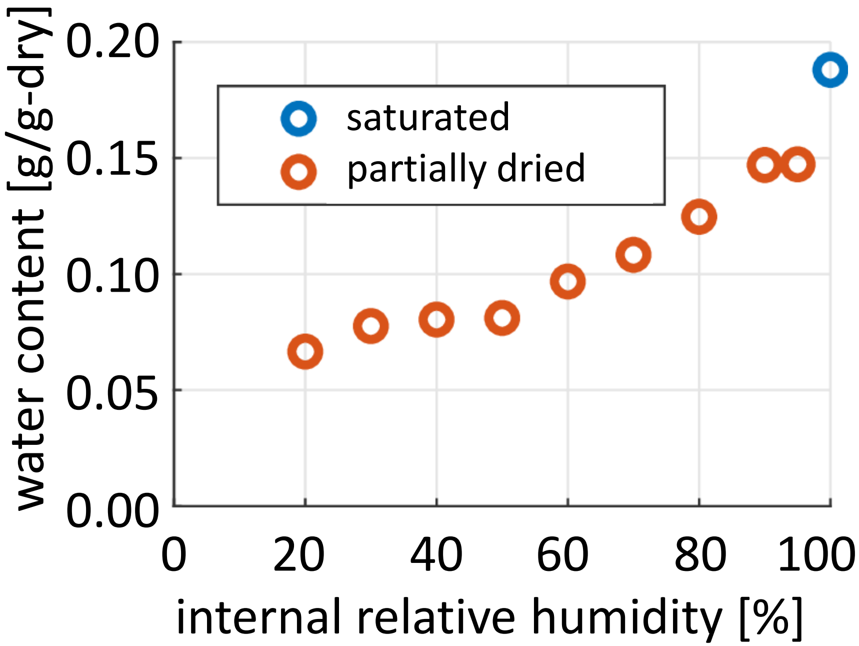
Pore size probability distribution $\phi_k^{pdf}(r) = \frac{1}{R_k} \exp\left(-\frac{r}{R_k}\right), \quad k \in [\,gpor\,;\,cpor\,]$

Modeled saturation degree

$$S_r^{mod} = \frac{\Delta m_{H_2O}(RH) + m_{H_2O}^{exp}(RH = 20\%)}{m_{dry}}$$

Experimental saturation degree

$$S_r^{exp} = \frac{m_{sample}(RH) - m_{dry}}{m_{dry}}$$

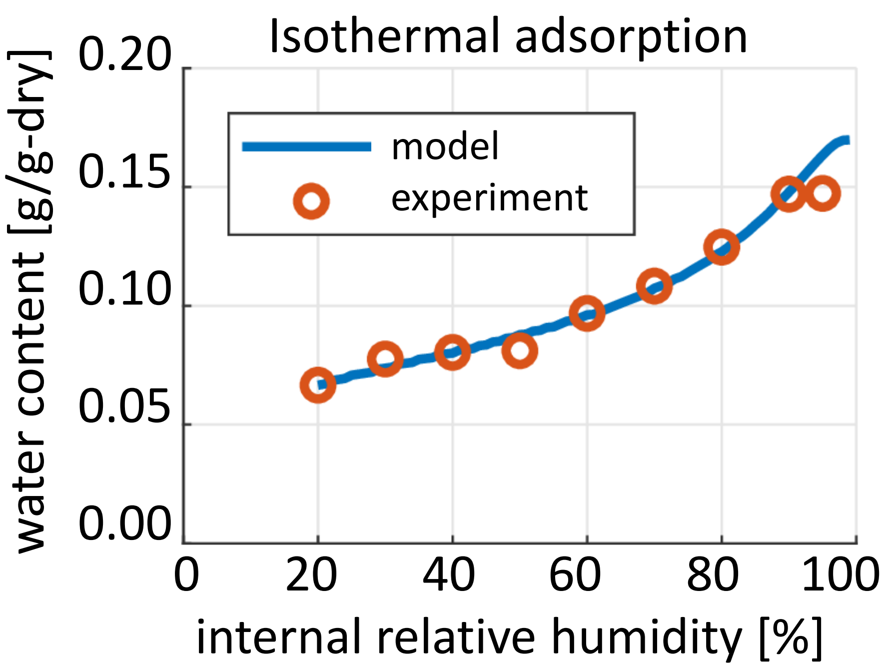


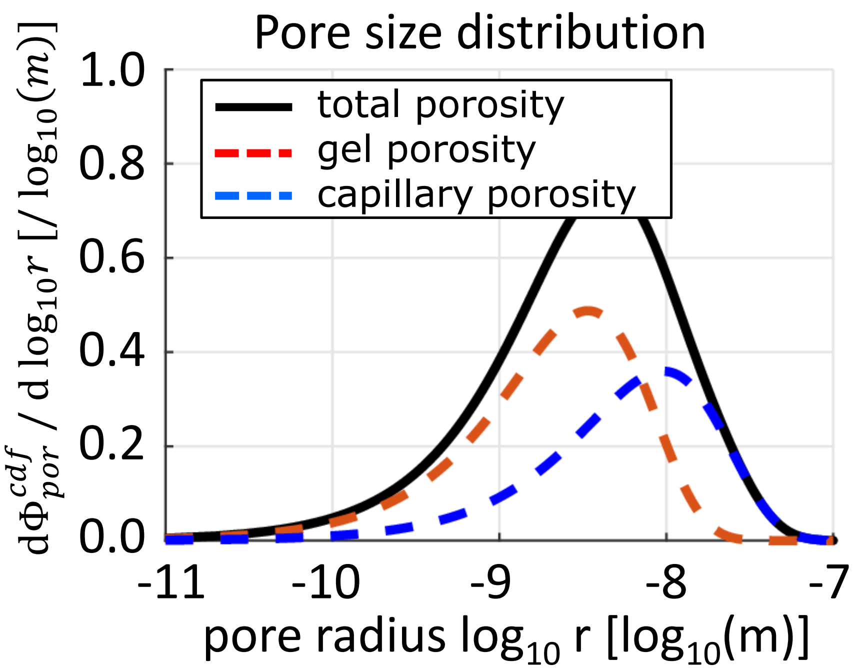
Identification of characteristic pore radii:

$$\varepsilon_{SRSS}\underbrace{\left(R_{gpor}, R_{cpor}\right)}_{\text{characteristic radii}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[S_r^{mod}\left(RH_i, R_{gpor}, R_{cpor}\right) - S_r^{exp}(RH_i)\right]^2} \;\rightarrow\; min$$

[Wang et al., Cement & Concrete Research, 2018] http://doi.org/csgw

Identification of pore radii





Pore size probability distribution $\phi_k^{pdf}(r) = \frac{1}{R_k} \exp\left(-\frac{r}{R_k}\right) , \quad k \in [\, gpor \,;\, cpor \,]$

$\Rightarrow$ $R_{gpor} = 3$ nm $\quad R_{cpor} = 10$ nm

Homogenization of eigenstressed elastic composites

Microscopic input

$$\forall \underline{x} \in V_k : \begin{cases} \mathbb{C}(\underline{x}) = \mathbb{C}_k \\ \boldsymbol{\sigma}^E(\underline{x}) = \boldsymbol{\sigma}_k^E \end{cases} , \quad f_k = \frac{V_k}{V} , \quad k \in [m\,;\,i]$$

Macroscopic expansion (eigenstrain)

$$\mathbf{E}^E_{\text{hom}} = -\mathbb{C}^{-1}_{\text{hom}} : \boldsymbol{\Sigma}^E_{\text{hom}}$$

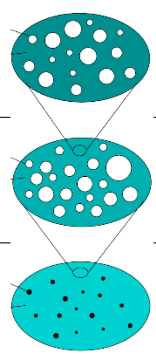
homogenized stiffness

$$\mathbb{C}_{\text{hom}} = f_m \mathbb{C}_m : \mathbb{A}_m + f_i \mathbb{C}_i : \mathbb{A}_i$$

homogenized eigenstress

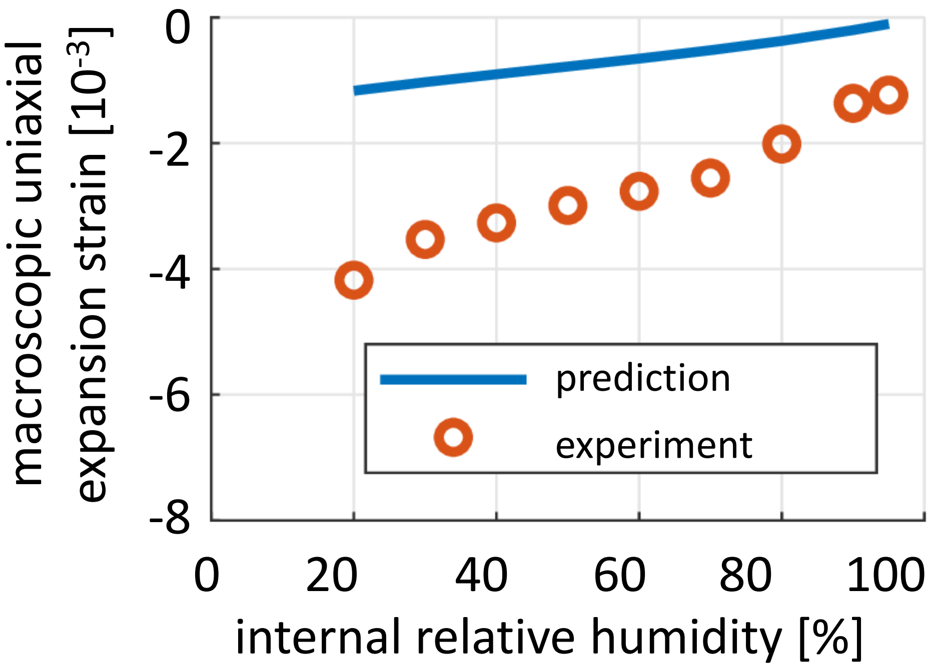
$$\boldsymbol{\Sigma}^E_{\text{hom}} = f_m \boldsymbol{\sigma}^E_m : \mathbb{A}_m + f_i \boldsymbol{\sigma}^E_i : \mathbb{A}_i$$

$\mathbb{A}_k$ – strain concentration tensor



Bottom-up homogenization	constituents	volume fraction	stiffness	eigenstress	homog. stiffness	homog. eigenstress
hydrate gel	solid hydrates	f^{gel}_{hyd}	$\mathbb{C}_{hyd}$	$\boldsymbol{\sigma}^E_{hyd} = 0$	$\mathbb{C}_{gel}$	$\boldsymbol{\Sigma}^E_{gel}$
	gel pores	f^{gel}_{gpor}	$\mathbb{C}_{gpor} = 0$	$\boldsymbol{\sigma}^e_{gpor} = -p_{gpor}\mathbf{1}$		
hydrate foam	hydrate gel	f^{hf}_{gel}	$\mathbb{C}_{gel}$	$\boldsymbol{\Sigma}^E_{gel}$	$\mathbb{C}_{hf}$	$\boldsymbol{\Sigma}^E_{hf}$
	capillary pores	f^{hf}_{cpor}	$\mathbb{C}_{cpor} = 0$	$\boldsymbol{\sigma}^e_{cpor} = -p_{cpor}\mathbf{1}$		
cement paste	hydrate foam	f^{cp}_{hf}	$\mathbb{C}_{hf}$	$\boldsymbol{\Sigma}^E_{hf}$	$\mathbb{C}_{cp}$	$\boldsymbol{\Sigma}^E_{cp}$
	clinker	f^{cp}_{clin}	$\mathbb{C}_{clin}$	$\boldsymbol{\sigma}^E_{clin} = 0$		

Prediction of macroscopic expansion resulting from changes of pore pressure $\left(\sigma_{hyd}^{E} = 0\right)$



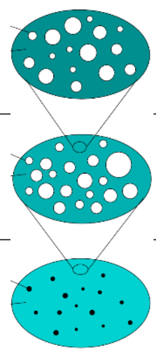
Changes of pore pressures

- contribute significantly to macroscopic expansion
- important but not sufficient

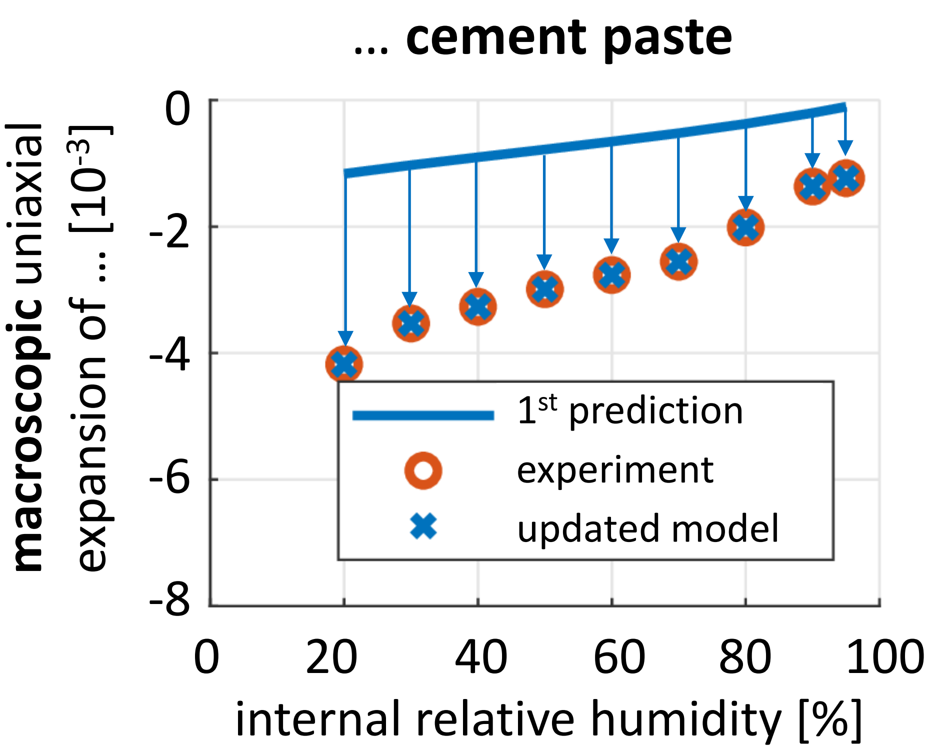
- Hydrates are swelling due to increase of RH
- **Aim:** identify RH-driven expansion of solid hydrates

[Maruyama, Journal of Advanced Concrete Technology, 2010] http://doi.org/fjm3vx

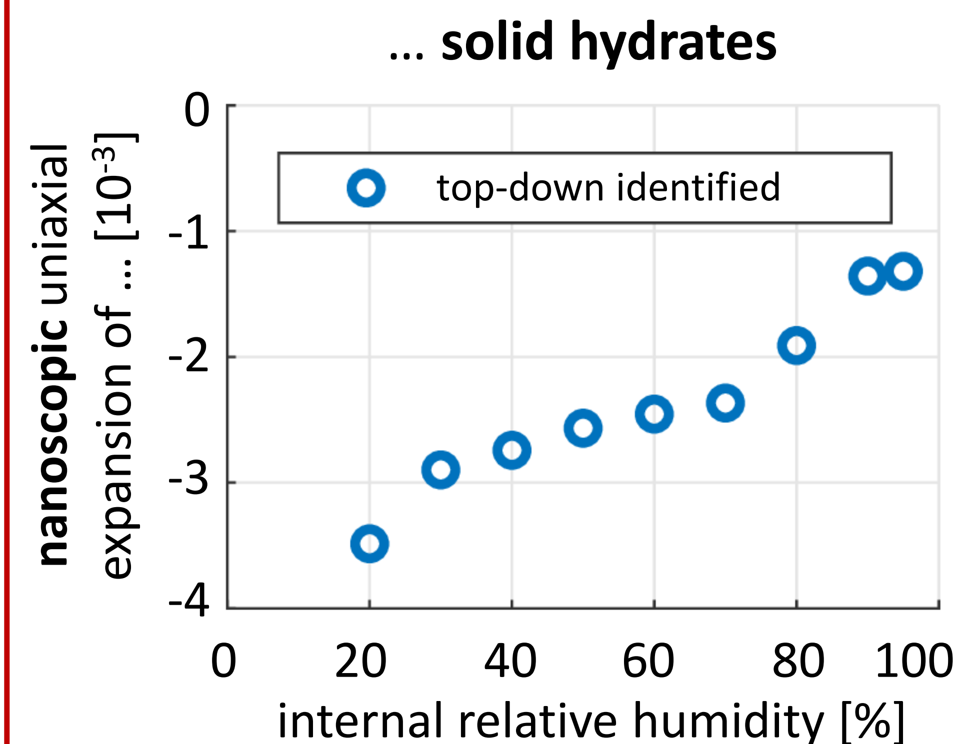
Top-down identification of eigenstress of solid hydrates $\boldsymbol{\sigma}^E_{hyd}(RH)$

Bottom-up homogenization	constituents	volume fraction	stiffness	eigenstress	homog. stiffness	homog. eigenstress
hydrate gel 	solid hydrates	f^{gel}_{hyd}	$\mathbb{C}_{hyd}$	$\boldsymbol{\sigma}^E_{hyd} = \boldsymbol{\sigma}^E_{hyd}(RH)$	$\mathbb{C}_{gel}$	$\boldsymbol{\Sigma}^E_{gel}$
	gel pores	f^{gel}_{gpor}	$\mathbb{C}_{gpor} = 0$	$\boldsymbol{\sigma}^e_{gpor} = -p_{gpor}\mathbf{1}$		
hydrate foam	hydrate gel	f^{hf}_{gel}	$\mathbb{C}_{gel}$	$\boldsymbol{\Sigma}^E_{gel}$	$\mathbb{C}_{hf}$	$\boldsymbol{\Sigma}^E_{hf}$
	capillary pores	f^{hf}_{cpor}	$\mathbb{C}_{cpor} = 0$	$\boldsymbol{\sigma}^e_{cpor} = -p_{cpor}\mathbf{1}$		
cement paste	hydrate foam	f^{cp}_{hf}	$\mathbb{C}_{hf}$	$\boldsymbol{\Sigma}^E_{hf}$	$\mathbb{C}_{cp}$	$\boldsymbol{\Sigma}^E_{cp}$
	clinker	f^{cp}_{clin}	$\mathbb{C}_{clin}$	$\boldsymbol{\sigma}^E_{clin} = 0$		

Top-down identification of eigenstress of solid hydrates $\boldsymbol{\sigma}_{hyd}^{E}(RH)$



➤ **Identification result**



[Maruyama, Journal of Advanced Concrete Technology, 2010] http://doi.org/fjm3vx

Conclusions

- Changes of relative humidity induce changes of effective pore pressures acting on the solid skeleton
- Changes of pore pressures induced by changes of relative humidity explain experimentally measured expansion of cement paste only partly
- Newly quantified RH-driven expansion of solid hydrates

Outreach: IES Alhama, Corella, Spain (29/3/2019)

Secondment: Saint Gobain, short visit October 2018
Heidelberg, starting February 2020