Numerical modelling of RC structure durability
- Multi-level concept and various coupled problems -

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Outline

1 - *Introduction*

2 - Modelling of isothermal **Cl^- transport** in concrete

- **2.1 -** Level 2: Multi-species transport model (sat. cond.)
- **2.2 -** Level 3: Advanced physical-chemical model (sat. cond.)
- **2.3 -** Level 4: Coupled moisture-ion transport model

3 - Modelling of **carbonation** of concrete

- **3.1 -** Level 2: Semi-analytical physical-chemical model - Probabilistic framework
- **3.2 -** Level 3: Numerical physical-chemical model

4 - Concluding remarks & further needed developments

1 - A BASIC ISSUE FOR CONCRETE STRUCTURES …

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coupled physical and chemical processes

Drying-wetting cycles → restrained def. → *cracking*

+

Freezing-thawing cycles + salts

• Chloride ingress
• Carbonation

• ASR
• Sulfate attack

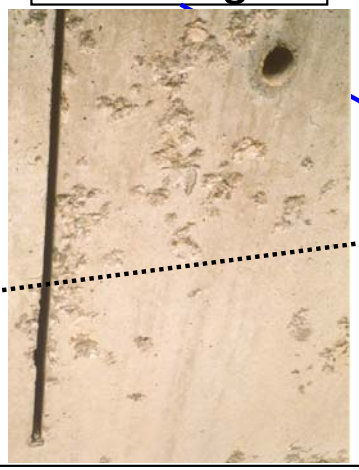
+ …

90% degradations

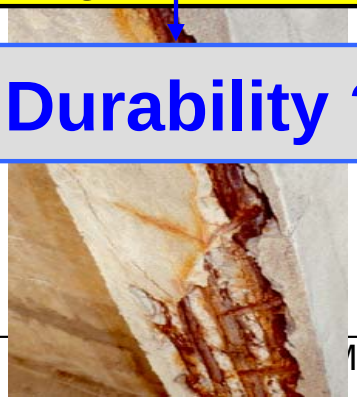
Microstructure → **"Pure" transport properties + fluid-matrix interactions**

degradations

• *Swelling*
• *Scaling*

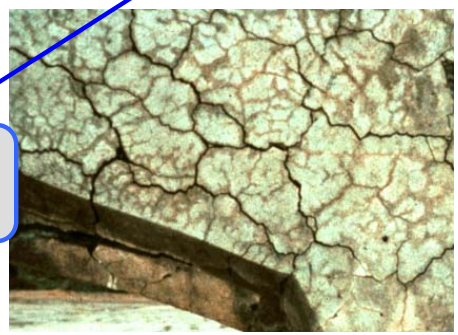


Reinforcement corrosion + concrete degradations



Swelling + cracking

+ …



Durability ?

fundamental aspect of sustainability

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• Chloride ingress
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+ …

Microstructure → **"Pure" transport properties + fluid-matrix interactions**

Durability indicators

degradations

• *Swelling*
• *Scaling*

Reinforcement corrosion + concrete degradations

Swelling + cracking

+ …

Durability ?

Monitoring parameters

Cost ?

1 - PURPOSES OF NUMERICAL MODELLING IN THE FIELD OF DURABILITY

*****

✷ Better understanding, description and implementation of phenomena

↪ multi-species & multi-phase transport, realistic field conditions (wetting-drying cycles, complex BCs...), coupling between ageing and degradation, physical-chemical-(mechanical) coupling, multi-scale problems

✷ Accurate prediction of ingress of aggressive species and of SL

↪ SL prediction at the design stage, prediction of future evolution of existing structures, selection of appropriate security margins (probabilistic framework)

➡ (very) long-term durability assessment (special structures)

➡ help diagnosis and optimise monitoring of RC structures

✷ Concrete mix-design or concrete cover design for a predefined SL

↪ multi-criteria optimisation of the composition of the material, probabilistic-based selection of optimum concrete cover

SCMs

➡ improve the link between **mix-design** & structural **lifetime**

➡ enhance the use of **"green" concretes** + ensure **durability**

→ life-cycle analysis

✷ Assessment of input data of models

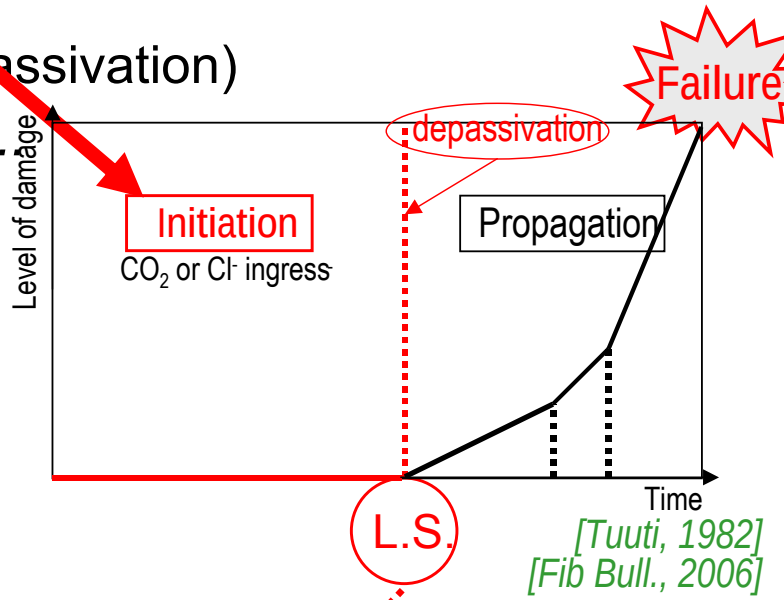
↪ transport properties & Cl- binding isotherms by **num. inverse analysis**

1 - NUMERICAL PREDICTIVE MODELS

✷✷✷✷✷

• Main features (protection against carbonation- or Cl^--induced corrosion) •

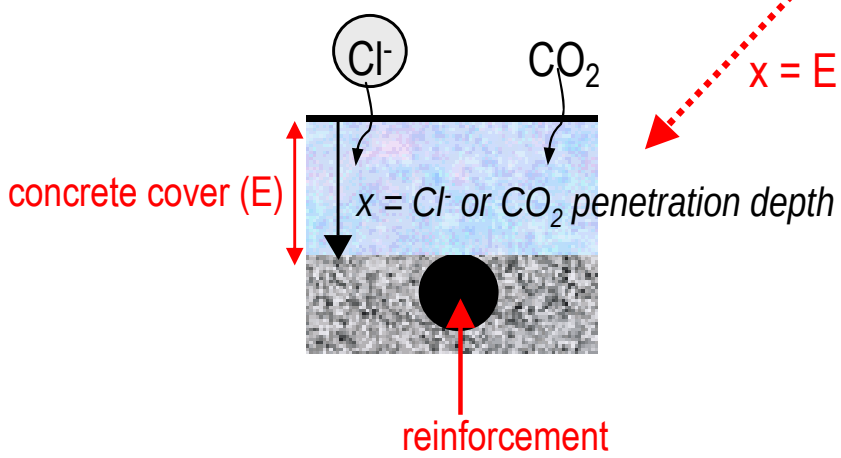
✷ **Assumption:** restriction to the initiation period
(limit state (L.S.) = reinforcement depassivation)
↪ ***conservative***, *material approach, ...*



[Tuuti, 1982]
[Fib Bull., 2006]

End of life: the aggressive species penetration front reaches the 1st layer of rebars

↪ uncracked concrete



✷ **Other approaches:** integration of part of propagation period (corrosion, cracking)

[Andrade, 2008], [Alexander, Microdurability, 2012], [Michel et al. Microdurability, 2012]

1 - NUMERICAL PREDICTIVE MODELS

✷✷✷✷✷

[ERLPC, 2008]

- Main features (protection against carbonation- or Cl^--induced corrosion)

✷ **Assumption:** restriction to the initiation period

- physically and chemically based
- deterministic or probabilistic framework
- **durability indicators** (transport prop., ...) ➔ main input data
- **monitoring parameters** (kinetics & conc. profiles) ➔ output data

➡ **set of numerical models** (macroscale, isoth. cond., uncracked concrete) with **different levels of sophistication** for each process

➔ *but the high d° of complexity may need in some cases to include analytical descriptions or coupling with analytical tools*

- Bil code (C++)
- 1-D Finite volume method (spatial discretization)
- Euler implicit scheme (time discretization)
- standard Newton algorithm

from simple tools to advanced physical-chemical models

e.g. - Cl^- ingress
- Carbonation

➡ **Multi-level platform**

1 - MULTI-LEVEL NUM. MODELLING PLATFORM FOR DURABILITY ASSESSMENT

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● Protection against carbo.- or Cl^--induced corrosion ●

(uncracked material & macro-scale - Isoth. cond. - 1-D physical-chemical models)

SCMs recycl. Mix-design

- chemical compo.
- binder type
- W/binder

Hydration models

Structural characteristics

Multi-species transport models in saturated cond.

(3 levels)

Moisture transport models

(2 levels)

Carbonation models

(3 levels)

Sustainable development

(carbon cycle)

Environment

- RH
- T°
- concentrations

Coupled moisture-ion/gas transport models

Durability & Service Life (RC structures)

LCA

Millau Bridge (France)

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2 - MULTI-LEVEL CONCEPT APPLIED TO MODELLING OF Cl^- TRANSPORT IN CONCRETE

*****

[Baroghel-Bouny et al., CCC, 2009]

• Multi-level platform (1-D physical numerical model) •

➡ **4 levels of sophistication**

Increasing level of sophistication

- **Level 1 - Chloride diffusion model (sat. cond.)**
  - **Cl^-** diffusion (in diluted solution) ➔ ***Fick's* 1st law**
  - (global) Cl^- binding ➔ ***Freundlich's*** non-linear isotherm
  - empirical law $D_{Cl^-} = f(c_{Cl^-})$

[Andrade, CCR, 1993]
[Masi et al., CCR, 1997]
[Samson et al., 1999]
[Truc et al., RILEM, 2000]

Multi-species approach

- **Level 2 - Multi-species transport model (sat. cond.)**
  - **4 ions + electrical interactions** between ions ➔ *Nernst-Planck/Poisson eq.*
  - equil. Cl^- binding ➔ **various options** ➡ *analytical formula* $s_{Cl} = s_{Cl}(c_{Cl^-})$
- **Level 3 - Advanced physical-chemical model (sat. cond.)**
  - **6 to 8 ions + 3 to 8 solid compounds**
  - Cl^- binding ➔ **physical adsorption** onto C-S-H **+ *Friedel's* salt formation** by (instant.) chemical reactions (dissol./precip.)
  - **microstructural** (and transport property) **changes** (induced by *Friedel's* salt precipitation, $Ca(OH)_2$ dissolution, ...)
- **Level 4 - Coupled moisture-ion transport model**
  - ↪ contribution of **advection** to the overall ionic transport
  - ↪ multi-species transport model (**level 2**) extended to **non-sat. cond.**

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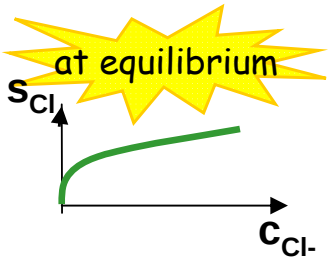
Global description (*Freundlich's* formula)

$$s_{Cl} = \mu c_{Cl^-}^{\gamma}$$

Freundlich's parameters

at equilibrium



Ion exchange theory description

$$s_{Cl} = \delta_3 N_{(C_3A)eq.} + N_{C\text{-}S\text{-}H} \frac{\alpha'' c_{Cl^-}}{c_{OH^-} + \beta'' c_{Cl^-}}$$

chemical

physical

fixed parameters

pH effect

s_{Cl} : total amount of bound Cl^- (mol / m^3 of mat.)
c_{Cl^-} : Cl^- conc. of the pore sol. (mol / m^3 of sol.)

[Baroghel-Bouny et al., CCR, 2012]

2.1 - MULTI-SPECIES TRANSPORT MODEL (SAT. COND.)

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Level 2

[Nguyen et al., C&C, 2006]

● Transport and mass balance equations ●

✷ **Ions: Cl^-, Na^+, K^+, OH^-**

Poisson's equation

$$\mathrm{div}(\mathrm{grad}\,\Psi) + \frac{F}{\varepsilon}\left(\sum c_i z_i\right) = 0$$

dielectric constant

[Samson et al., 1999 → 2003]

✷ **Transport of each ion → *Nernst-Planck* equation**

Flux *(mol.m^{-2}.s^{-1})* (i = Cl^-, Na^+, K^+, OH^-) →

$$J_i = -D_i\left[\mathrm{grad}c_i + c_i\,\mathrm{grad}(\ln\gamma_i) + \frac{z_i F}{RT}c_i\,\mathrm{grad}\Psi\right]$$

(constant) effective ionic **diffusion coef.** of the saturated mat. (m^2.s^{-1})

chemical activity coef. (-)

local elec. potential (V)

(ion-ion interactions)

c_i : (free) conc. in ion i of the pore solution (mol / m^3 of sol.)

z_i : valence number of ion i (-)

T : absolute temperature (K)

R : ideal gas constant (8.3143 J.mol^{-1}.K^{-1})

F : Faraday constant (9.64846· 10^4 C.mol^{-1})

$\gamma_i = 1$

[Truc et al., RILEM, 2000]
[Marchand et al.,M&S, 2002]
[Nguyen et al., C&C, 2006]

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(constant) effective ionic **diffusion coef.** of the saturated mat. (m^2.s^{-1})

chemical activity coef. (-)

local elec. potential (V) (ion-ion interactions)

✷ **Mass balance equation for each element** (i = Cl, Na, K, O, H)

$$\frac{\partial n_i}{\partial t} + \mathrm{div}J_i = 0$$

total content (mol / m^3 of mat.)

(e.g. $n_{Cl} = \phi c_{Cl^-} + s_{Cl}$)

total amount of bound Cl^- (mol / m^3 of mat.)

(free) Cl^- conc. of the pore sol. (mol / m^3 of sol.)

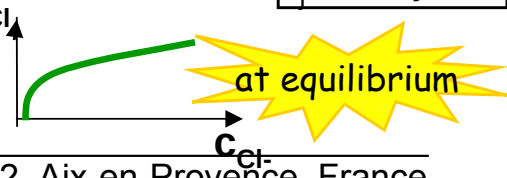
e.g. *Freundlich's* formula: $s_{Cl} = \mu c_{Cl^-}^{\gamma}$

and s_j=0 for j≠Cl

porosity (-) (constant)

$s_{Cl} = s_{Cl}(c_{Cl^-})$

→ **Cl^- binding isotherm**



2.1 - MULTI-SPECIES TRANSPORT MODEL (SAT. COND.)

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few inputs

Level 2

● Input data required for the model ●

Durability indicators

assumed independent of age and depth (non-reactive porous solid)

ϕ	Porosity accessible to water ($m^3.m^{-3}$)
D_{Cl-}	*Effective* Cl^- diff. coefficient ($m^2.s^{-1}$)
$s_{Cl} = s_{Cl}(c_{Cl-})$	Cl^- binding isotherm (at equilibrium)
I.C. (pore sol.) c_{Na+}^0, c_{K+}^0, c_{OH-}^0	*Initial* chemical compo. of the pore solution

exp. or anal. formula or num. inverse analysis

$(C_{Cl-}^0=0)$

\+ **B.C.**: T° (constant), ionic conc. of the contact solution, ...

c_{Na+}^0, c_{K+}^0: mix-compo. + cement chem. compo. + initial alkali binding *[Taylor, ACR, 1987]* + hydration model + sat. sol. compo.

$c_{OH-}^0 = c_{Na+}^0 + c_{K+}^0$

[Mounanga et al., CCR, 2004]
[Nguyen, PhD thesis, 2009]

$$\frac{D_i}{D_i^0} = \frac{D_{Cl^-}}{D_{Cl^-}^0} (= \tau \cdot \phi) = \frac{1}{F} \quad (i \neq Cl^-)$$

[Samson, 1999]

at infinite dilution

τ : tortuosity (-)
F : formation factor (-)

2 - MULTI-LEVEL CONCEPT APPLIED TO MODELLING OF Cl^- TRANSPORT IN CONCRETE

*****

[Baroghel-Bouny et al., CCC, 2009]

• Multi-level platform (1-D physical numerical model) •

➡ **4 levels of sophistication**

Increasing level of sophistication

- **Level 1 - Chloride diffusion model (sat. cond.)**
  - **Cl^-** diffusion (in diluted solution) ➔ ***Fick's* 1st law**
  - (global) Cl^- binding ➔ ***Freundlich's*** non-linear isotherm
  - empirical law $D_{Cl-} = f(c_{Cl-})$

(Equil.) thermodynamic modelling
[Johannesson et al., M&S, 2007]
[Hosokawa & Yamada, C&S, 2009]
[Lothenbach et al., CCR, 2010]

- **Level 2 - Multi-species transport model (sat. cond.)**
  - **4 ions + electrical interactions** between ions ➔ *Nernst-Planck/Poisson eq.*
  - equil. Cl^- binding ➔ **various options**

Transport-chemistry coupling

- **Level 3 - Advanced physical-chemical model (sat. cond.)**
  - **6 to 8 ions + 3 to 8 solid compounds**
  - Cl^- binding ➔ **physical adsorption** onto C-S-H **+ *Friedel's* salt formation** by (instant.) chemical reactions (dissol./precip.)
  - **microstructural** (and transport property) **changes** (induced by *Friedel's* salt precipitation, $Ca(OH)_2$ dissolution, ...)

- **Level 4 - Coupled moisture-ion transport model**
  - ↪ contribution of **advection** to the overall ionic transport
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➡ **4 levels of sophistication**

Chemical equilibriums (*Friedel's* salt formation)	$-\log K$
$H_2O \rightleftharpoons H_3O^+ + OH^-$	14
$Ca(OH)_2 \rightleftharpoons Ca^{2+} + 2OH^-$	5,05
$3CaO.Al_2O_3 + 6H_2O \rightleftharpoons 3Ca^{2+} + 4OH^- + 2Al(OH)_4^-$	22,5
$3CaO.CaCl_2.Al_2O_3.10H_2O \rightleftharpoons 4Ca^{2+} + 4OH^- + 2Al(OH)_4^- + 2Cl^-$	29,1

additional eqs associated with dissol./precip. reactions

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2.2 - ADVANCED PHYSICAL-CHEMICAL MODEL (SAT. COND.)

*****

Level 3

• Transport and mass balance equations •

- **Ions**: Cl^-, Na^+, K^+, OH^-, Ca^{2+}, $Al(OH)_4^-$, ...
- **Solid compounds**: $Ca(OH)_2$, equiv. aluminates, ***Friedel's*** salt

- **Transport of each ion** → ***Nernst-Planck*** equation

Flux *(mol.m^{-2}.s^{-1})* →

$$J_i = -D_i \left[\text{grad}c_i + c_i \text{grad}(\ln\gamma_i) + \frac{z_i F}{RT} c_i \text{grad}\Psi \right]$$

effective ionic **diffusion coef.** of the saturated mat. (m^2.s^{-1})

chemical activity coef. (-)

local elec. potential (V)

- **Mass balance equation for each element** (in ion or solid compound)

$$\frac{\partial}{\partial t}\left[\phi c_i + s_i\right] + \text{div}\, J_i = 0$$

[Nguyen et al., RILEM, 2006]
[Nguyen et al., ICCC'07, 2007]

Transport-chemistry coupling

Microstructural evolution ⟺ Transport property changes

Porosity $\phi = \phi_0 + \sum \nu_i \Delta s_i$

Effective diffusion coef. $D_i = D_i^0 \frac{\phi}{\phi_0} \left(\frac{\phi_0 - 0.18}{\phi - 0.18} \right)^2$ derived from *[Bentz et al., CCA, 1998]*

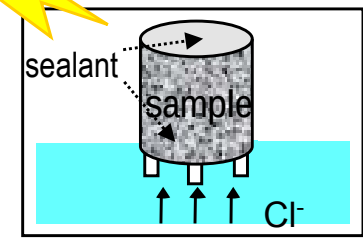
s_i: amount of solid compound i (mol / m^3 of mat.)
ν_i: molar vol. of solid compound i (m^3 / mol)

2.2 - ADVANCED PHYSICAL-CHEMICAL MODEL (SAT. COND.)

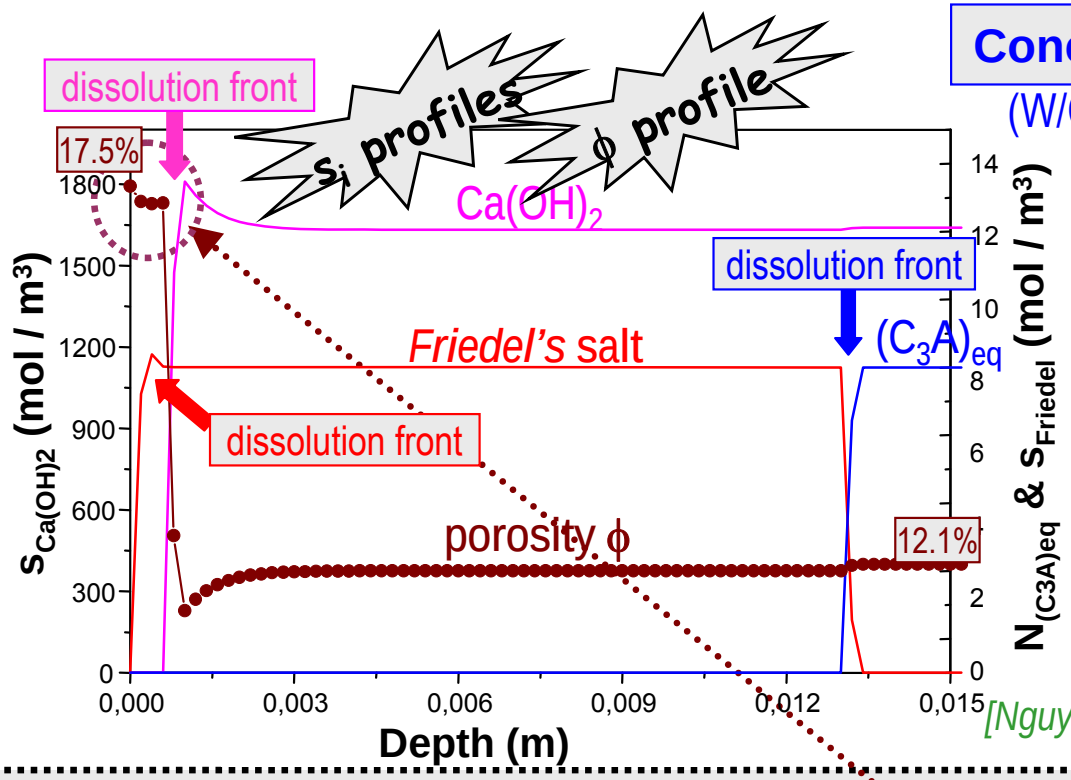
*****

Level 3

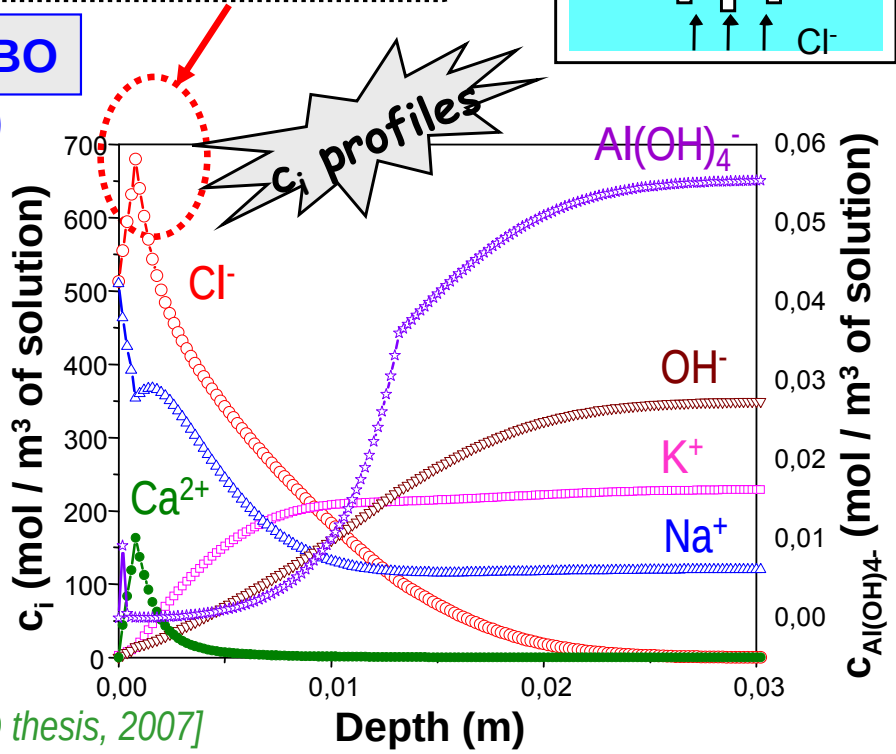
- Example of simulations (nss diffusion test in lab)



- **B.C.: 90-day** exposure to 30 g.L^{-1} NaCl (*i.e.* c_{Cl^-} = 517, c_{Na^+} = 517 mol.m^{-3})



Concrete BO
(W/C=0.49)



[Nguyen, Ph.D thesis, 2007]

- Cl^- ingress → aluminates dissolution → *Friedel's* salt precipitation
- B.C.: → $Ca(OH)_2$ dissolution → porosity ↗ in the surf. zone
  → c_{Ca2+} ↗ → c_{Cl^-} ↗ in the surf. zone (> B.C.)
  (*Friedel's* salt dissolution)

Evolution of pore solution & solid phase composition and of microstructure

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  - (global) Cl^- binding ➡ ***Freundlich's*** non-linear isotherm
  - empirical law $D_{Cl^-} = f(c_{Cl^-})$

[Nilsson et al., 1996]
[Johannesson, CCR, 2003]
[Samson, 2005]

- **Level 2 - Multi-species transport model (sat. cond.)**
  - **4 ions + electrical interactions** between ions ➡ *Nernst-Planck/Poisson eq.*
  - equil. Cl^- binding ➡ **various options**
- **Level 3 - Advanced physical-chemical model (sat. cond.)**
  - **6 to 8 ions + 3 to 8 solid compounds**
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  - ↪ contribution of **advection** to the overall ionic transport
  - ↪ multi-species transport model (**level 2**) extended to **non-sat. cond.**

Non-saturated conditions

2.3 - COUPLED MOISTURE-ION TRANSPORT MODEL

★★★★★

• Description •

Level 4

For (concentrated) non-ideal sol.

$\ln a_w = f(I)$

I : ionic strength of the solution (mol.m^{-3})

[Lin & Lee, FPE, 2003]

$$p_c = -\frac{\rho_w}{M_w} RT \left[\ln \frac{p_v}{p_{vs}(T)} - \ln a_w \right]$$

h: relative humidity (-)

[Baroghel-Bouny et al., CCR, 1999]
[Thiery et al., REGC, 2007]

degree of saturation

Moisture transport

- **ionic** transport ➔ ***Nernst-Planck/Poisson* eq.** (incl. γ effects)
- **liquid phase** & gas movement ➔ ***extended Darcy's* law**
- **water vapour** & dry air relative diffusion ➔ ***Fick's* 1st law**
- **water-ions coupling** ➔ water activity a_w ➔ ***extended Kelvin's* law**
- transport properties variations ***vs.*** S_l ➔ *integral or analytical laws*
  e.g. permeabilities ➔ *[Mualem, 1976]*
- equil. Cl^- binding ➔ **various options**
  + possible **delay effect** ➔ *kinetics equation*

$$ds^*_{Cl}/dt = -(s^*_{Cl} - \mu c_{Cl^-}{}^{\gamma}) / \tau$$

characteristic (delay) time
[Francy, Ph.D thesis, 1998]

➔ multi-species & multi-phase!

➔ natural drying, wick action, **wetting-drying** cycles, … ➔ tidal zones

2.3 - COUPLED MOISTURE-ION TRANSPORT MODEL

[Baroghel-Bouny et al., CCR, 2011]

Level 4

• Transport and mass balance equations •

✷ **Ions: Cl^-, OH^-, Na^+, K^+**

✷ **Transport of each ion → *Nernst-Planck* equation**

account for chemical activity effects

Flux *(mol.m^{-2}.s^{-1})* →

$$J_i = -D_i \, d_{ri}(S_l) \left[\text{grad}c_i + c_i \cdot \text{grad}(\ln\gamma_i) + \frac{z_i F}{RT} c_i \cdot \text{grad}\Psi \right]$$

effective ionic **diffusion coef.** of the saturated mat. (constant)

relative diffusion coef.

$$d_{rCl^-} = D_{Cl^-}(S_l)/D_{Cl^-}(S_l = 1) = S_l^{\lambda}$$

[Buchwald, 2000]

and

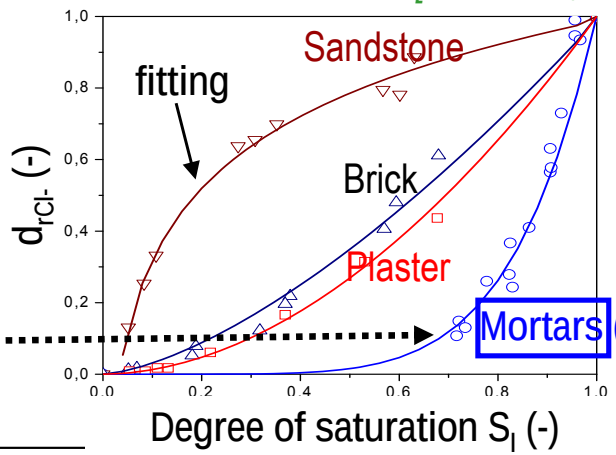
at $S_l = 1$ $(i \neq Cl^-)$

$$\frac{D_i}{D_i^0} = \frac{D_{Cl^-}}{D_{Cl^-}^0} (= \tau \cdot \phi) = \frac{1}{F}$$

[Samson, 1999]

at infinite dilution

τ : tortuosity (-)
F : formation factor (-)



[Francy, Ph.D thesis, 1998]

Calibration → $\lambda = 6$

2.3 - COUPLED MOISTURE-ION TRANSPORT MODEL

[Baroghel-Bouny et al., CCR, 2011]

Level 4

*****

• Transport and mass balance equations •

✷ Overall transport equation

Total flux → (mol.m^{-2}.s^{-1})

$$w_\alpha = v_l c_\alpha + J_\alpha \quad (\alpha = w \text{ or } i) \rightarrow \textbf{extended } \textit{Nernst-Planck} \textbf{ eq. } (\alpha = i)$$

or

$$w_\alpha = v_g c_\alpha + J_\alpha \quad (\alpha = v \text{ or } a)$$

Advection **Diffusion**

c_α : conc. in phase α (mol.m^{-3}) with $\sum \upsilon_\alpha c_\alpha = 1$ when α = w or i, where υ_α is the molar vol. of phase α in sol. (m^3.mol^{-1})

✷ Mass balance equations (for moisture w+v, dry air a, and species j in ion or in solid compound

$$\begin{cases} \dfrac{\partial}{\partial t}\left(\phi S_l c_w + \phi(1-S_l)\dfrac{\rho_v}{M_v}\right) = -\mathrm{div}(w_w + w_v) \\ \dfrac{\partial}{\partial t}\left(\phi(1-S_l)\dfrac{\rho_a}{M_a}\right) = -\mathrm{div}(w_a) \\ \dfrac{\partial}{\partial t}\underbrace{\left(\phi S_l c_j + s_j\right)}_{n_j} = -\mathrm{div}(w_j) \end{cases}$$

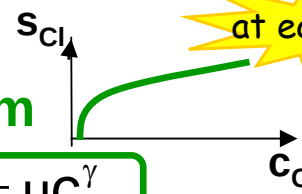
n_j : total content (mol / m^3 of mat.)

porosity (constant)

s_{Cl} : total amount of bound Cl$^-$ (mol / m^3 of mat.) and s_j=0 for j≠Cl

$s_{Cl} = s_{Cl}(c_{Cl^-})$ at equilibrium

→ **Cl$^-$ binding isotherm**



e.g. *Freundlich's* formula: $s_{Cl} = \mu c_{Cl^-}^{\gamma}$

2.3 - COUPLED MOISTURE-ION TRANSPORT MODEL

*****

Level 4

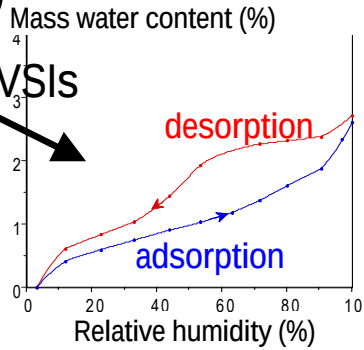
Durability indicators

few inputs

- Input data required for the model -

ϕ	Porosity accessible to water ($m^3.m^{-3}$)
D_{Cl-}	*Effective* Cl^- dif. coef. in saturated cond. ($m^2.s^{-1}$)
K_g, K_l	*"Intrinsic"* permeabilities (m^2)
$s_{Cl} = s_{Cl}(c_{Cl-})$	Cl^- binding isotherm (in sat. cond.) at equilibrium
$p_C = p_C(S_l)$	Capillary pressure curve → derived from exp. WVSIs
I.C. S_l^0	*Initial* degree of saturation (-)
I.C. c_{Na+}^0, c_{K+}^0, c_{OH-}^0	*Initial* chemical compo. of the pore solution ($C_{Cl-}^0=0$)

exp. or anal. formula or num. inverse analysis



\+ **B.C.**: ionic conc. of the contact solution, S_l at the boundary of the test specimen, T° (constant), ...

c_{Na+}^0, c_{K+}^0: mix-compo. + cement chem. compo. + initial alkali binding *[Taylor, ACR, 1987]* + hydration model + sat. sol. compo. + S_l^0

$c_{OH-}^0 = c_{Na+}^0 + c_{K+}^0$

[Mounanga et al., CCR, 2004]
[Nguyen, PhD thesis, 2009]

*****

• Simulation of wetting by a NaCl solution (after drying) •

Level 4

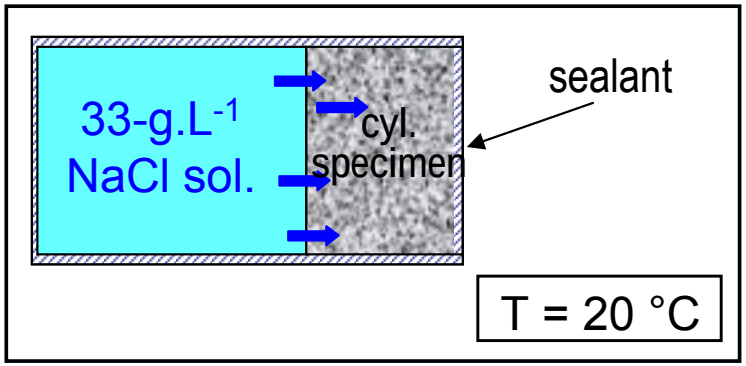
Mortar M1N
(W/C=0.50)

Experimental conditions

1) 90-day water curing

2) drying at RH=4%
   ↳ **I.C.:** $S_l^0 = 0.09$
   $c_{Cl^-}^0 = 0$, $c_{OH^-}^0 = 722$, $c_{Na^+}^0 = 144$,
   $c_{K^+}^0 = 578$ mol.m^{-3}

3) 24-h expo. to **33 g.L^{-1}** NaCl + 1 g.L^{-1} NaOH + 4.65 g.L^{-1} KOH by 1 face



[Francy, Ph.D thesis, 1998]

Material properties

- ϕ = **0.13** ➔ **exp.**
- D_{Cl^-} = **2.1 · 10^{-12} m^2.s^{-1}** ([Cl^-_{tot}] profile after 7-d nss diffusion test ➔ **inv. analysis**)
- K_l = **15 · 10^{-21} m^2** (drying kinetics at RH = 4% ➔ **inv. analysis**)
- $p_c = p_c(S_l)$ from **exp.** WVAI *[Bonnet, Ph.D thesis, 1997]*
- $S_{Cl} = S_{Cl}(c_{Cl^-})$ ➔ **exp. data** + *Freundlich's* description + **delay effect** ($\tau \approx$ 6h)

Level 2

Moisture transport

[Francy, Ph.D thesis, 1998]

high-rate advective transport in the short term

Level 4

*****

- Simulation of wetting by a NaCl solution (after drying): impact of binding description -

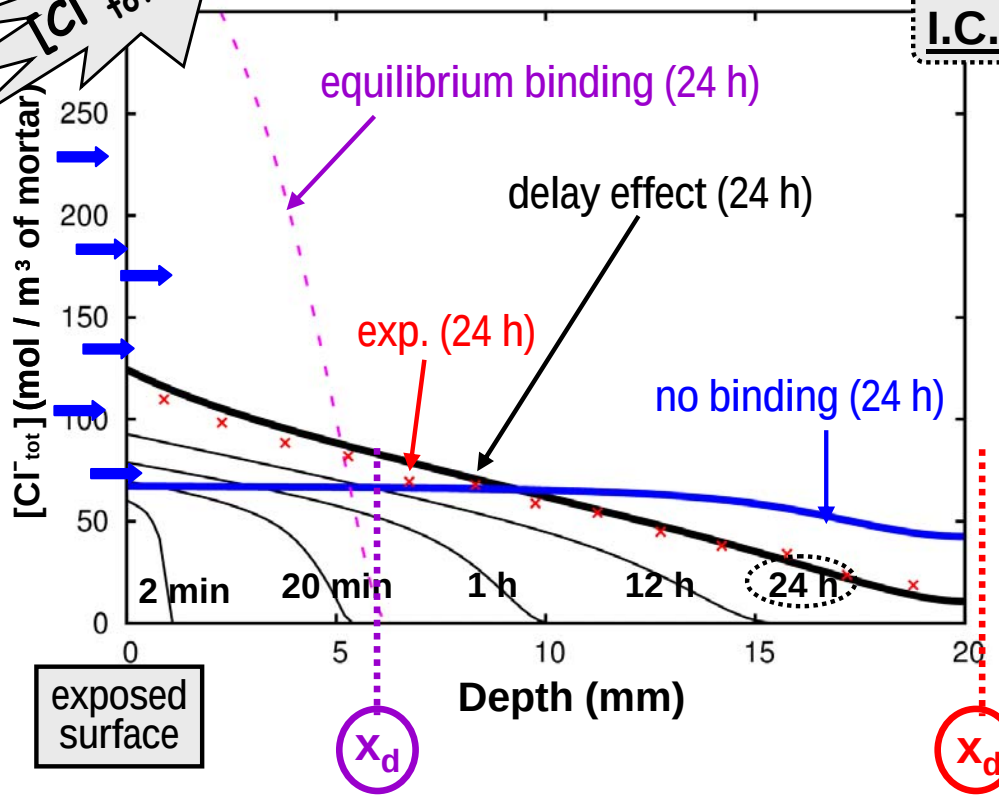
[Baroghel-Bouny et al., CCR, 2011]

Mortar M1N

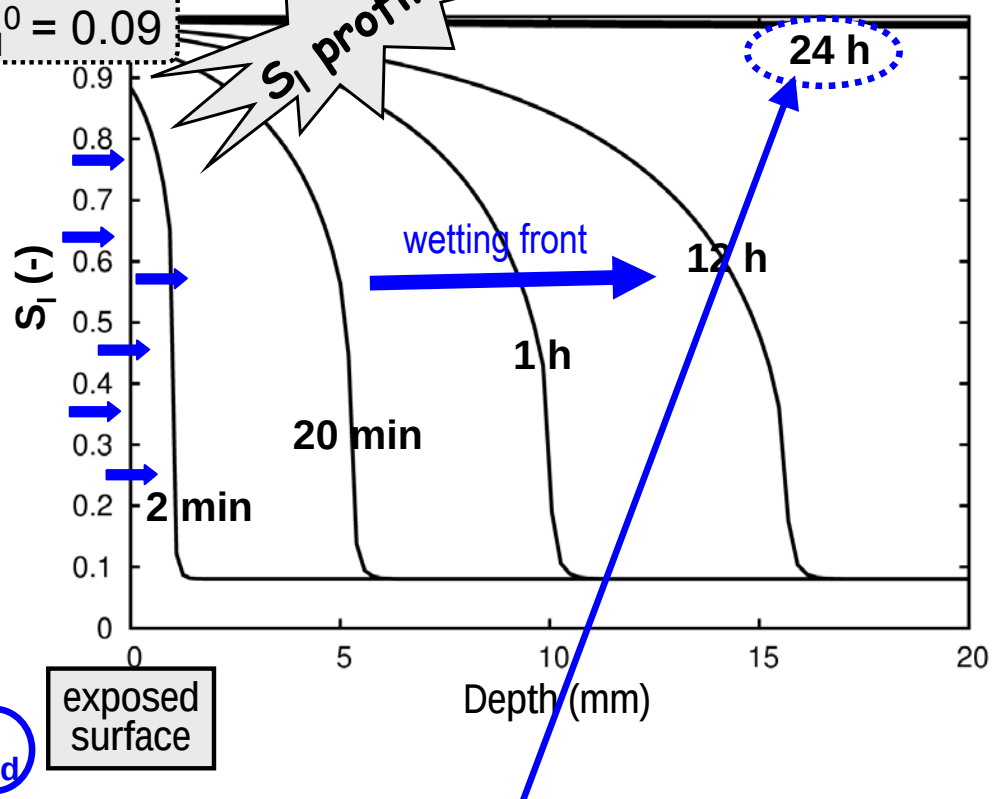
(W/C=0.50)

I.C.: $S_l^0 = 0.09$

$[Cl^-_{tot}]$ profiles



S_l profiles



- after 24-h exposure → wetting front has reached the specimen boundary
  → $S_l = 1$ throughout the specimen thickness

- *Freundlich's* description + **delay effect** → best agreement with exp.data

Models → *importance to account for appropriate Cl^- binding description (structural safety)*

*****

[Baroghel-Bouny et al., CCR, 2011]

• Diffusion *vs.* advection •

Mortar M1N
(W/C=0.50)

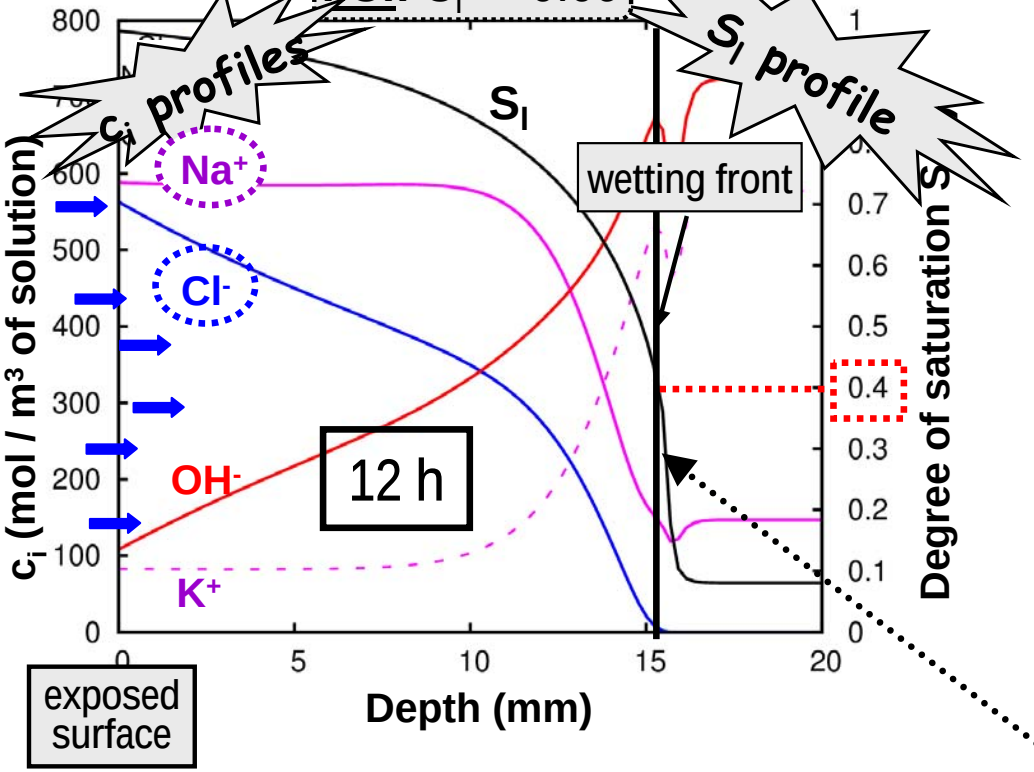
Level 4

Diffusion + Advection

I.C.: $S_l^0 = 0.09$

c_i profiles

S_l profile



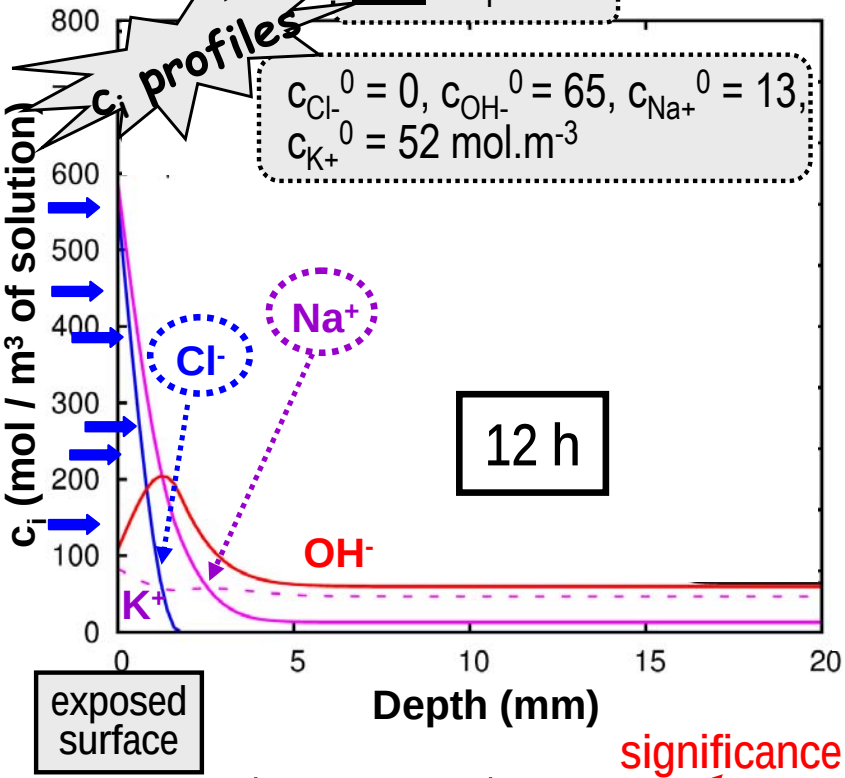
Level 2

Diffusion

I.C.: $S_l^0 = 1$

$c_{Cl^-}^0 = 0$, $c_{OH^-}^0 = 65$, $c_{Na^+}^0 = 13$, $c_{K^+}^0 = 52$ mol.m^{-3}

c_i profiles



significance of K_l!

➡ **$S_l^0 = 0.09$** | ➡ ions move along with the liquid phase (advection)
➡ faster Cl⁻ (and Na⁺) ingress and higher c_{Cl^-} compared to **$S_l^0 = 1$**

➡ **$S_l^0 = 1$** (diffusion) ➡ larger Na⁺ penet. depth (no binding) than Cl⁻ (equil. binding)

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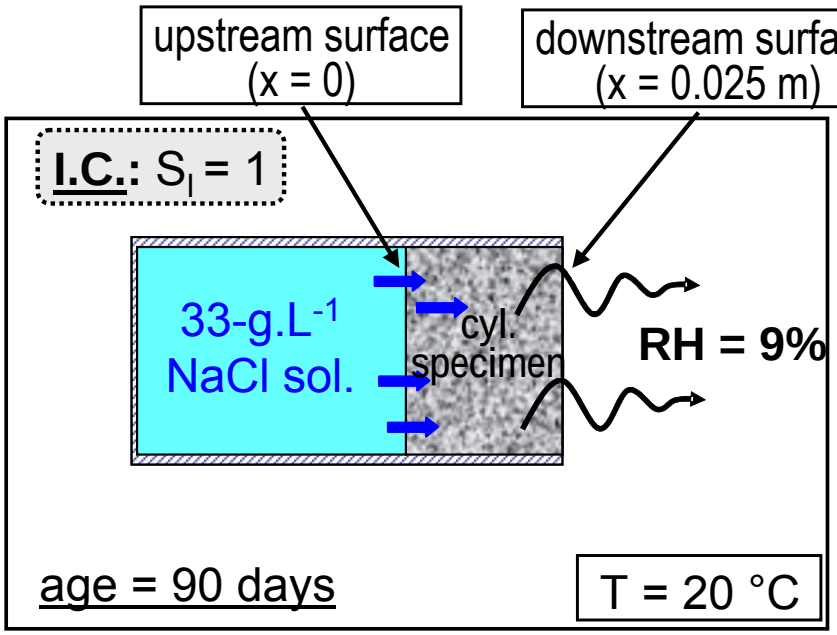
• Simulation of wick-action test •

Level 4

Mortar M1N

(W/C=0.50)

Experimental conditions



[Francy, Ph.D thesis, 1998]

I.C.: $c_{Cl^-}^0 = 0$, $c_{OH^-}^0 = 65$, $c_{Na^+}^0 = 13$, $c_{K^+}^0 = 52$ mol.m^{-3}

Material properties

Moisture transport

- ϕ = **0.13** ➔ **exp.**
- D_{Cl^-} = **2.1 · 10^{-12} m^2.s^{-1}** ([Cl^-_{tot}] profile after 7-d nss diffusion test ➔ **inv. analysis**)
- K_l = **15 · 10^{-21} m^2** (drying kinetics at RH = 4% ➔ **inv. analysis**)
- $p_c = p_c(S_l)$ from **exp.** WVAI & WVDI *[Bonnet, Ph.D thesis, 1997]*
- $S_{Cl} = S_{Cl}(c_{Cl^-})$ ➔ **exp. data** + *Freundlich's* description

Level 2

[Francy, Ph.D thesis, 1998]

*****

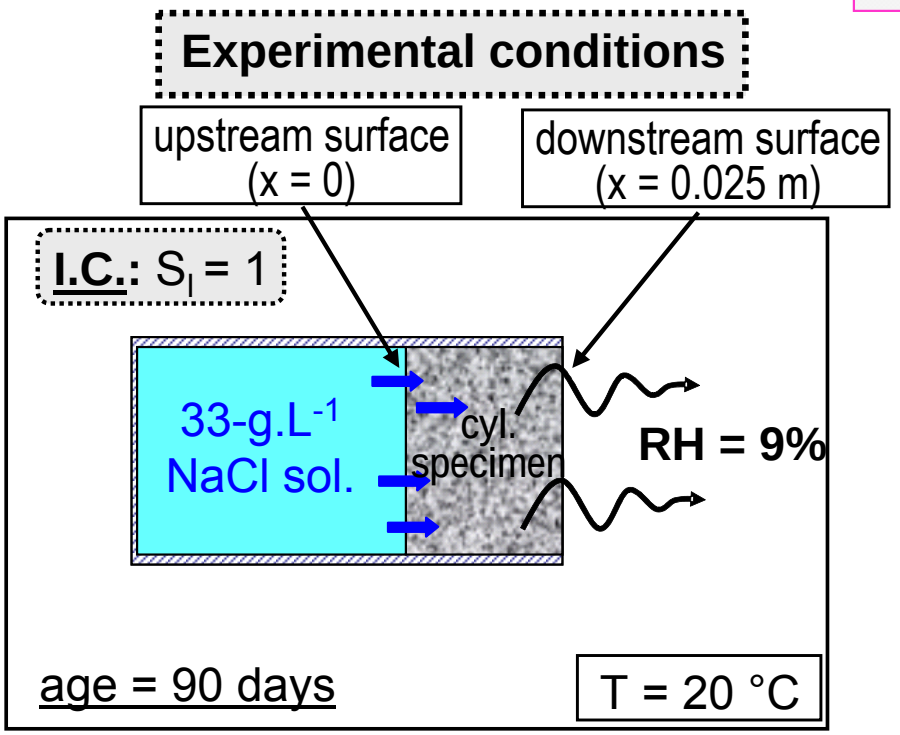
• Simulation of wick-action test •

Level 4

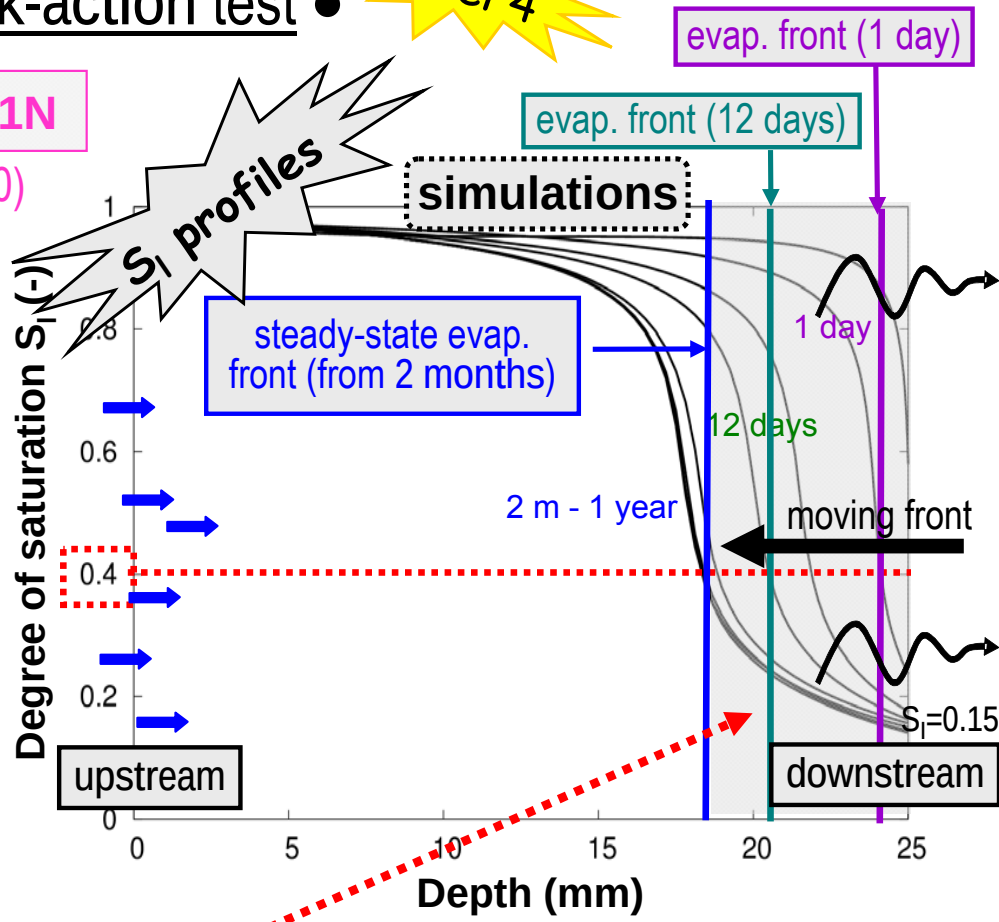
Mortar M1N

(W/C=0.50)

Experimental conditions



[Francy, Ph.D thesis, 1998]



[Baroghel-Bouny et al., CCR, 2011]

- RH = 9% at x = 0.025
  - ➔ strong drying
  - ➔ formation of a zone with $S_l < 0.40$ (from x = 0.025) ➔ **no liquid transport**
  - ➔ **evaporation front**

➡ after a given time ➔ **steady-state regime** (S_l profile & evap. front)

*****

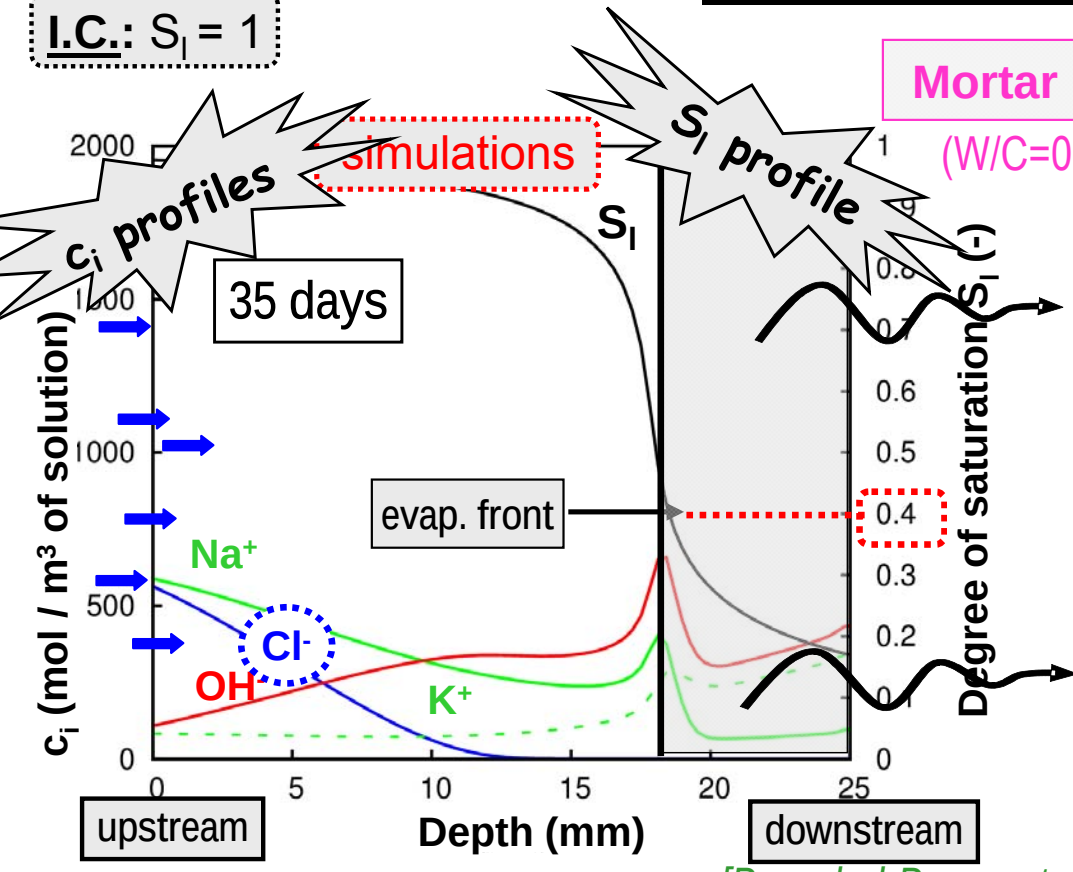
● Simulation of wick-action test ●

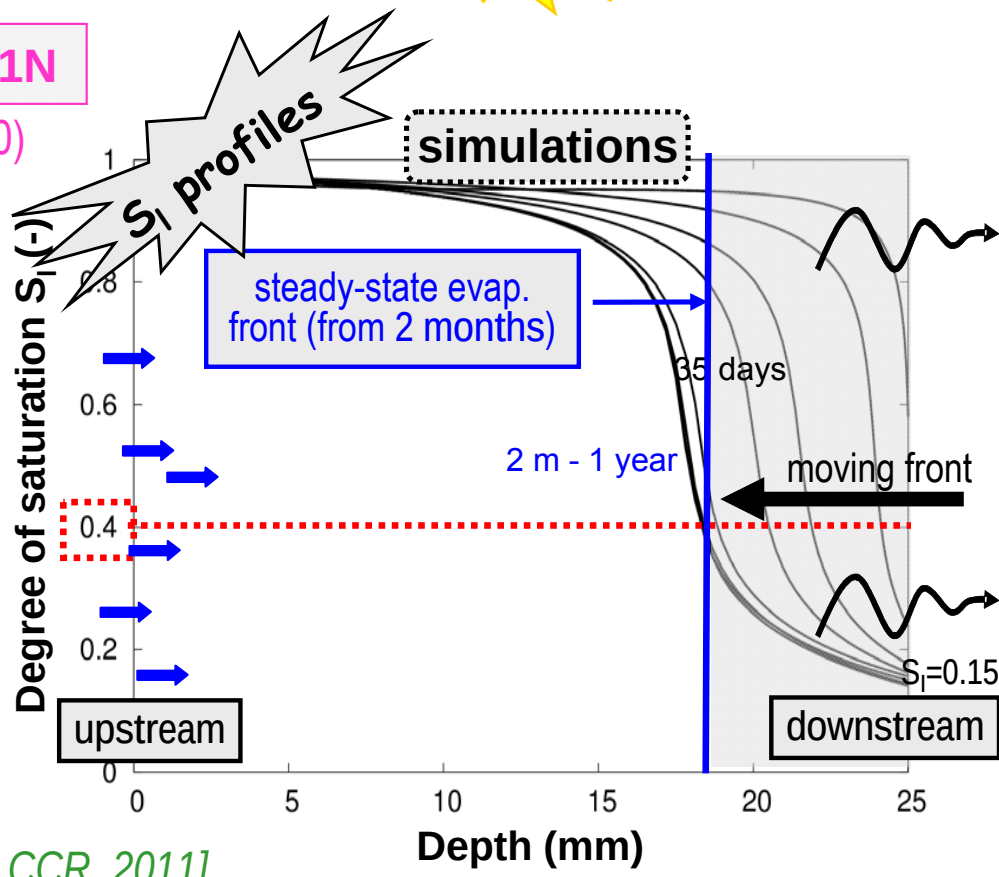
Level 4

I.C.: $S_l = 1$

Mortar M1N

(W/C=0.50)





[Baroghel-Bouny et al., CCR, 2011]

● Close to the upstream surface (x = 0) → **Cl^-** move by diffusion + advection towards the downstream surface (x = 0.025)

*****

• Simulation of wick-action test •

Level 4

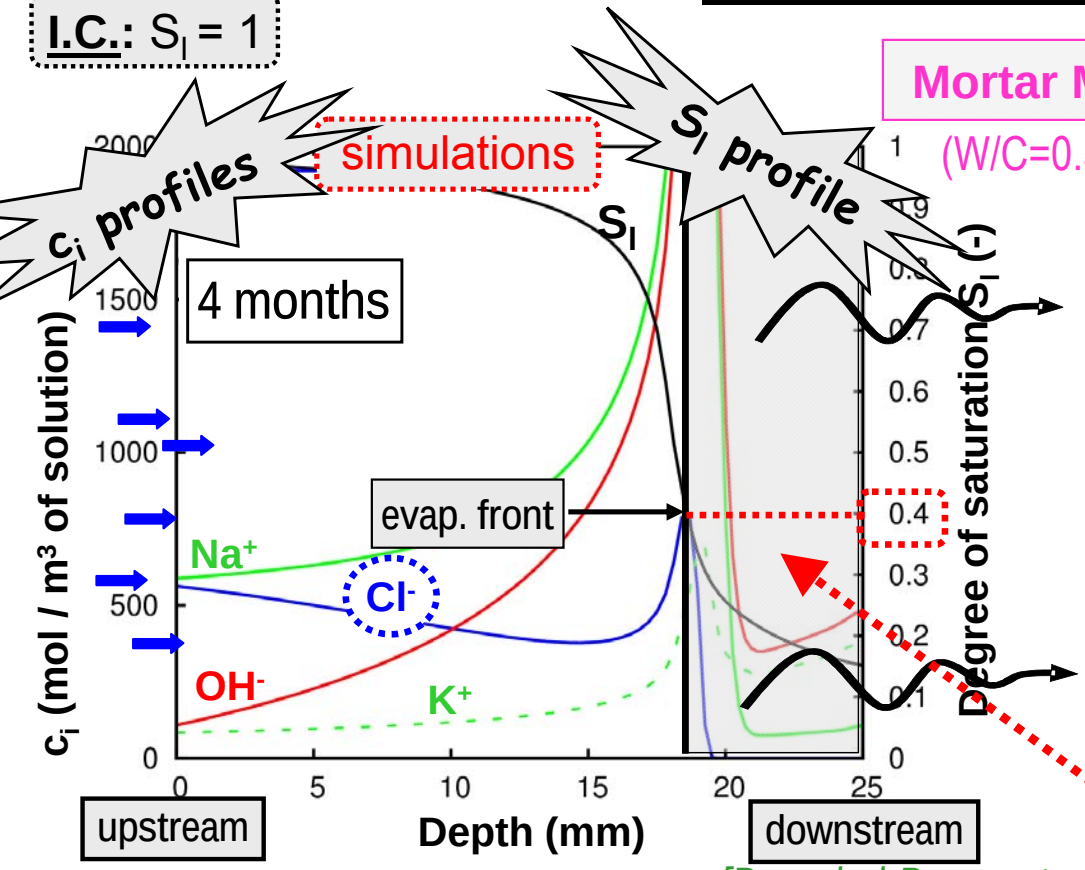
Exp. data

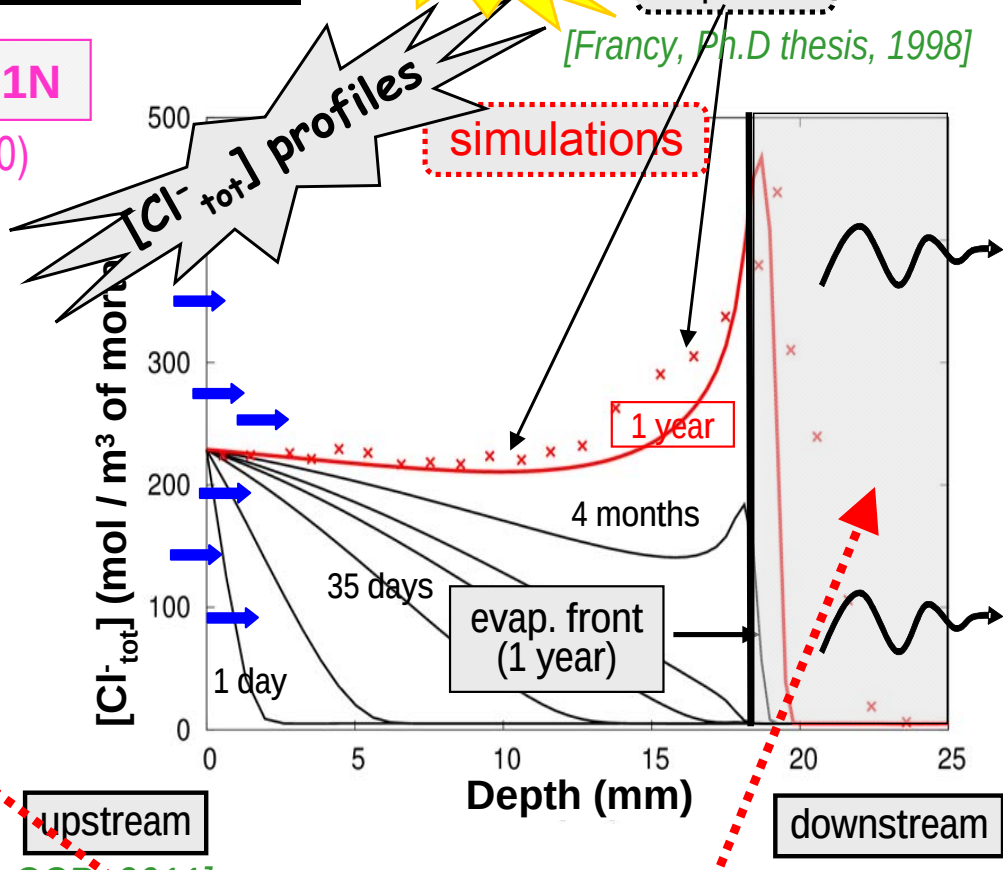
[Francy, Ph.D thesis, 1998]

I.C.: $S_l = 1$

Mortar M1N

(W/C=0.50)





[Baroghel-Bouny et al., CCR, 2011]

- Close to the upstream surface (x = 0) → **Cl^-** move by diffusion + advection towards the downstream surface (x = 0.025)
- RH = 9% at x = 0.025 → strong drying → significant liquid flow → advection prominent
  - → **no liquid transport** in the zone where $S_l < 0.40$
  - → **Cl^- accumulation** at the evaporation front

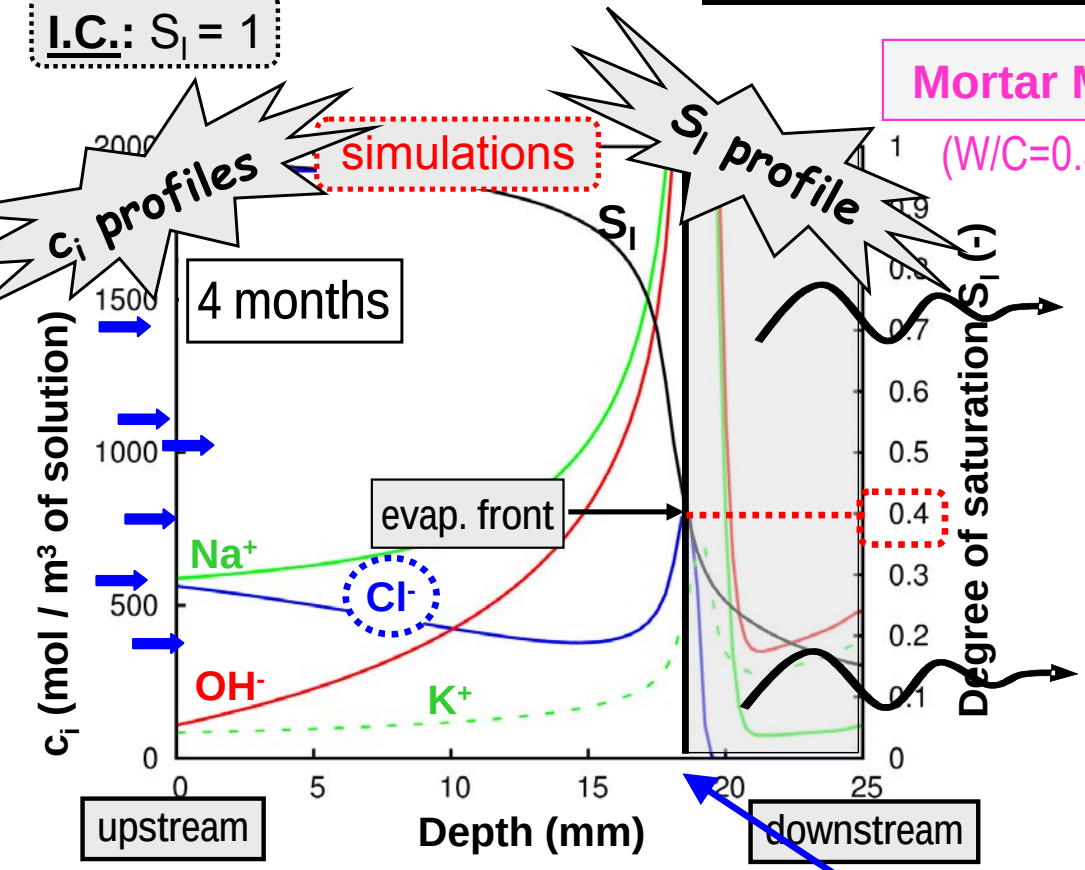
significance of K_l !

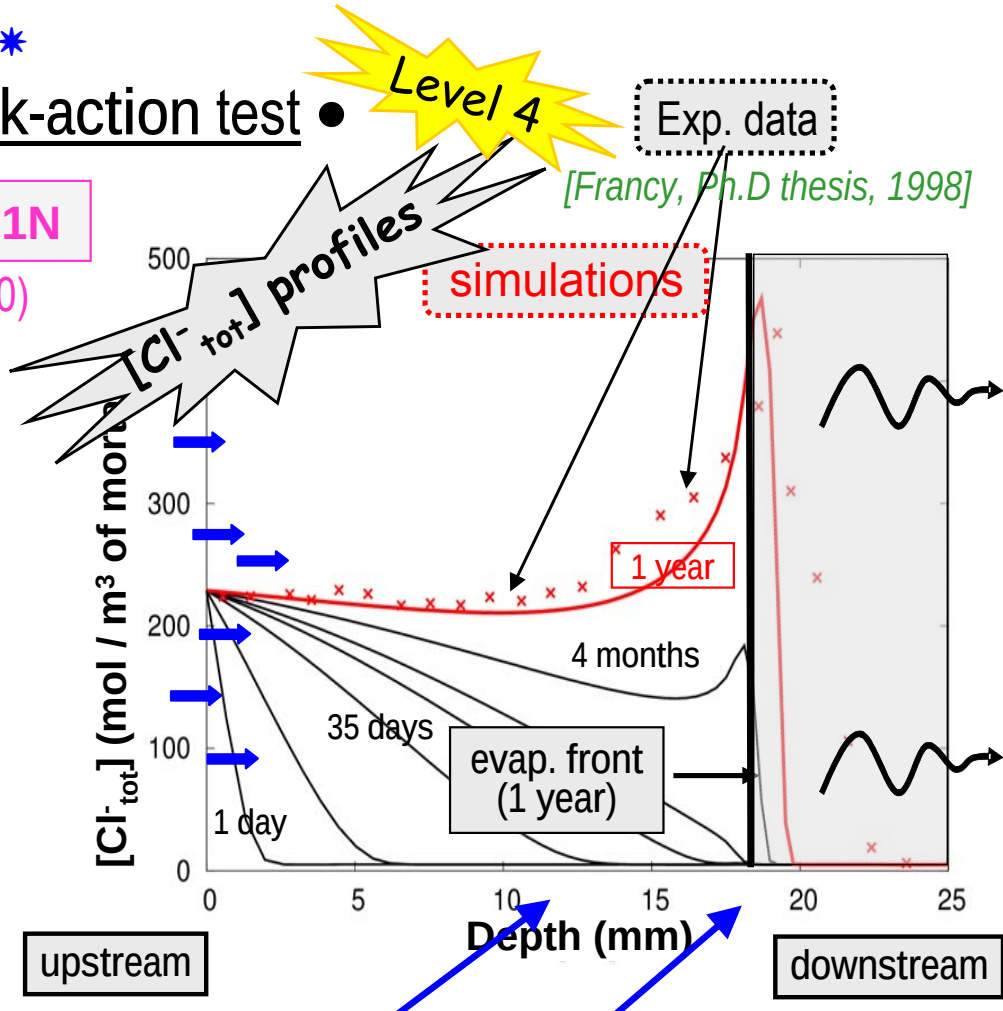
*****

• Simulation of wick-action test •

I.C.: $S_l = 1$

Mortar M1N (W/C=0.50)





[Baroghel-Bouny et al., CCR, 2011]

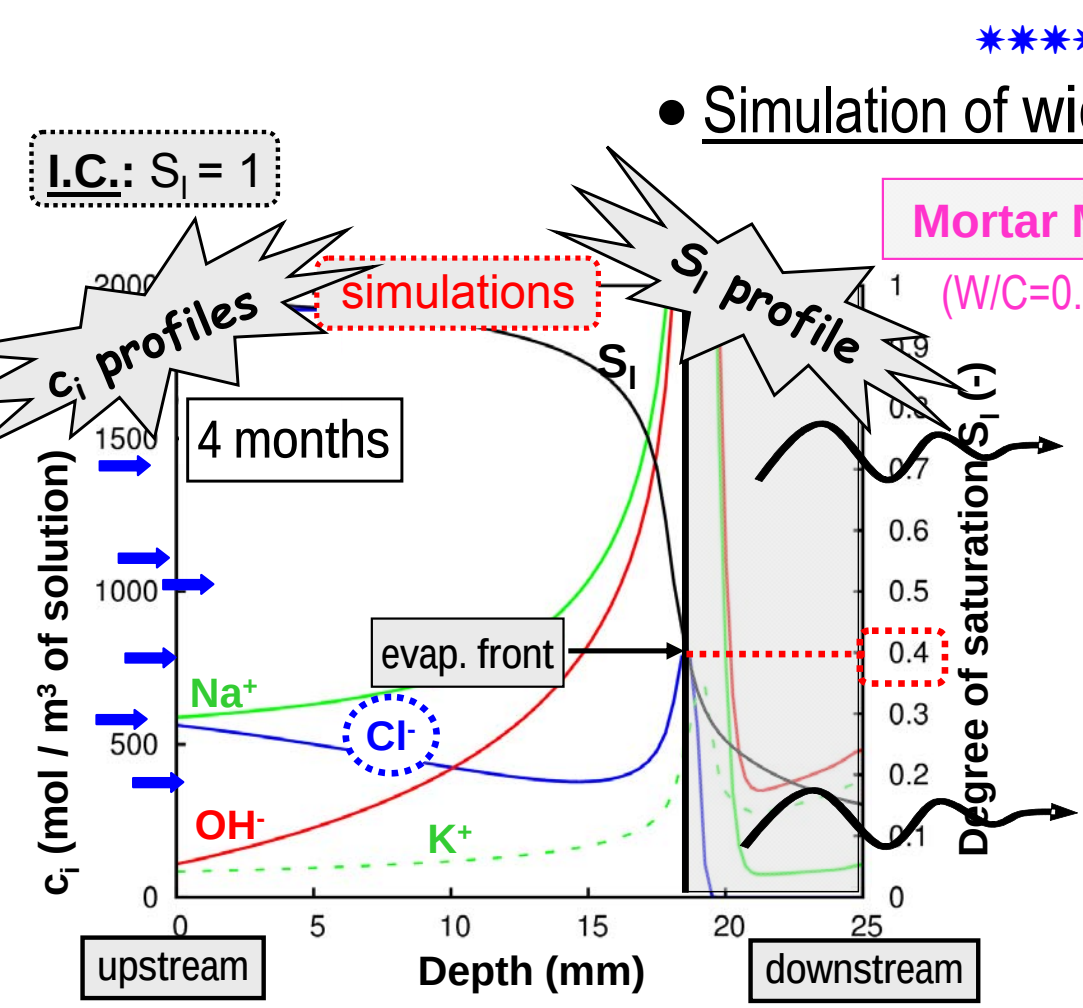
- consistence between **evap. fronts** deduced from $[Cl^-_{tot}]$, c_i & S_l profiles
- peculiar shape of the num. ionic & $[Cl^-_{tot}]$ profiles
- good agreement between **num. simulations** and **exp. data** (at 1 year)
  - ↳ *location of the evap. front **experim**. and **theor**. pointed out*

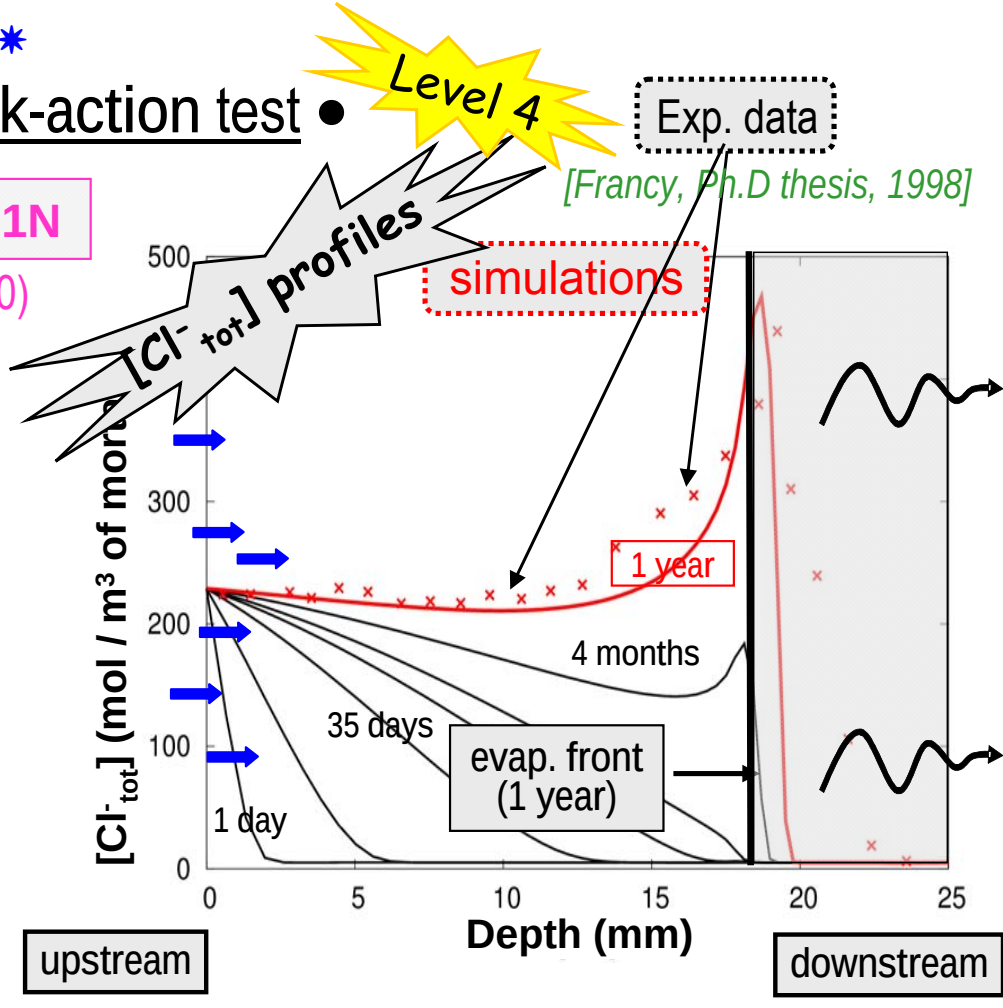
*****

● Simulation of wick-action test ●

I.C.: $S_l = 1$

Mortar M1N (W/C=0.50)





[Baroghel-Bouny et al., CCR, 2011]

➡ Simulation of all the complex effects associated with coupled moisture-ion transport on profiles (e.g. in the vicinity of the evap. front)

➡ **Validation of the level-4 model** in lab cond. for prediction (1st stage of validation)

Outline

1 - Introduction

2 - Modelling of isothermal **Cl^- transport** in concrete

- **2.1 -** Level 2: Multi-species transport model (sat. cond.)
- **2.2 -** Level 3: Advanced physical-chemical model (sat. cond.)
- **2.3 -** Level 4: Coupled moisture-ion transport model

☞ ***3 - Modelling of carbonation of concrete***

- **3.1 -** Level 2: Semi-analytical physical-chemical model - Probabilistic framework
- **3.2 -** Level 3: Numerical physical-chemical model

4 - Concluding remarks & further needed developments

3 - MULTI-LEVEL CONCEPT APPLIED TO MODELLING OF CARBONATION OF CONCRETE

*****

Increasing level of sophistication

- **Level 1 - Analytical** physical-chemical models *[Papadakis et al., ACI, 1991]*
  - ↳ √t law → sharp carbonation front

SLD — Easy coupling with probabilistic methods

- **Level 2 - Semi-analytical** physical-chemical models
  - ↳ **analytical** *Papadakis'* approach + weathering **cycles** *[Bakker, 1993], [Hyvert, 2009]*
  - ↳ **analytical** *Papadakis'* approach + **numerical** physical moisture transport model + no carbo. for RH≥90% *[Thiery et al., CONMOD'08, 2008]*

Advanced models

- **Level 3 - Numerical** physical-chemical models
  - ↳ comprehensive **speciation** models *[van der Lee et al., C&G, 2006], [Matschei, Lothenbach et al., CCR, 2007]*
    thermodynamic (equil.) modelling (+ mod. of hydrodynamic processes in sat. cond.)
  - ↳ (coupled) **transport-chemistry** models *[Steffens, CCR, 2002], [Bary & Sellier, CCR, 2004], [Saetta et al., CCR, 2004], [Mai-Nhu et al., SSCS, 201*
    - chemistry: thermodynamic modelling → phase assemblages at equilibrium (0-D)
      - chemistry of the pore solution ($[K^+]$, $[Na^+]$, ...)
      - evolution of the solid phases (e.g. C-S-H decalcification)

      → pH evolution
    - chemical reaction kinetics ($Ca(OH)_2$) → *soften up the carbonation profile*
    - physics: **microstructural** changes → evolution of porosity, transport properties, ...
    - coupling with advanced **transport** model (non-sat. cond.) → S_l evolution

[Thiery et al., 2005-2012]

3.2 - NUMERICAL PHYSICAL-CHEMICAL MODEL

*****

Level 3

[Thiery et al., CANMET/ACI, 2006]

• Chemical aspects: speciation in the pore solution •

local thermod. equilibrium

free & bound alkalis are taken into account

	Chemical reactions (aqueous solution)	$\log(K_i)$	r_i
(1)	$OH^- + H^+ \Leftrightarrow H_2O$	14	r_1
(2)	$Ca^{2+} + 2OH^- \Leftrightarrow Ca(OH)_2^0$	0	r_2
(3)	$Ca^{2+} + H_2O \Leftrightarrow Ca(OH)^+ + H^+$	−12.78	r_3
(4)	$Na^+ + H_2O \Leftrightarrow NaOH^0 + H^+$	−14.18	r_4
(5)	$K^+ + H_2O \Leftrightarrow KOH^0 + H^+$	−14.46	r_5
(6)	$CO_2^0 + H_2O \Leftrightarrow H_2CO_3$	–2.77	r_6
(7)	$H_2CO_3 + OH^- \Leftrightarrow HCO_3^- + H_2O$	7.65	r_7
(8)	$HCO_3^- + OH^- \Leftrightarrow CO_3^{2-} + H_2O$	3.66	r_8
(9)	$Ca^{2+} + HCO_3^- \Leftrightarrow CaHCO_3^-$	1.11	r_9
(10)	$Na^+ + HCO_3^- \Leftrightarrow NaHCO_3^0$	−0.25	r_{10}
(11)	$Na^+ + HCO_3^- \Leftrightarrow NaCO_3^- + H^+$	−9.10	r_{11}
(12)	$H_2SiO_4^{2-} + 2H^+ \Leftrightarrow H_4SiO_4^0$	23.14	r_{12}
(13)	$H_2SiO_4^{2-} + H^+ \Leftrightarrow H_3SiO_4^-$	13.33	r_{13}
(14)	$H_2SiO_4^{2-} + Ca^{2+} \Leftrightarrow CaH_4SiO_4^0$	4.60	r_{14}
(15)	$H_3SiO_4^- + Ca^{2+} \Leftrightarrow CaH_3SiO_4^+$	1.20	r_{15}

reaction rate

CO_2 dissol./dissociation in the pore solution

➥ **evolution of the chemical compo. of the pore solution**

➥ **pH value**

3.2 - NUMERICAL PHYSICAL-CHEMICAL MODEL

★★★★★ Level 3 [Morandeau et al., CONMOD, 2010]

- Chemical aspects: chemical reactions between ionic & solid phases (dissol./precip.) - kinetic effect -

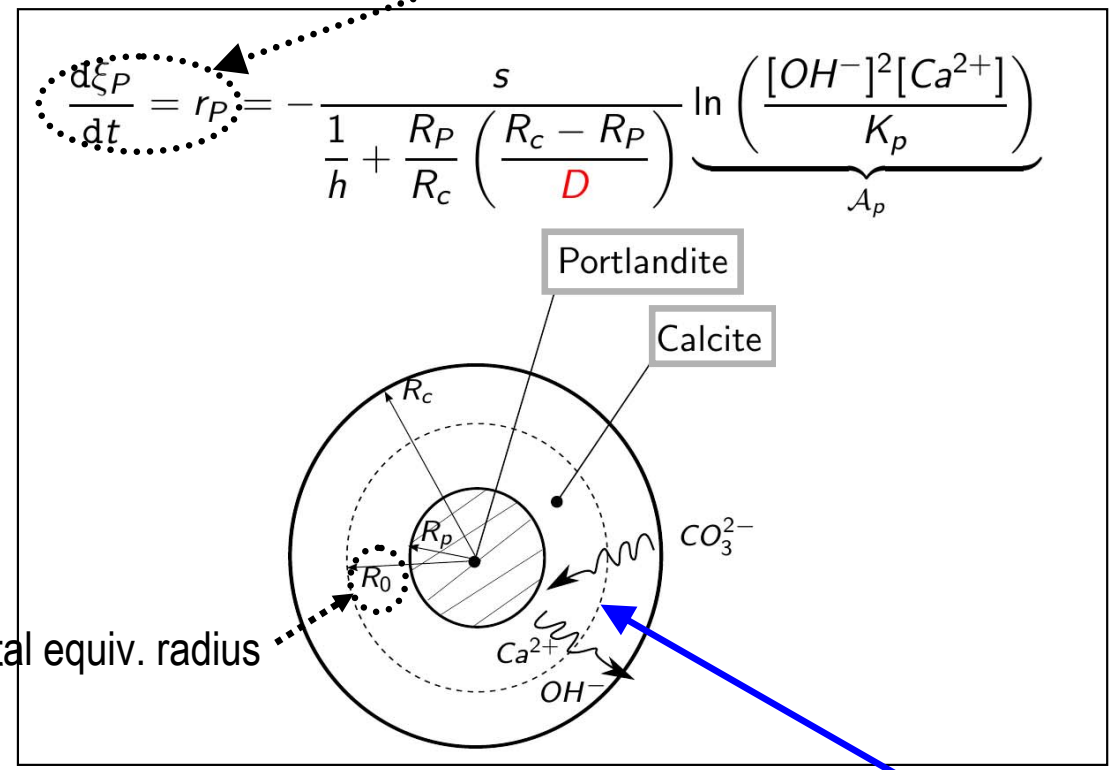
evolution of solid phases

	Heterogeneous chemical reactions	$\log(K_i)$	r_i
(P)	$Ca^{2+} + 2OH^- \Leftrightarrow CH$	5.19	r_P
(C)	$Ca^{2+} + CO_3^{2-} \Leftrightarrow C\overline{C}$	8.45	r_C

reaction rate

➔ **$Ca(OH)_2$** dissolution and $CaCO_3$ precipitation

$$\frac{d\xi_P}{dt} = r_P = -\frac{s}{\frac{1}{h} + \frac{R_P}{R_c}\left(\frac{R_c - R_P}{D}\right)} \underbrace{\ln\left(\frac{[OH^-]^2[Ca^{2+}]}{K_p}\right)}_{\mathcal{A}_p}$$



Initial $Ca(OH)_2$ crystal equiv. radius

kinetic effect
↪ *softens up the front*

➔ reduction of accessibility ($CaCO_3$ layer)

3.2 - NUMERICAL PHYSICAL-CHEMICAL MODEL

★★★★★ Level 3 [Morandeau et al., CONMOD, 2010]

- Chemical aspects: chemical reactions between ionic & solid phases (dissol./precip.) - kinetic effect -

evolution of solid phases

	Heterogeneous chemical reactions	$\log(K_i)$	r_i ← reaction rate
(P)	$Ca^{2+} + 2OH^- \Leftrightarrow CH$	5.19	r_P
(C)	$Ca^{2+} + CO_3^{2-} \Leftrightarrow C\overline{C}$	8.45	r_C
(C-S-H)	$C_xS_yH_z \Leftrightarrow xCa^{2+} + 2xOH^- + yH_4SiO_4^0 + (z-x-2y)H_2O$	variable	r_{CSH}

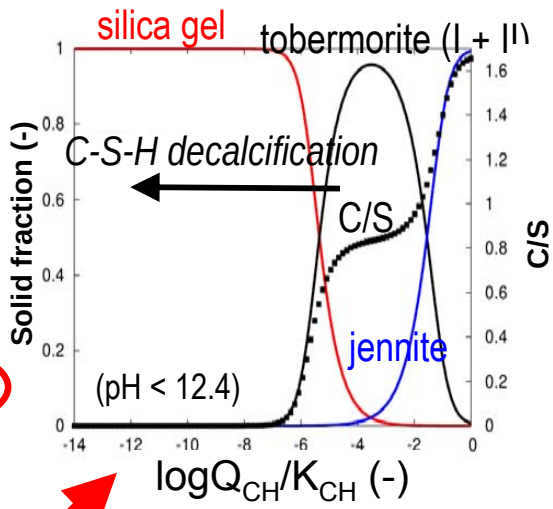
SCMs !

➔ progressive decalcification of **C-S-H** (& $CaCO_3$ precipitation)

(Ideal) solid solution model *[Kulik & Kersten, JACS, 2001]*

2 ideal C-S-H binary solid solution phases
↳ 4 end-members

Amorphous silica:	$C_0S_1H_1$	C/S	=0	$\log(K_i)$=-2.71
Tobermorite II:	$C_{1.5}S_{1.8}H_3$	C/S	=0.83	$\log(K_i)$=-21.19
Tobermorite I:	$C_2S_{2.4}H_4$	C/S	=0.83	$\log(K_i)$=-28.26
Jennite:	$C_{1.5}S_{0.9}H_{2.4}$	C/S	= 1.7	$\log(K_i)$=-15.62



For each end-member i: molar solid fraction $f_i = Q_i/K_i$ with $\Sigma f_i = 1$

activity product / solubility product

↳ constitutive chemical law which depends on Q_{CH} ➔ *easy implementation*
↳ pH value

3.2 - NUMERICAL PHYSICAL-CHEMICAL MODEL

Level 3

*****

• Transport equations (macroscale - partially saturated material) •

[Thiery et al., CANMET/ACI, 2006]

1 Gaseous CO_2 diffusion

CO_2 molar flux $\mathbf{w}_{CO_2} = -D_{CO_2}(\phi,\ S_l)\,\mathbf{grad}\,[CO_2]$ **(*Fick's 1st* law)**

diffusion coef. in the air

$$D_{CO_2}(\phi,\ S_l) = D^0_{CO_2}\,\phi^{2,74}(1-S_l)^{4,20}$$

reduction factor

2 Liquid water transport

filtration rate: $\mathbf{V}_l = -\frac{K_l}{\eta} k_{rl}(S_l)\,\mathbf{grad}\,p_l$ **(extended *Darcy's* law)**

$p_l(S_l) = p_g - p_c(S_l)$: capillary pressure curve

3 Transport of ionic species

(e.g. Ca^{2+} from $Ca(OH)_2$ dissolution)

advection

mole flux of species i: $\mathbf{w}_i = -D_i\,\mathbf{grad}\,[i] - \frac{z_i F}{RT} D_i\,\mathbf{grad}\,\psi + [i]\mathbf{V}_l$ **(extended *Nernst-Planck* equation)**

$$D_i = \frac{D^0_i}{D^0_{Ca^{2+}}} \times 2,35.10^{-13}\exp(9,95\phi)\,\frac{1}{[1+625(1-S_l)^2]}$$

[Tognazzi, 1998], [Thiery, 2005]

3.2 - NUMERICAL PHYSICAL-CHEMICAL MODEL

Level 3

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● Balance equations and related main unknown variables ●

[Thiery et al., CANMET/ACI, 2006]

	Equations		Related variables
(1) Global mass balance equation	$\frac{\partial m}{\partial t} = -\mathrm{div}\,\mathbf{w}_m$	$\Longleftrightarrow$	S
(2) Charge balance	$\mathrm{div}\,\mathbf{w}_q = \mathbf{0}$	$\Longleftrightarrow$	Ψ
(3) C-balance	$\frac{\partial n_C}{\partial t} = -\mathrm{div}\,\mathbf{w}_C$	$\Longleftrightarrow$	$[CO_2]$
(4) Na-balance	$\frac{\partial n_{Na}}{\partial t} = -\mathrm{div}\,\mathbf{w}_{Na}$	$\Longleftrightarrow$	$[Na^+]$
(5) K-balance	$\frac{\partial n_K}{\partial t} = -\mathrm{div}\,\mathbf{w}_K$	$\Longleftrightarrow$	$[K^+]$
(6) Ca-balance	$\frac{\partial n_{Ca}}{\partial t} = -\mathrm{div}\,\mathbf{w}_{Ca}$	$\Longleftrightarrow$	$n_{C\bar{C}}$
(7) Si-balance	$\frac{\partial n_{Si}}{\partial t} = -\mathrm{div}\,\mathbf{w}_{Si}$	$\Longleftrightarrow$	$n_{\text{C-S-H}}$
(8) Local electroneutrality	$q = 0$	$\Longleftrightarrow$	$[OH^-]$
(9) solid solution model	$\sum_i f_i = 0$	$\Longleftrightarrow$	$[H_3SiO_4^-]$

Coupling between transport equations & chemical reactions

3.2 - NUMERICAL PHYSICAL-CHEMICAL MODEL

Level 3

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- Input data required for the model (accelerated carbonation in lab) -

few inputs

I.C.	c_{Na+}^0, c_{K+}^0	*Initial* chemical compo. of the pore solution
	$n^0_{Ca(OH)2}$	*Initial* $Ca(OH)_2$ content in concrete ($mol.m^{-3}$)
	$n^0_{C\text{-}S\text{-}H}$	*Initial* C-S-H content in concrete ($mol.m^{-3}$)
	$R^0_{Ca(OH)2}$	*Initial* $Ca(OH)_2$ crystal equiv. radius (µm)
	ϕ^0	*Initial* porosity accessible to water ($m^3.m^{-3}$)
	K_l^0	*Initial* intrinsic permeability to liquid water (m^2)
	S_l^0	*Initial* degree of saturation (-)
	$p_C = p_C(S_l)$	Capillary pressure curve
B.C.	x_{CO2}, $RH_{ext.}$	*External* CO_2 concentration ($mol.m^{-3}$) and RH
	S_l	Degree of saturation at the boundary of the sample

Durability indicators

exp. (TGA)

Chemical

hydration model

literature

Physical

$$K_l = K_l^0 \left[\frac{\phi}{\phi^0}\right]^3 \left[\frac{1-\phi}{1-\phi^0}\right]^2$$

[van Genuchten, 1982]

3.2 - NUMERICAL PHYSICAL-CHEMICAL MODEL: EXAMPLES OF SIMULATION

Level 3

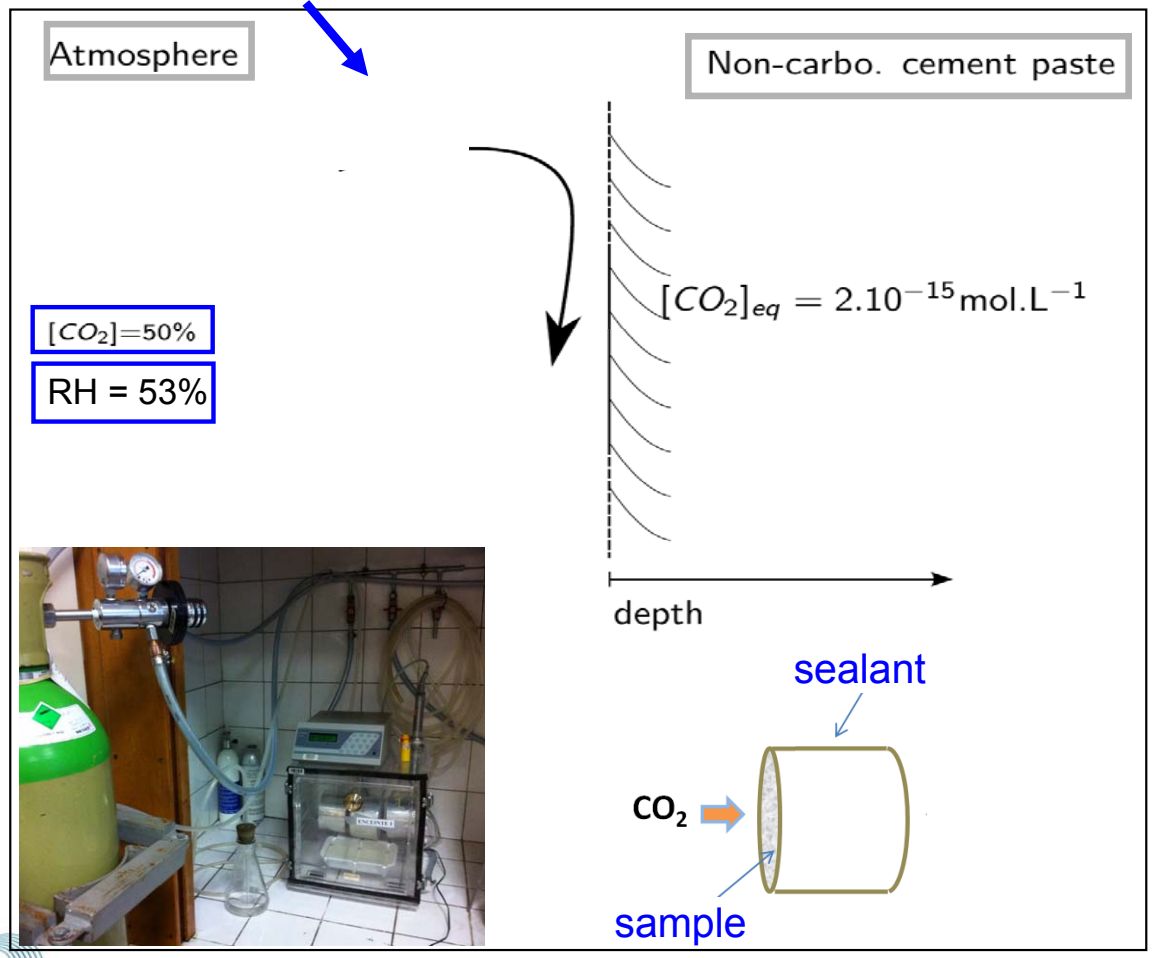
★★★★★

Hcp

(CEM I ; W/C=0.45)

(accelerated carbonation in lab)

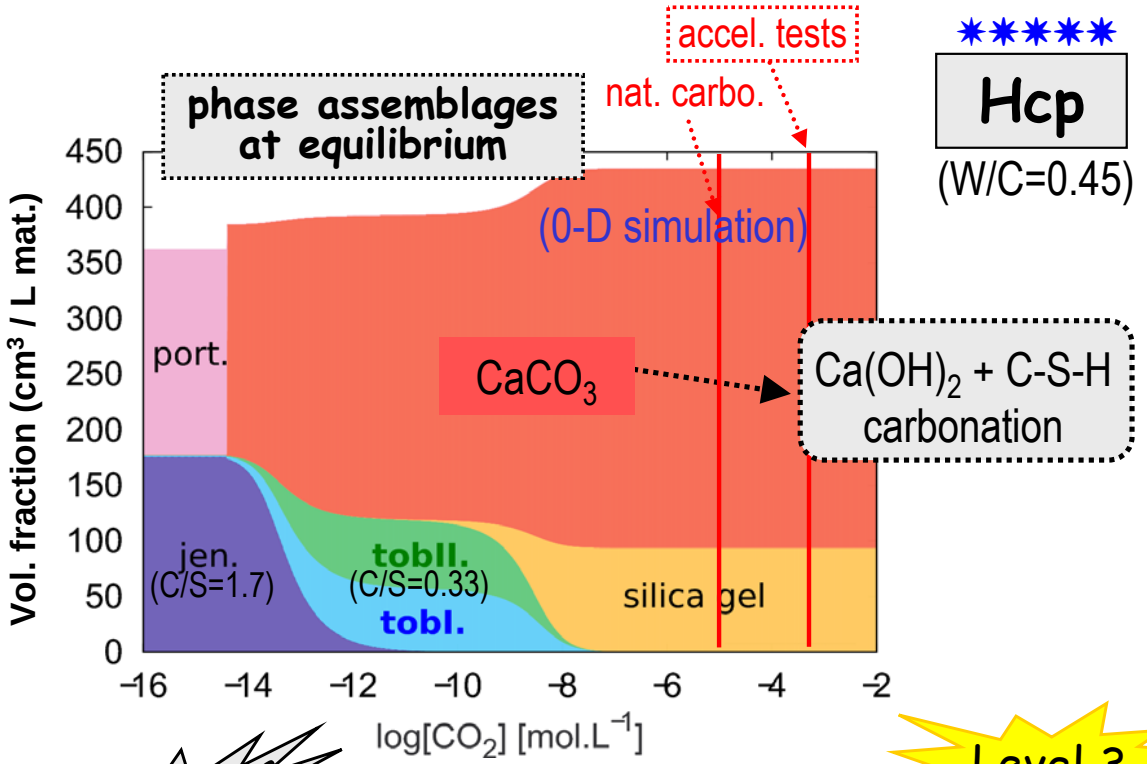
1) 1-year sealed curing
2) 1-year exposure to 1-D drying at RH=53%
3) **1-D carbonation**



Input data		value
Physical	ϕ_0 (%)	42.0
	K_l^0 (10^{-20} m^2)	2
	S_{0_l}(-)	RH = 53%
	$p_c = p_c(S_l)$	exp. WVDI
Chemical	n_{CH}^0 (mol.L^{-1})	5.6
	$n_{C\text{-}S\text{-}H}^0$ (mol.L^{-1})	2.4
	$[Na^+]$ (mol.L^{-1})	0.12
	$[K^+]$ (mol.L^{-1})	0.24
	R_0 (μm)	30

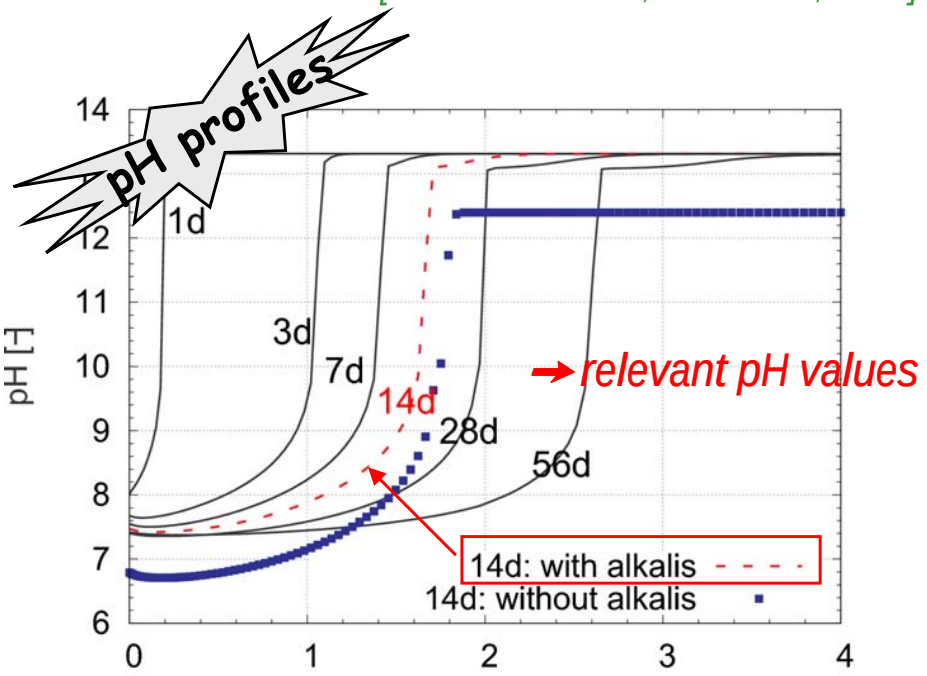
3.2 - NUMERICAL PHYSICAL-CHEMICAL MODEL: EXAMPLES OF SIMULATION

[Morandeau et al., CONMOD, 2010]



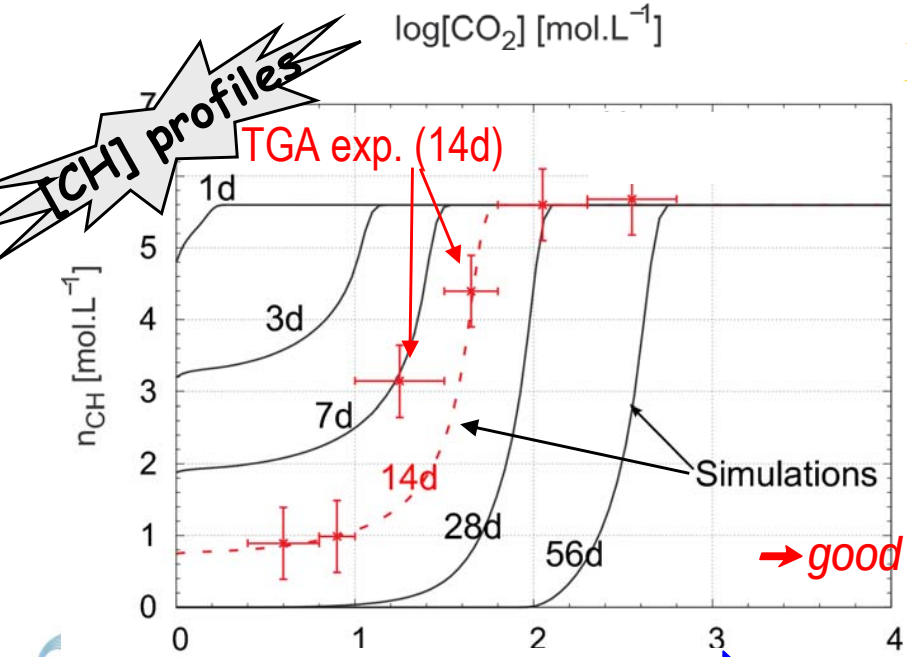
Hcp

(W/C=0.45)

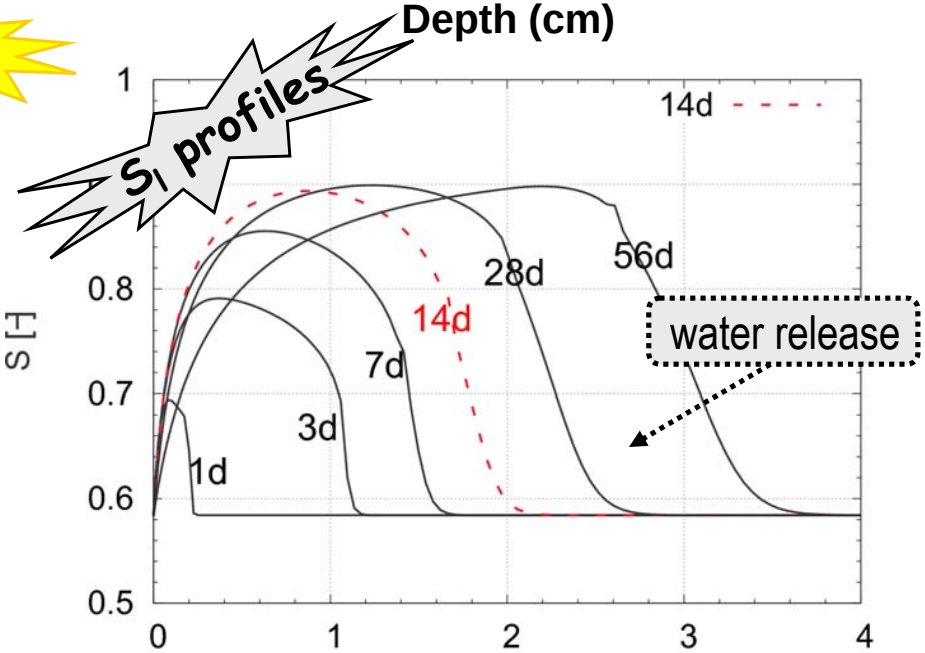


→ *relevant pH values*

Level 3



→ *good agreement*



➡ detailed & accurate predictions

Outline

1 - Introduction

2 - Modelling of isothermal **Cl^- transport** in concrete

- **2.1 -** Level 2: Multi-species transport model (sat. cond.)
- **2.2 -** Level 3: Advanced physical-chemical model (sat. cond.)
- **2.3 -** Level 4: Coupled moisture-ion transport model

3 - Modelling of **carbonation** of concrete

- **3.1 -** Level 2: Semi-analytical physical-chemical model - Probabilistic framework
- **3.2 -** Level 3: Numerical physical-chemical model

☞ ***4 - Concluding remarks & further needed developments***

4 - CONCLUDING REMARKS

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✷ Multi-level platform of numerical models for durability

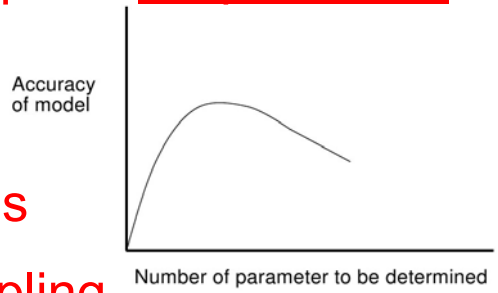
flexibility

- ➥ *intended for different issues*
- ➥ *selection according to accuracy required, target lifetime, available data, ...*

Engineering approaches

- **Intermediate levels**
  - num. inverse analysis (➟ input data K_l, D, μ, γ)
  - probabilistic approaches (➟ account for uncertainties)
  - [Cl^-] profile / carbonation depth & **SL** prediction

➥ *compromise between refinement & application*
(sufficient accuracy for various practical cases)



Advanced models

- **High levels**
  - validation of assumptions/mechanisms
  - integration of transport-chemistry coupling
  - integration of coupling between moisture & ionic/gaseous transports

- Integrated **exp./num.** and performance-based approach
  - input
  - validation

4 - FURTHER DEVELOPMENTS NEEDED / OTHER APPROACHES

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... in order to improve the prediction of long-term durability

[Biernacki et al., ACI, 2001], [Buffo-Lacarrière et al., CCR, 2007], [Kolani, PhD, 2012]

1 - Further **coupling** with hydration models

SCMs

➔ account for early-age characteristics in field cond. ("covercrete")

[Zhang et al., Microdurability, 2012]

2 - Better account for **hysteresis** effects (scanning curves) on **moisture transport**

[Johannesson & Janz, B&E, 2009]
[Zhang et al., SSCS 2012]

3 - Better description of **nano/microstructure** & its evolution

[Bentz, 1997], [Ye, PhD, 2003], [Bishnoi & Scrivener, CCR, 2009]

4 - Account for impact of **cracking** on transport processes

5 - Advanced physical-chemical models ➔ **Probabilistic** framework?

↪ *appropriate data bases !*

6 - Further physical-chemical **coupling** or coupling with mechanics

realistic SLD

➔ e.g. coupled moisture-ions-CO_2 transport model

➔ chemo-thermo-hygro-mechanical models ➔ e.g. sulfate attack, frost action with deicing salts

[Schrefler, SSCS, 2012]

7 - Integration of part of **propagation** period (corrosion, cracking, ...)

[Alexander, Microdurability, 2012], [Michel et al. Microdurability, 2012]

8 - Enhanced **multi-scale** approach (nano➔micro➔macro ; material➔**structure** ; 1D➔2D➔3D)

engineering applications

e.g. *[Maekawa & Ishida, 2001→2012]*

➔ e.g. 3-D integrated micro-material-structural modelling platform DuCOM-COM3

Thank you for your attention ...