STADIUM model

Technical basis

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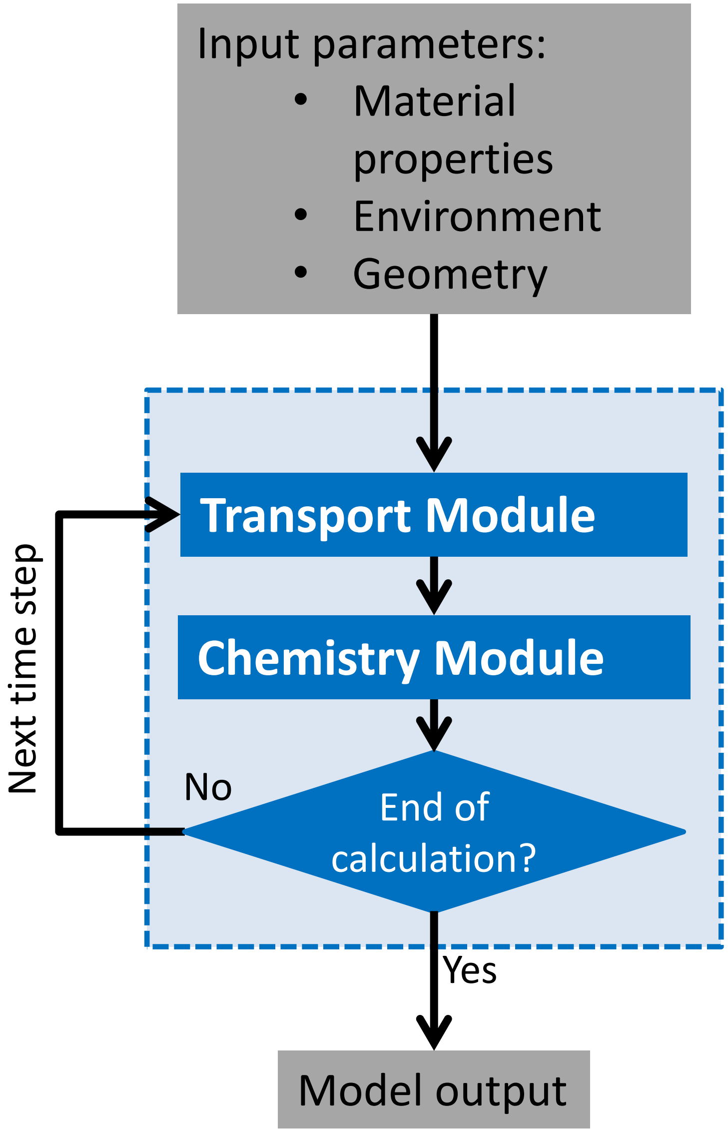
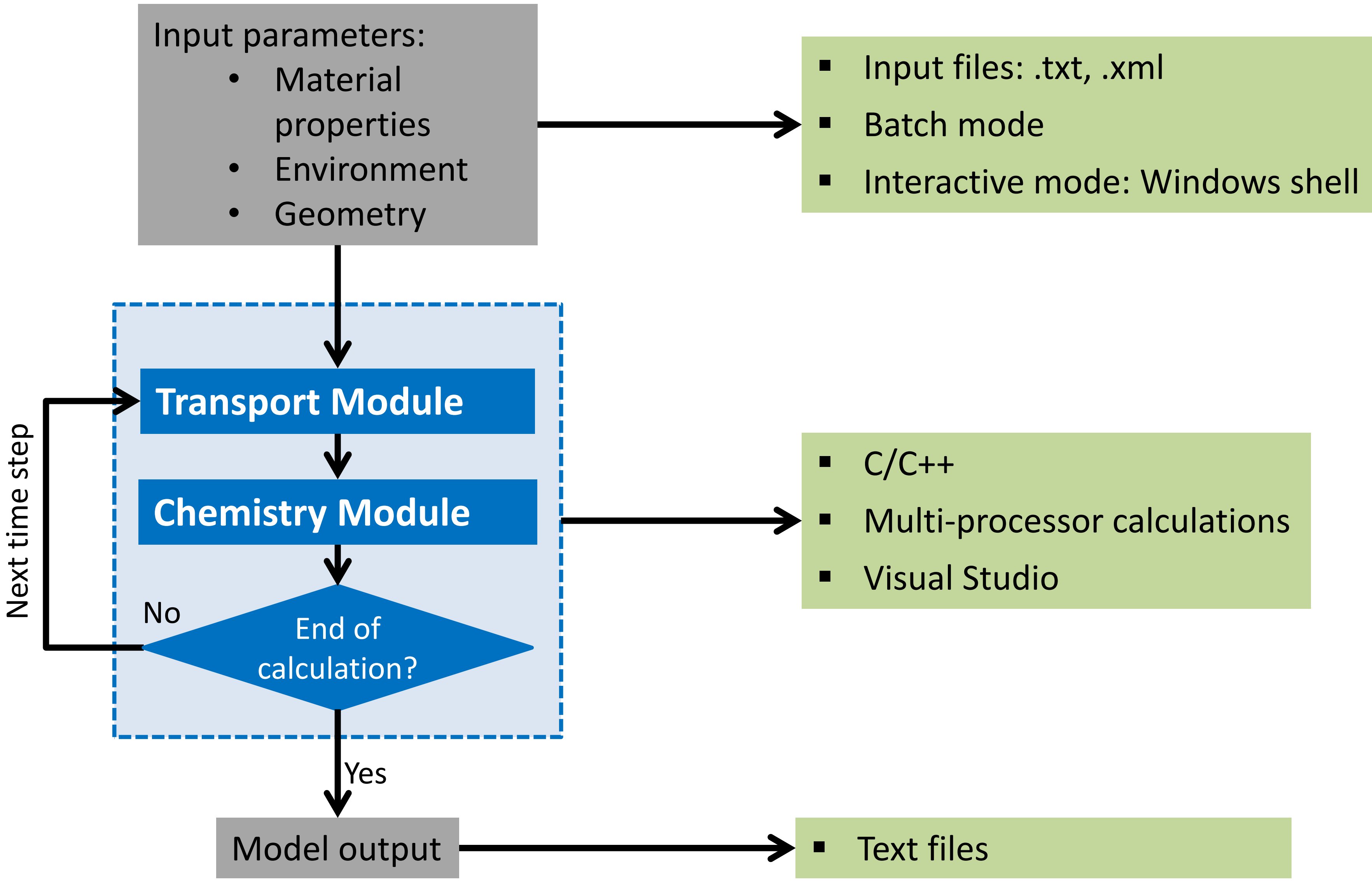
STADIUM Overview



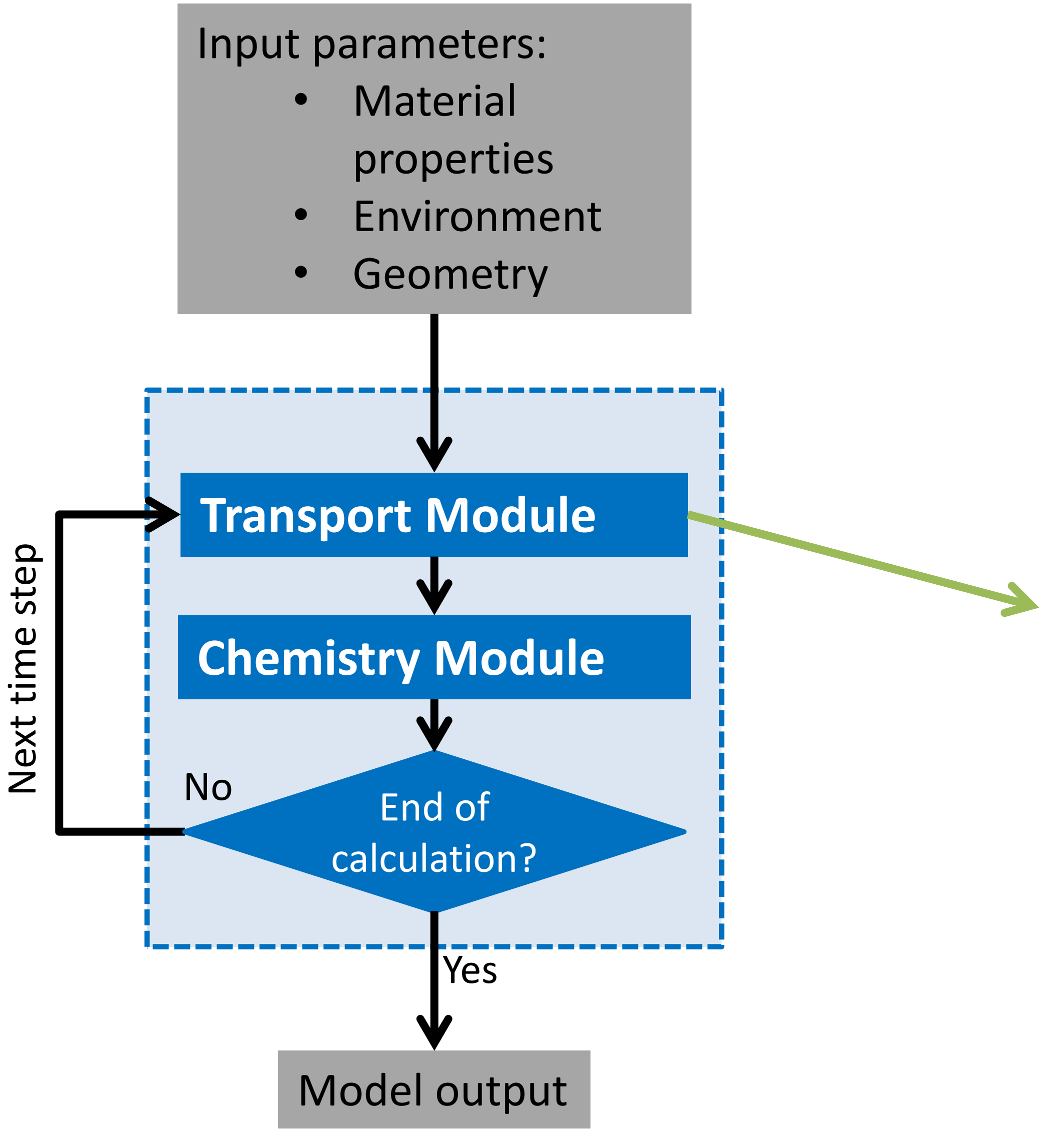
The model is divided in 2 main modules:

- The transport module makes the species move during one time step,
- The chemistry module simulates the reactions between species in the pores and the hydrated paste.

STADIUM Overview

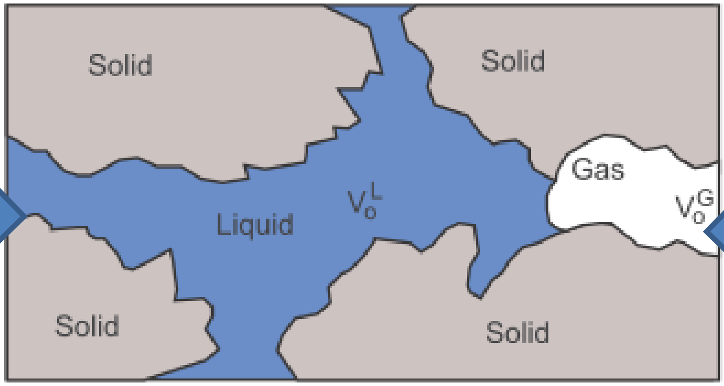


Transport Module



- Coupled species diffusion
- Moisture/Temperature coupling
- Transport of main species
- Feedback effect
- Time-dependent transport properties (hydration)
- Time-dependent B.C.

Moisture Transport



$$\mathbf{v_l} = -\frac{k_l}{\mu}\text{grad}(p_l)$$

$$\mathbf{j_v} = -\theta_g \tau_g D_v^o \text{grad}(\rho_v)$$

Averaging over REV
Assumption: diffusion-only movement of vapor

$$\frac{\partial w}{\partial H}\frac{\partial H}{\partial t} + \frac{\partial w}{\partial T}\frac{\partial T}{\partial t} - \text{div}\big(D_{mH}\text{grad}(H) + D_{mT}\text{grad}(T)\big) = 0$$

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Moisture Transport

$$\frac{\partial w}{\partial H}\frac{\partial H}{\partial t} + \frac{\partial w}{\partial T}\frac{\partial T}{\partial t} - \mathrm{div}\left(D_{mH}\,\mathrm{grad}(H) + D_{mT}\,\mathrm{grad}(T)\right) = 0$$

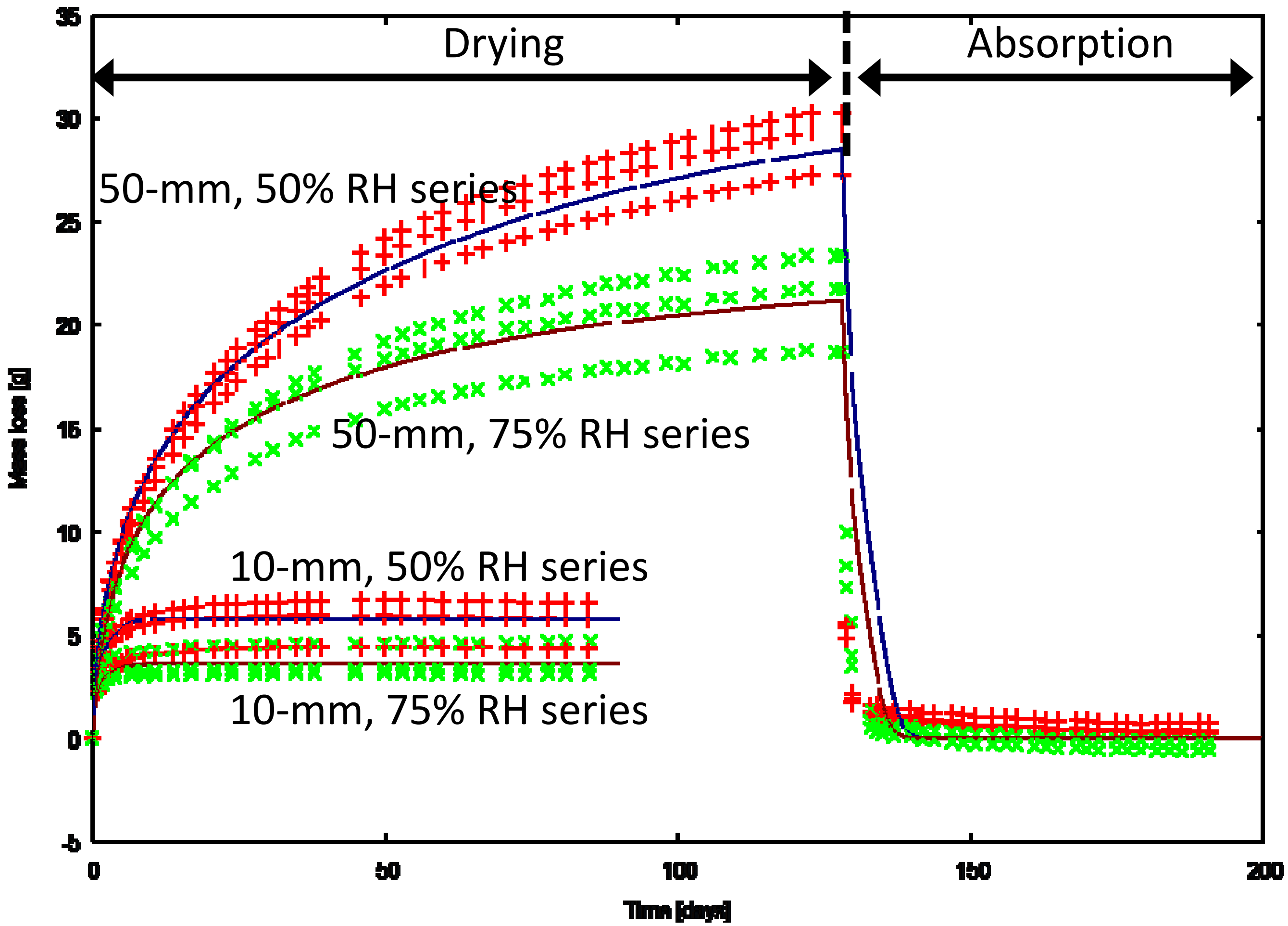
$$S = \frac{1}{\beta(H^{\delta} - 1) + 1}$$

$$D_{mH} = \frac{k_s k_r^l \rho_l R}{\mu M_w}\frac{T}{H} + \frac{D_v^o \tau_s \tau_r^g M_w p_v^s}{\rho_l R}\frac{(\phi - w)}{T}$$

$$k_r^l = \frac{1}{1 - a + aS^b}$$

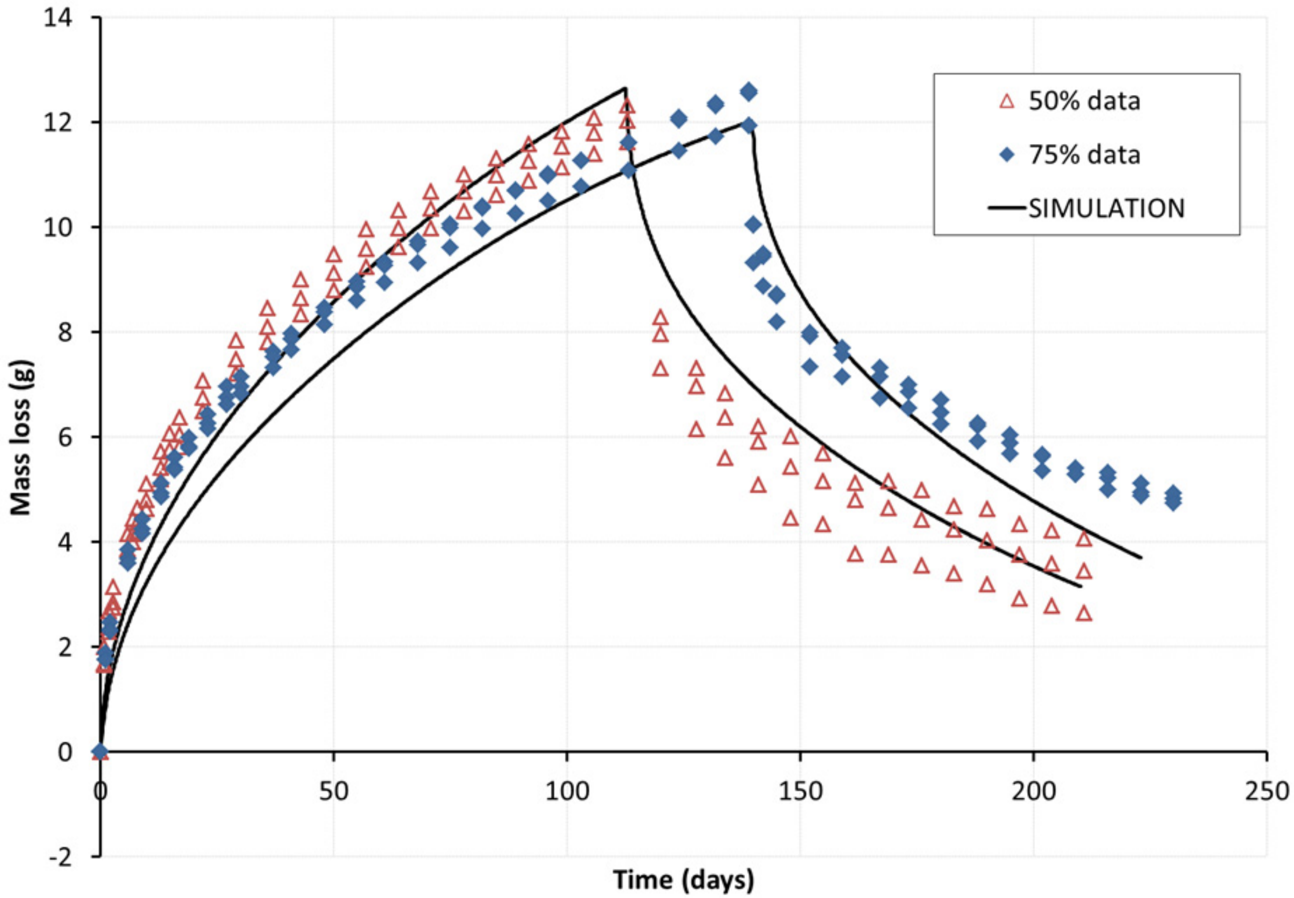
Moisture Transport

0.65 w/c opc concrete



Moisture Transport

0.40 w/c opc concrete + dampproofer



Species Transport

The transport of ions in **STADIUM** is modeled using the extended Nernst-Planck equation with an advection and temperature term:

Mass conservation equation: $$\frac{\partial(wc_i)}{\partial t} + \mathrm{div}(\mathbf{j_i}) = 0$$

Flux of ions:

$$\mathbf{j_i} = -D_i w \,\mathrm{grad}(c_i) - \frac{D_i z_i F}{RT} w c_i \,\mathrm{grad}(\psi) - D_i w c_i \,\mathrm{grad}(\ln \gamma_i) - \frac{D_i c_i \ln(\gamma_i c_i)}{T} w \,\mathrm{grad}(T) - c_i \boldsymbol{v_l}$$

Variables:

- **Concentrations *c_i***
- **Diffusion potential *ψ***
- **Relative humidity *H***
- **Temperature *T***

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Species Transport

To complete the system of equations, the following relationships are considered:

Poisson:
$$\mathrm{div}\,(\tau w\,\mathrm{grad}\,\psi) + \frac{F}{\epsilon}\,w\left(\sum_{i=1}^{N} z_i c_i\right) = 0$$

Heat conduction:
$$\rho C_p \frac{\partial T}{\partial t} - \mathrm{div}\big(\kappa\,\mathrm{grad}(T)\big) = 0$$

The system of equations is solved using the finite element method:

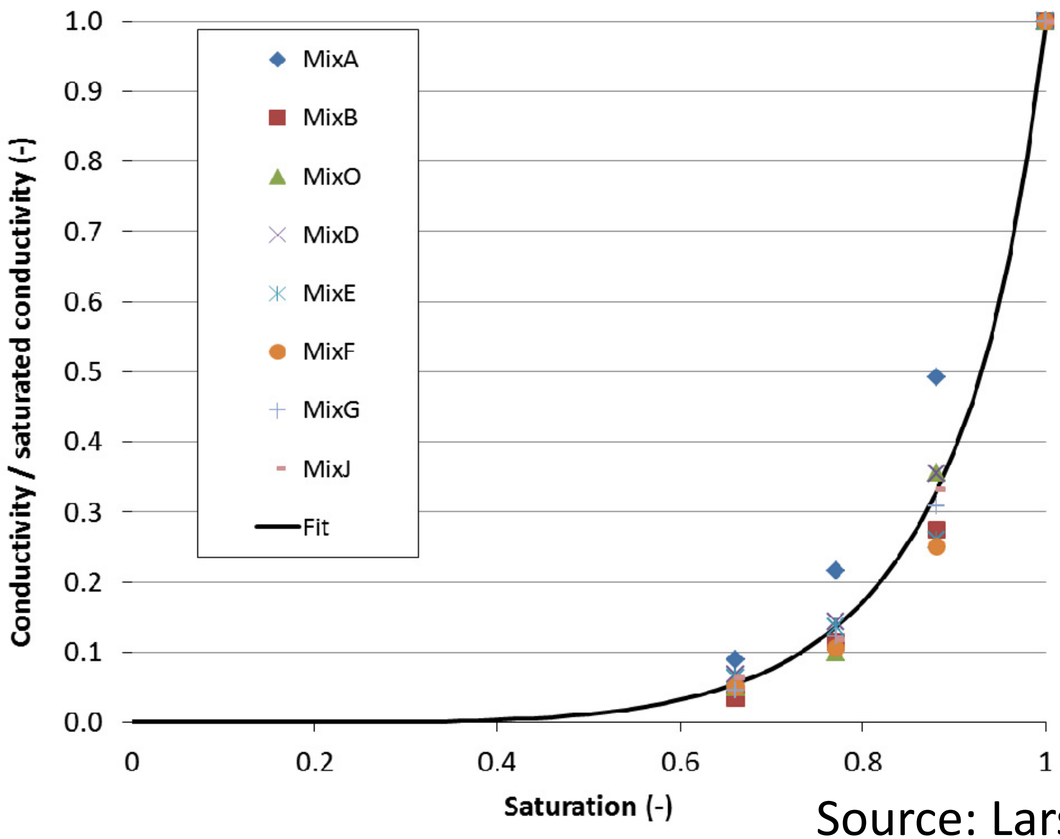
- **N+3 unknowns: N x c_i + H + ψ + T**
- **N+3 equations: N conservation + Poisson + moisture + Heat**

Species Transport

Diffusion coefficient: $D_i = \tau_s \tau_l^r D_i^o$

- τ_s: intrinsic tortuosity
- τ_l^r: relative tortuosity
- D_i^o: self-diffusion coefficient = *f(T)*

Effect of saturation on tortuosity:

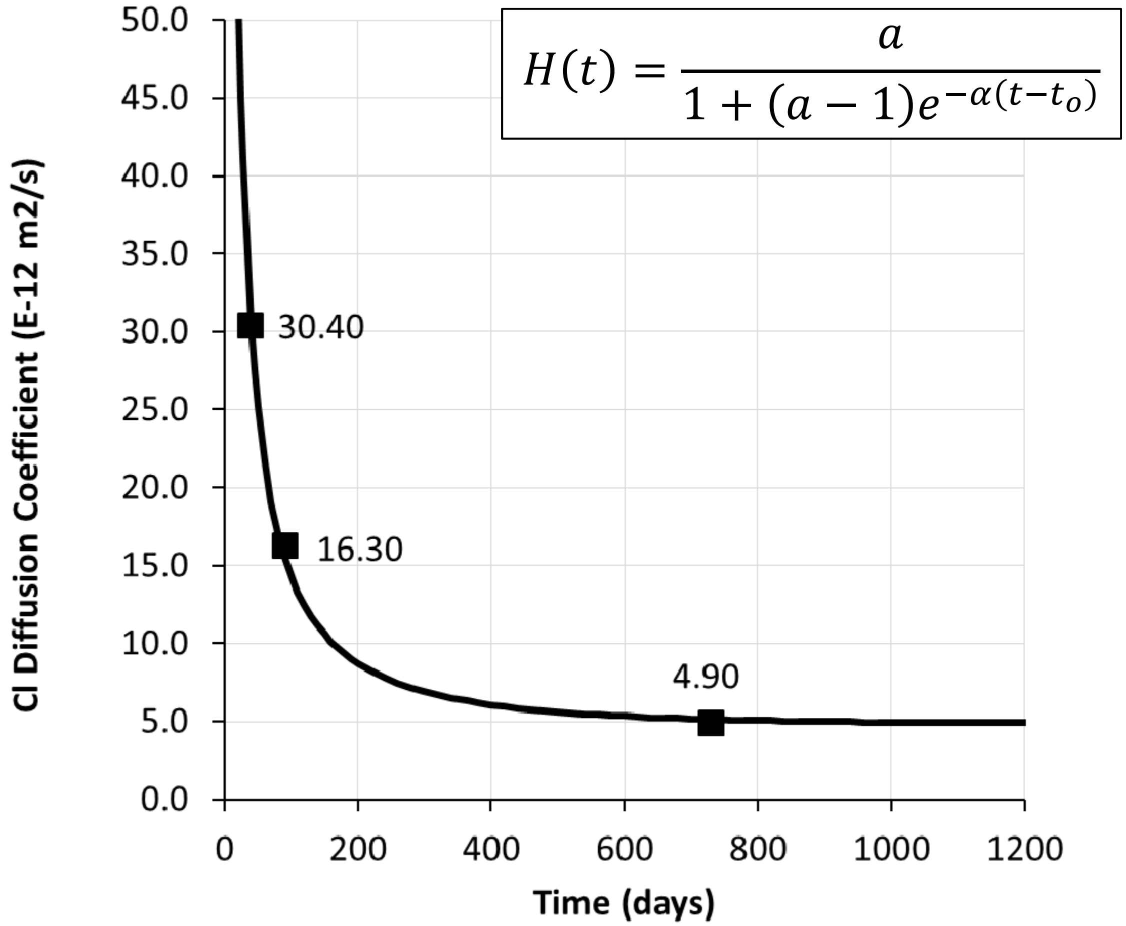


$$\tau_l^r = \frac{D(s)}{D_{sat}} = \frac{\sigma(s)}{\sigma_{sat}}$$

Source: Larsen et al., RILEM pro-051 2006

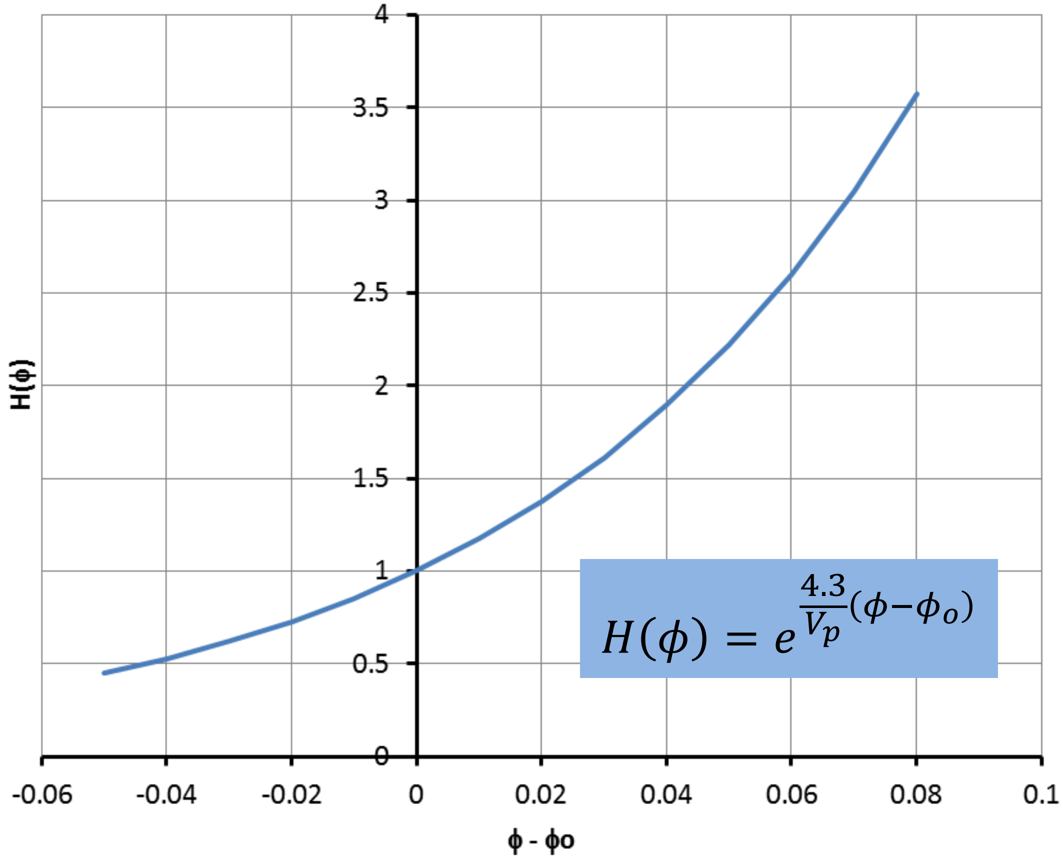
Species Transport

Effect of hydration on tortuosity:



Species Transport

Effect of dissolution/precipitation on tortuosity:



Species Transport

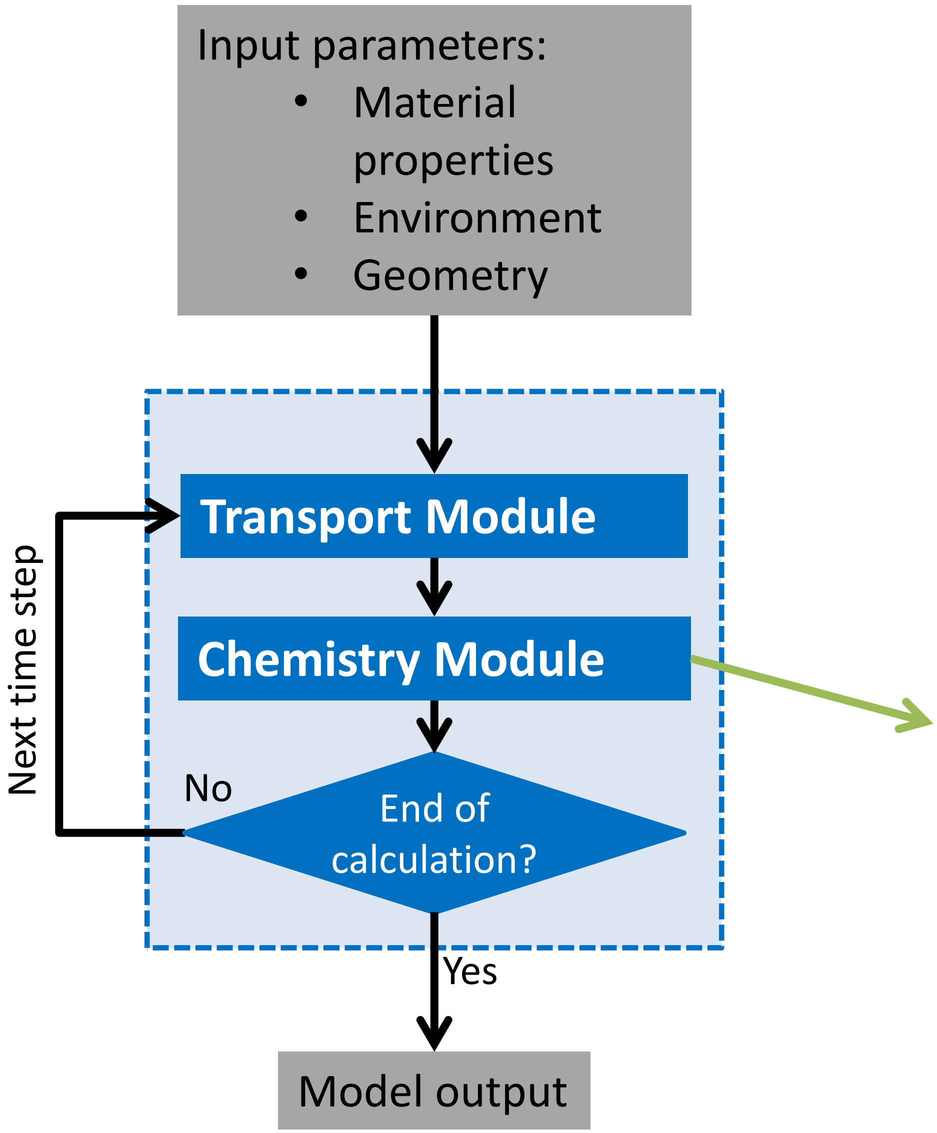
Mechanisms	Properties	Lab tests
Electrodiffusion of species	Diffusion coefficient	Migration test
	Porosity	ASTM C642
Moisture transport (liquid & vapor)	Permeability	Drying test
	Moisture isotherm	Drying test
Heat conduction	Thermal conductivity	Estimated
	Heat capacity	Estimated

Species Transport

Numerical methods:

- All equations are coupled to each other (e.g. temperature influences moisture and diffusion),
- The equations are solved using FEM,
- 1D and 2D versions are available.
- Euler implicit time-stepping.
- Adaptative time-stepping.

Chemistry Module



- Local Equilibrium Assumption
- Dissolution/precipitation
- Solid solutions
- Chemical/Pitzer database in separate text file
- Effect of temperature on chemistry

The chemical reactions are modeled according to dissolution/precipitation equilibrium relationships:

- **Dissolution/precipitation:** $K_m = \prod_{i=1}^{N} c_i^{\nu_{mi}} \gamma_j^{\nu_{mi}} \quad \text{with} \quad m = 1, \ldots, M$

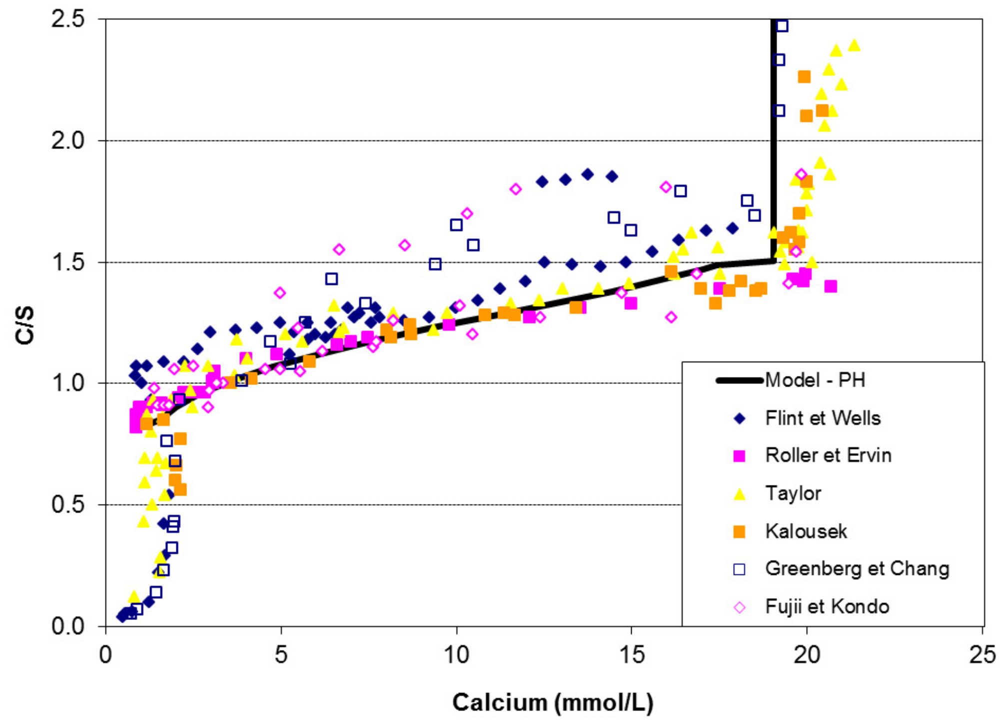
In the case of chlorides, the formation of Friedel's salts is modeled according to an ionic exchange relationship:

- **Friedel's salts formation:** $\underbrace{[\mathrm{AF}_m^+ - \mathrm{SO}_4^{2-}]}_{\text{monosulfates}} + 2\mathrm{Cl}^- \rightleftharpoons \underbrace{[\mathrm{AF}_m^+ - 2\mathrm{Cl}^-]}_{\text{Friedel's salt}} + \mathrm{SO}_4^{2-}$

- **Relationship:** $K_{Cl/SO_4} = \frac{\{\mathrm{Cl}\}^2}{\{\mathrm{SO}_4\}} \frac{[\mathrm{AFm}_{SO4}]}{[\mathrm{AFm}_{Cl}]}$

C-S-H model:

- Berner's approach: C-S-H ⟶ $CaH_2SiO_4 + 1.65\ Ca(OH)_2$
- Kps = f(C/S) for CaH_2SiO_4 and $Ca(OH)_2$



Chemistry Module

INPUT TO CHEMISTRY MODULE

- Mix composition
- Cement chemistry
- SCMs chemistry
- Chemistry database

CALCULATED PARAMETERS

- Hydrated cement paste composition
- Pore solution composition

STADIUM Output

At the end of calculations, the model provides the following information:

- Space and time distribution of species concentrations,
- Space and time distribution of mineral contents,
- Space and time distribution of temperature and humidity,
- Analysis of the main variables to get: total calcium, sulfur and chloride content.
- Space and time distribution of pH.
- Chloride content at specific depth to estimate the time to initiate corrosion for different rebar depths.

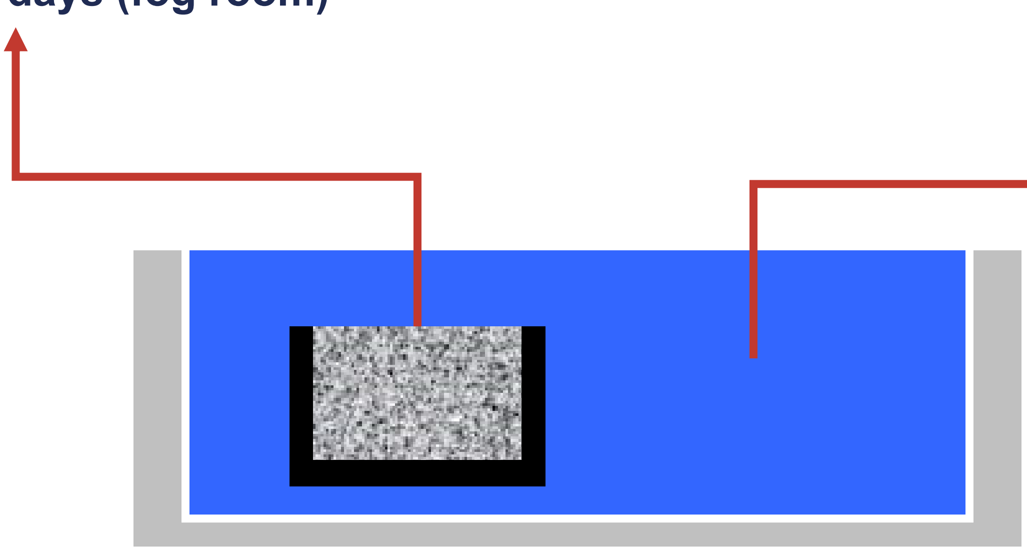
Lab Validation

Sulfate exposure

- Volume of solution: 30 L
- Regularly renewed to maintain stable conditions
- Exposure duration: 12 months

- Solutions: 50 mM Na_2SO_4

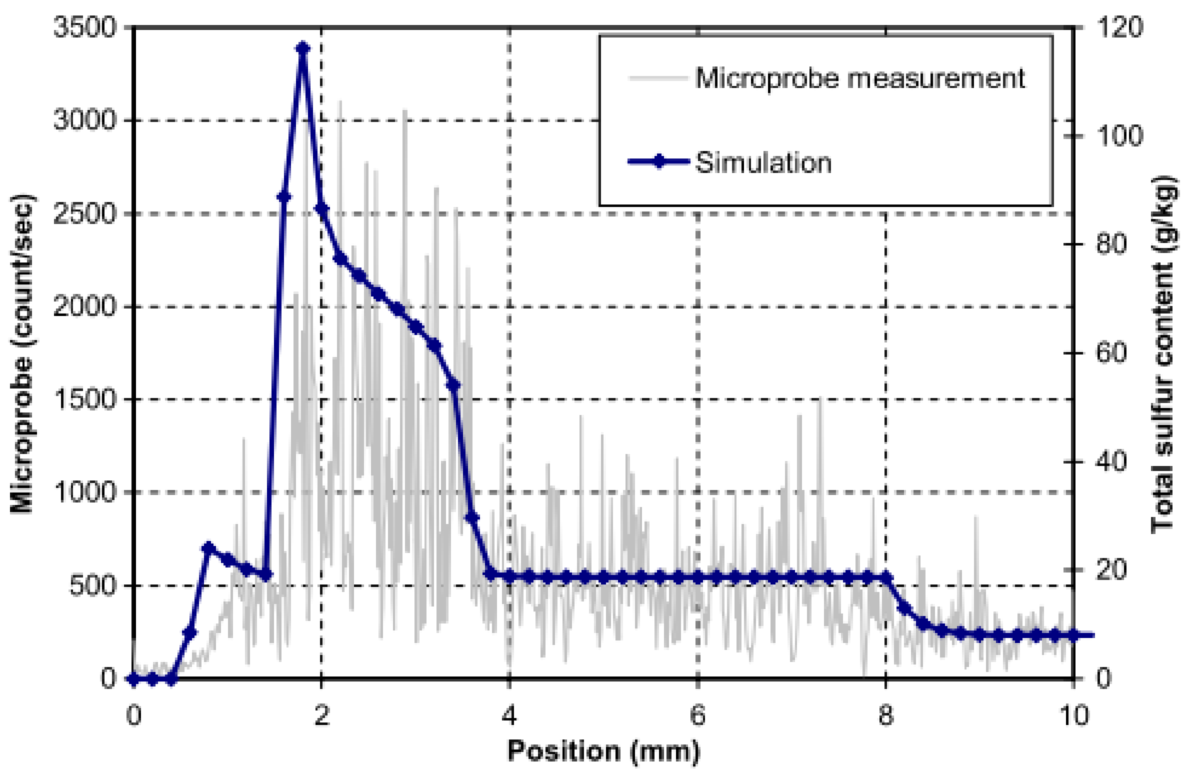
- Paste sample
- Thickness: 25 mm
- Sealed except on top
- Hydration: 28 days (fog room)



Lab Validation

Sulfate exposure

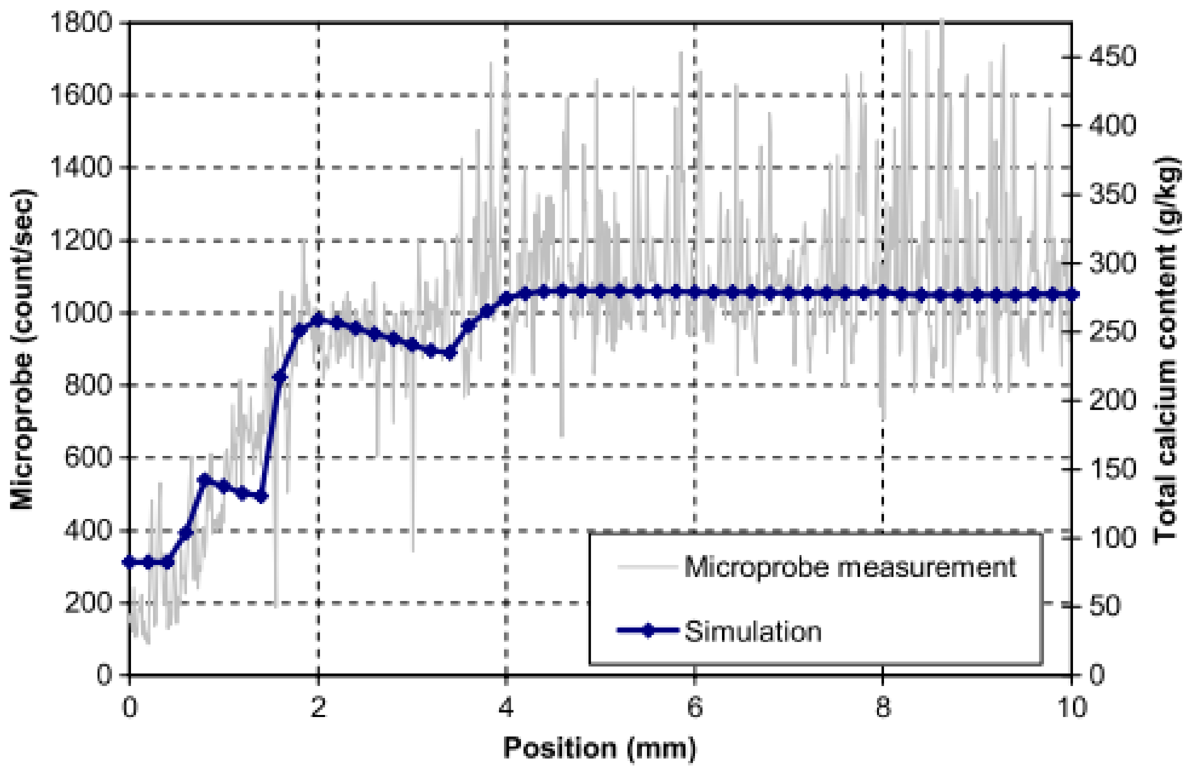
Microprobe sulfur profile



Lab Validation

Sulfate exposure

Microprobe calcium profile



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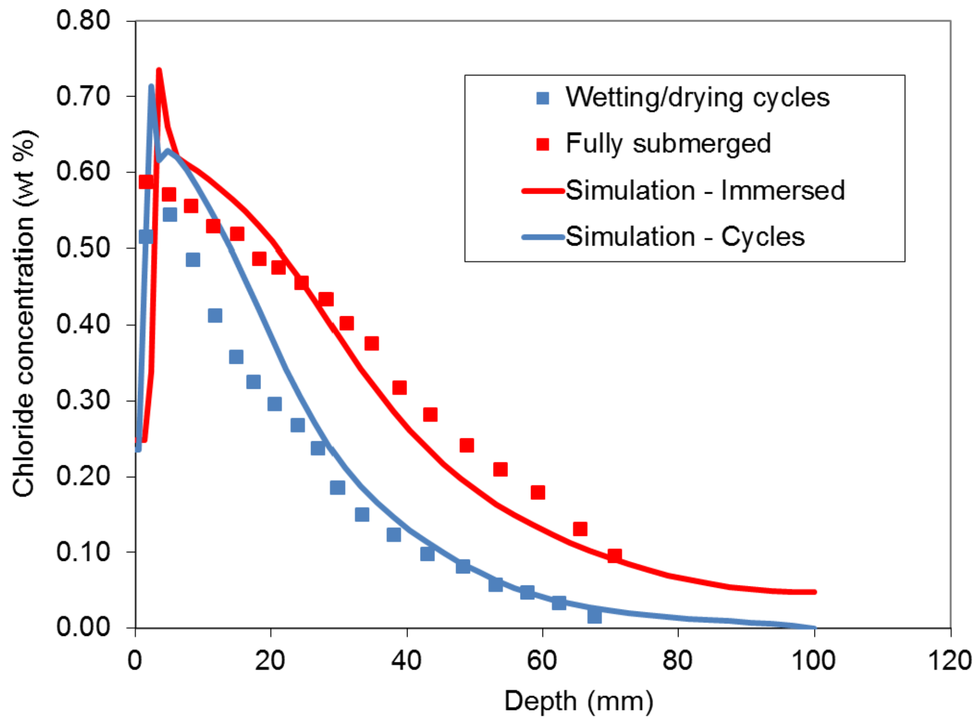
Lab Validation

Chloride profiles: wetting/drying cycles vs. immersed

- Solution: 0.5 M NaCl
- Cycles: 3 days in solution, 4 days drying at 50% RH
- Duration: 2.5 years



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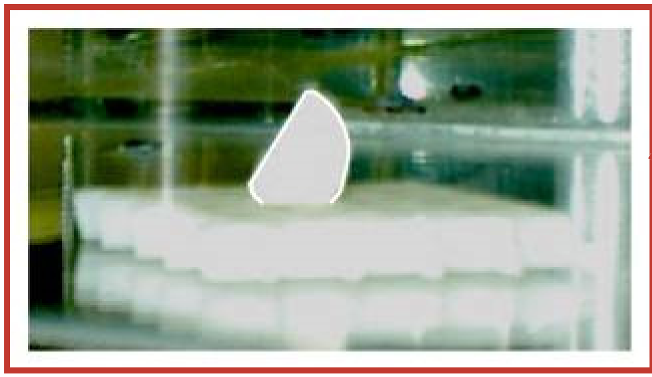
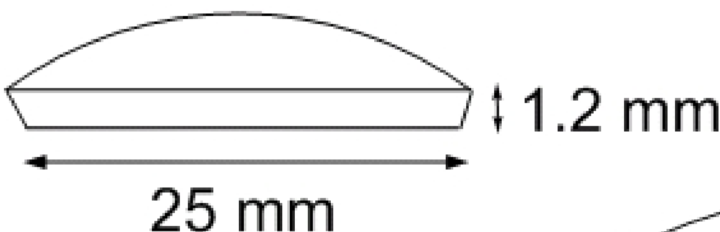
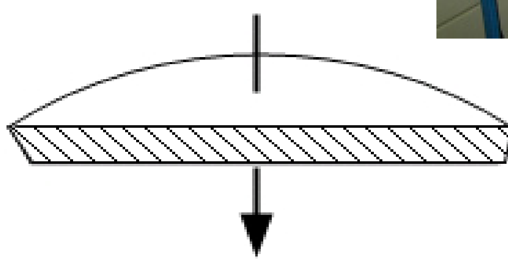
Lab Validation

C3S paste exposed to pure water







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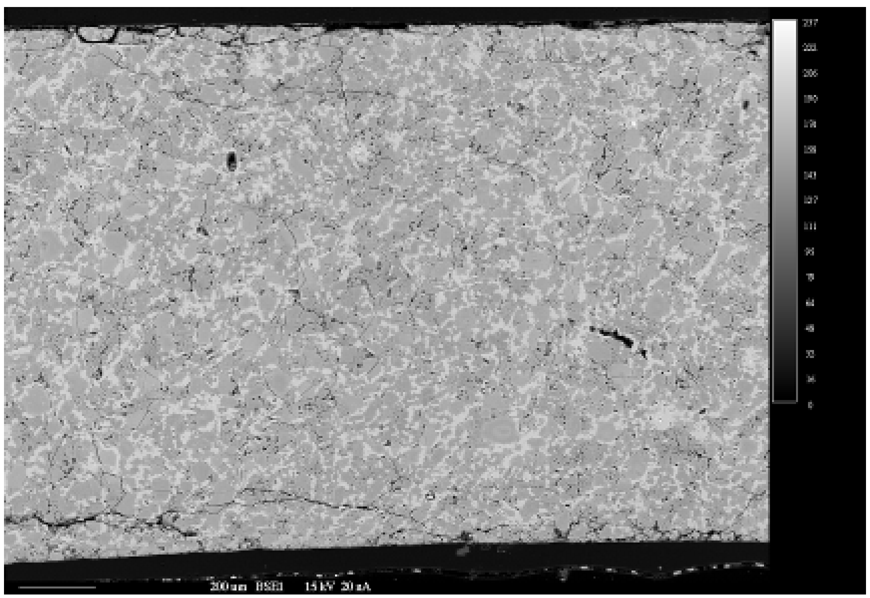
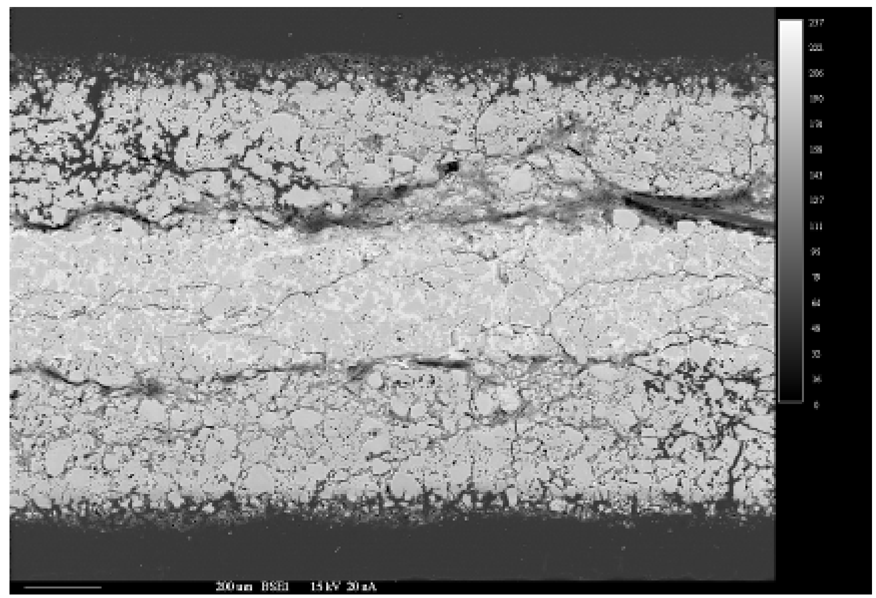
Lab Validation

C3S paste exposed to pure water

Sound C_3S paste

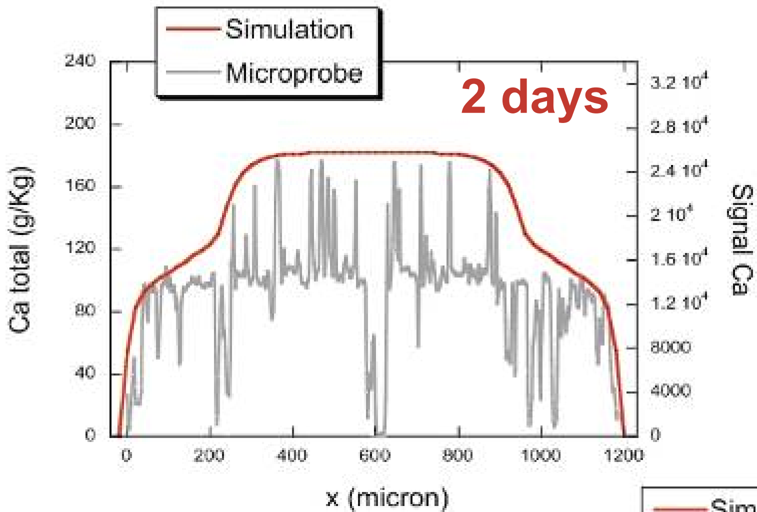


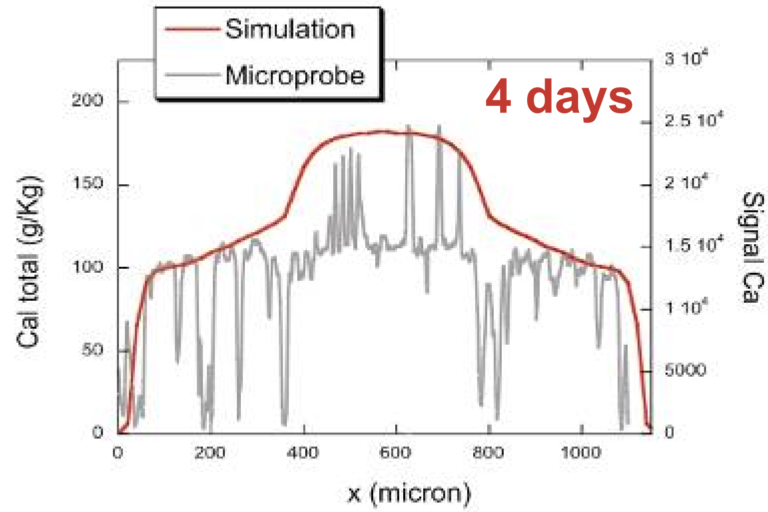
Leached C_3S paste

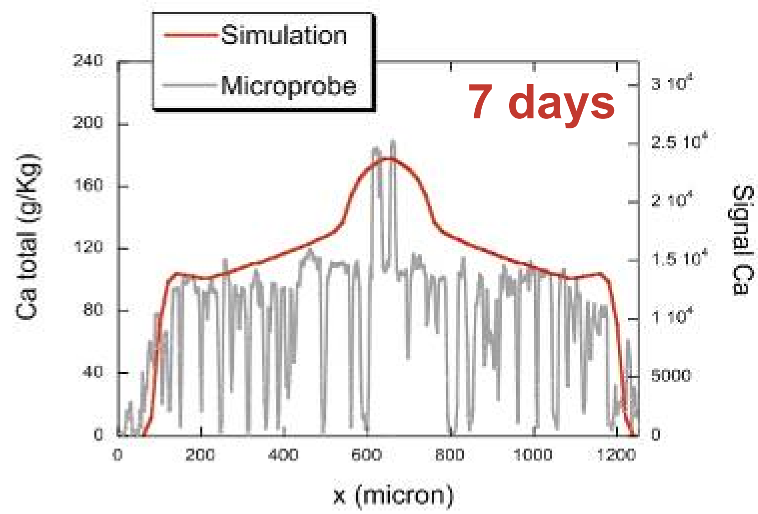


Lab Validation

C3S paste exposed to pure water – Ca profiles

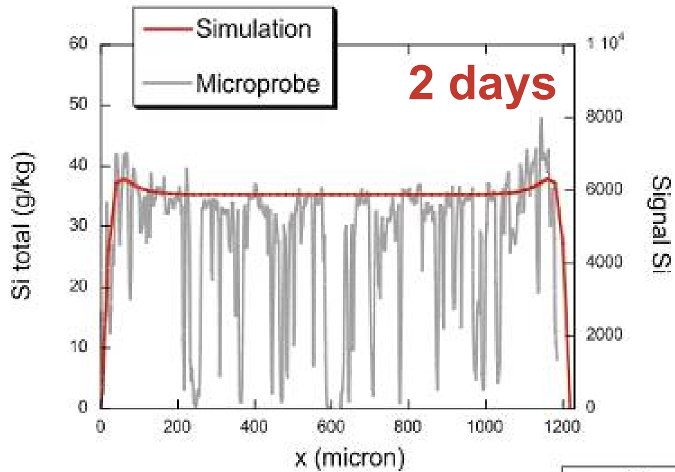


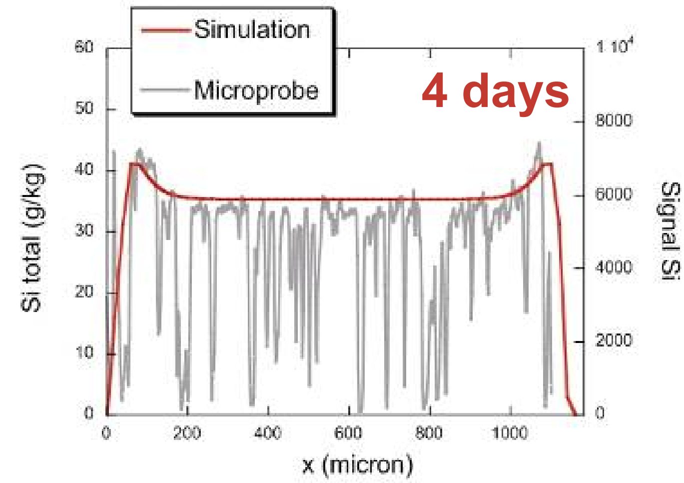


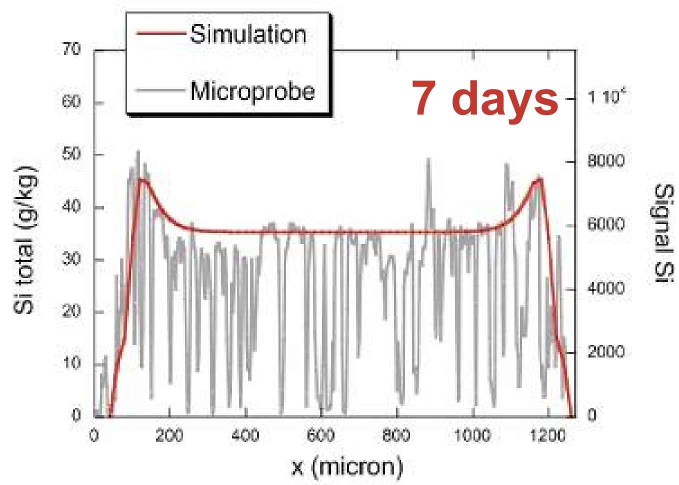


Lab Validation

C3S paste exposed to pure water – Si profiles







Questions?