Two-scale model for moisture transport in concrete carbonation process

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Outline of this talk

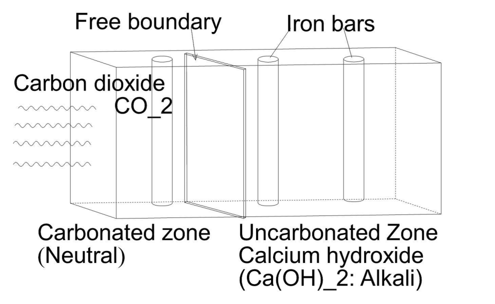
Aims: Introduce our results on concrete carbonation process: Model and mathematical results

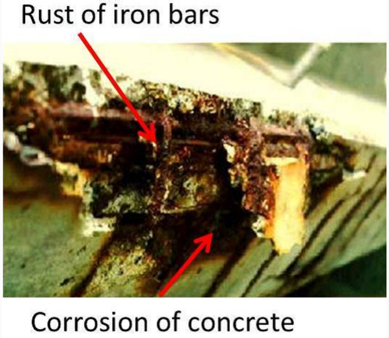
1. 1D model: free boundary model (with A. Muntean): 2009-2015
2. In 3D domain(with N. Sato, Y. Murase, K. Shirakawa, K. Kumazaki): Since 2011

Contents

1. Concrete carbonation process
2. 1D model: FBP
3. Model of concrete carbonation process in 3D domain
4. Multi-scale model
5. Summary, future works

1. Concrete carbonation process





Porous media, many holes.

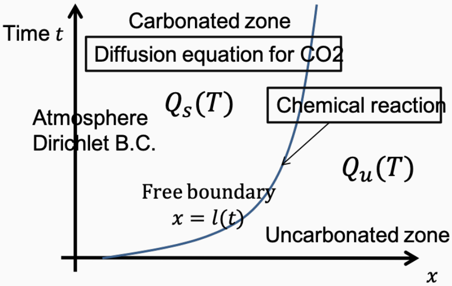
$$CO_2(aq) + Ca(OH)_2(aq) \to CaCO_3(aq) + H_2O$$

Purpose : To construct a model for concrete carbonation

By mathematical models we can measure depth of carbonation.

2. 1D model: Free boundary problem

Muntean, Böhm, 2007, 2009



1D FBP: Existence and uniqueness of solutions

A., Muntean, 2009-2011

Simplified model, large time behavior of carbonation depth $l(t)$:

$$c\sqrt{t} \le l(t) \le C\sqrt{t} \quad \text{for } t \ge 0.$$

Experimental law:

"Carbonation Depth $\propto \sqrt{t}$"

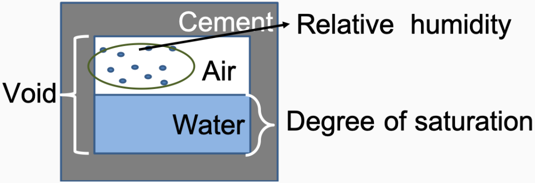
Our mathematical result guarantees the law.

3. Concrete carbonation process in 3D domain (1)

Maekawa-Chaube-Kishi(1999, book), Maekawa-Ishida-Kishi(1999)

Our model:

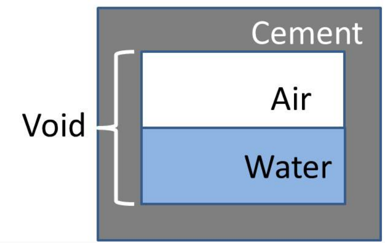
- Moisture transport & CO_2 diffusion(Kumazaki)
- Moisture transport $=$ conservation of H_2O(Two types)



- Diffusion equation & relationship between relative humidity and degree of saturation in concrete.

3. Concrete carbonation process in 3D domain (2)

Porous material

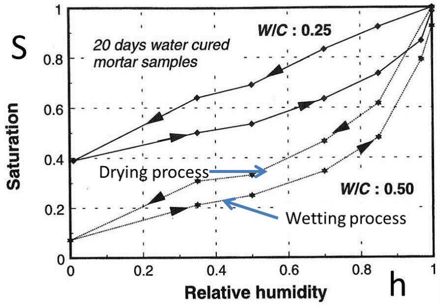


ϕ: porocity $\phi = \dfrac{\text{(Void)}}{\text{(Unit Volume)}}$

s: degree of saturation

$$s = \frac{\text{(water region)}}{\text{(Void)}}$$

Experimental results



Hysteresis with anti-clockwise trend

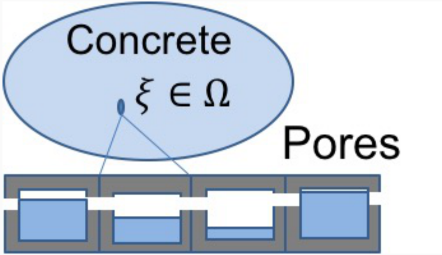
Our aim Find mathematical formula of this relationship

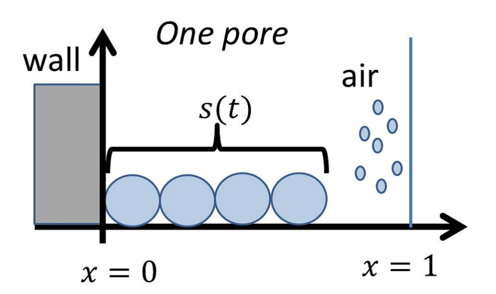
4. Multi-scale model(1): Outline

Concrete $=$ Porous material

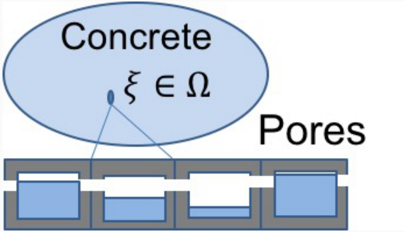
$$\text{Multi-scale model}: \begin{pmatrix} \text{Macro-domain} \\ \text{Concrete building} \\ \text{Diffusion equation} \end{pmatrix} \& \begin{pmatrix} \text{Micro-domain} \\ \text{One pore} \\ \text{1D FBP} \end{pmatrix}$$

Let Ω be a macro-domain in $\mathbb{R}^3$, bounded.





4. Multi-scale model(2): Domains and variables

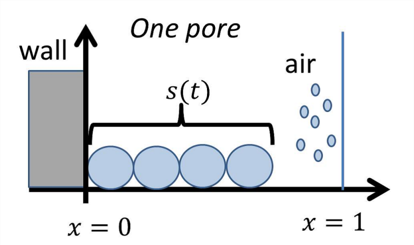


macro domain: $\xi \in \Omega$

relative humidity $h = h(t, \xi)$ on Ω

degree of saturation:

$$s = s(t, \xi) = \frac{\text{(water region)}}{\text{(Void)}}$$



micro domain: $x \in (0, 1)$

water region: $[0, s(t)]$

air region: $[s(t), 1]$

wall : $x = 0$

Connection to macro domain: $x = 1$

relative humidity: $u = u(t, \xi, x)$

4. Multi-scale model(3): FBP in micro domain

Find u and s s.t.

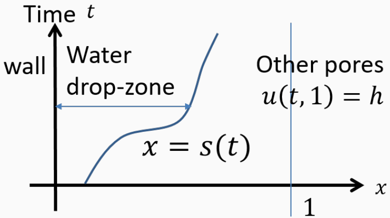
$$\rho_a u_t - \kappa u_{xx} = 0 \text{ on } (s(t), 1),$$
$$u(t,1) = h(t), t > 0,$$
$$\kappa u_x(t, s(t)) = (\rho_l - \rho_a u(t, s(t)))s'(t), t > 0,$$
$$s'(t) = a(u(t, s(t)) - \varphi(s(t))), t > 0,$$
$$s(0) = s_0, u(0, x) = u_0(x), s_0 \le x \le 1.$$

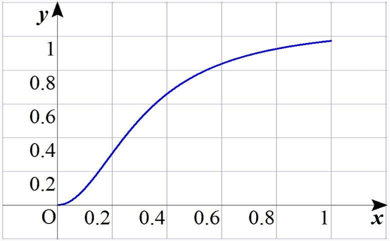
ρ_a, ρ_l: density of H_2O in air, liquid (resp.)

κ: diffusion coefficient

a: a positive constant

$\varphi : \mathbb{R} \to \mathbb{R}$





4. Multi-scale model(4): Free boundary condition

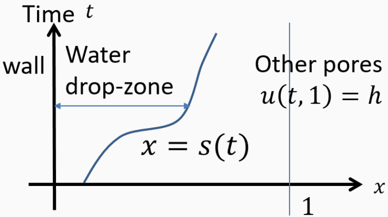
Key: $s(t) \to 1$?

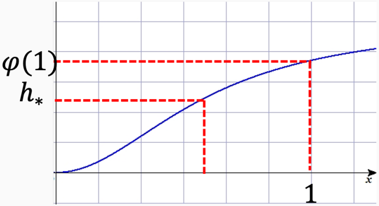
$$s'(t) = a(u(t, s(t)) - \varphi(s(t))), t > 0.$$

Assumption: $h \leq h^* < \varphi(1)$.

If $s(t) \to 1$, then $s'(t) = a(u(t, s) - \varphi(s(t))) \to a(u(t, 1) - \varphi(1))$ and $s'(t) < 0$.

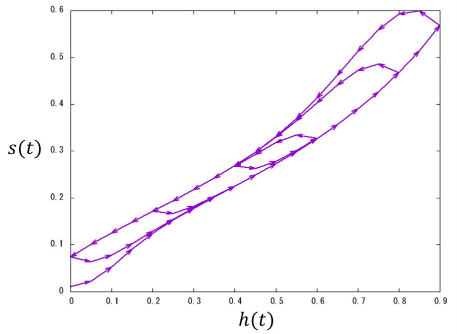
Then, s does not touch the fixed boundary $x = 1$.



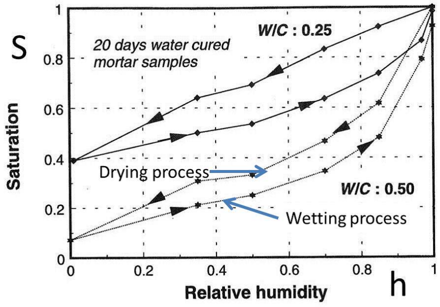


4. Multi-scale model(5): Numerical result

Numerical result



Experimental result



4. Multi-scale model(6): Previous results on 1D FBP

- Sato, A., Murase, Shirakawa(2013, 2014):
  Derivation of the free boundary problem
  Local existence in time and uniqueness
- A., Murase(2017):
  - Global existence, since s does not touch the fixed boundary $x = 1$.
  - Convergence to the steady solution as $t \to \infty$,
    namely, $s(t) \to s_*$ and $u(t) \to u_*$ as $t \to \infty$, where s_* and u_* are constants.
- Sato, A.(2018):
  If the boundary function h is periodic in time, then the FBP has a periodic solution in time. The uniqueness of periodic solutions is an open problem.

4. Multi-scale model(7): Mathematical formulation (Macro Scale)

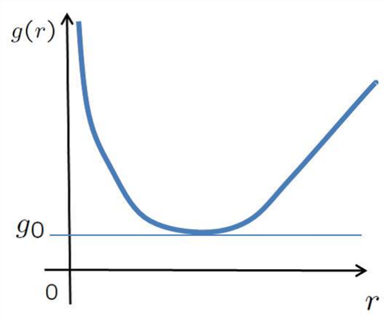
$\Omega \subset \mathbb{R}^3$. We suppose that $h = h(t, \xi)$ on $Q(T) := (0, T) \times \Omega$ satisfies

$$\rho_l h_t - \operatorname{div}_\xi(g(h)\nabla_\xi h) = sf \quad \text{in } Q(T),$$
$$h = h_b \quad \text{on } (0, T) \times \partial\Omega, \quad h(0) = h_0 \quad \text{on } \Omega.$$

$f : Q(T) \to [0, \infty)$: generation rate of H_2O by chemical reaction(given)

h_b, h_0: given

$g : (0, \infty) \to \mathbb{R}$, continuous



4. Multi-scale model(8): Mathematical formulation

Find $h = h(t, \xi)$ and $s = s(t, \xi)$ on $Q(T) := (0, T) \times \Omega$,
$u = u(t, \xi, x)$ on $\Sigma_s(T) = \{(t, \xi, x) | 0 < t < T, \xi \in \Omega, s(t, \xi) < x < 1\}$;

$$
\begin{aligned}
&\rho_l h_t - \operatorname{div}_\xi(g(h)\nabla_\xi h) = sf \quad \text{in } Q(T),\\
&h = h_b \quad \text{on } (0, T) \times \partial\Omega, \quad h(0) = h_0 \quad \text{on } \Omega,\\
&\rho_a u_t - \kappa u_{xx} = 0 \text{ on } (s(t, \xi), 1),\\
&u(t, \xi, 1) = h(t, \xi) \text{ for } (t, \xi) \in Q(T),\\
&(\rho_l - \rho_a u(t, \xi, s(t, \xi)))s'(t, \xi) = \kappa u_x(t, \xi, s(t)) \text{ for } t > 0,\\
&s'(t, \xi) = a(u(t, \xi, s(t, \xi)) - \varphi(s(t, \xi))) \text{ for } (t, \xi) \in Q(T),\\
&s(0, \xi) = s_0(\xi), u(0, \xi, x) = u_0(\xi, x) \text{ for } s_0 \le x \le 1, \xi \in \Omega.
\end{aligned}
$$

4. Multi-scale model(9): Mathematical results on Multi-scale model

- Kumazaki(2016, 2017): Measurability of s w.r.t. (t, ξ) for given h.
- Kumazaki, A., Murase, Sato(2017): Local existence in time and uniqueness
- Kumazaki(2019): Global existence in time and uniqueness:
  Assume $f = (1 - \psi(h))v$, $v \in L^\infty(Q(T)) \cap W^{1,2}(0, T; H^1(\Omega))$, $v \geq 0$,
  and $\psi : \mathbb{R} \to \mathbb{R}$, continuous, $0 \leq \psi \leq 1$ on $\mathbb{R}$, $\psi(r) = 1$ for $r \geq h^*$.
  If $h_b \leq h^*$ and $h_0 \leq h^*$, then the multi-scale problem has a unique solution on $[0, T]$ for any $T > 0$.

5. Summary, future works (1): Summary

- (Concrete carbonation process in 3D domain)
  $=$ (Moisture transport) & (Diffusion CO_2)
- (Moisture transport)
  1. Nonlinear diffusion H_2O
  2. Hysteresis relationship between degree of saturation and relative humidity

     $\Longrightarrow$ 1D FBP
- Moisture transport by multi-scale model
  $\Longrightarrow$ Global Existence (by Kumazaki)

$$\rho_l h_t - \operatorname{div}(g(h)\nabla h) = s(1 - \psi(h))v \quad \text{on } \Omega.$$

5. Summary, future works (2): Future problems

As a next step, we would like to consider the system of moisture transport and CO_2 diffusion. For example: v: concentration of CO_2.

$$
\begin{aligned}
&\rho_l h_t - \operatorname{div}((g(h) + \phi(v)(1-s))\nabla h) = s(1-\psi(h))v,\\
&(\phi(v)(1-s)v)_t - \operatorname{div}((1-s)\nabla v) = -kvw,
\end{aligned}
$$

where ϕ is the porosity and a function of v, k is a positive constant and w is a given function.

Thus we need the estimate for $\dfrac{\partial s}{\partial \xi}$.

5. Summary, future works (3): Estimate for ∇s

$$\rho_a u_t - \kappa u_{xx} = 0 \text{ on } (s(t,\xi),1),$$
$$u(t,\xi,1) = h(t,\xi) \text{ for } (t,\xi) \in Q(T),$$
$$(\rho_l - \rho_a u(t,\xi,s(t,\xi)))s'(t,\xi) = \kappa u_x(t,\xi,s(t)) \text{ for } t > 0,$$
$$s'(t,\xi) = a(u(t,\xi,s(t,\xi)) - \varphi(s(t,\xi))) \text{ for } (t,\xi) \in Q(T),$$
$$s(0,\xi) = s_0(\xi), u(0,\xi,x) = u_0(\xi,x) \text{ for } s_0 \le x \le 1, \xi \in \Omega.$$

Lemma (A., Kumazaki)
If $\nabla_\xi h, \nabla_\xi h_t \in L^2(0,T)$, $\nabla_\xi s_0 \in \mathbb{R}$ and $\nabla_\xi u_0 \in W^{1,2}(s_0,1)$, then $\nabla_\xi s \in W^{1,2}(0,T)$ and

$$|\nabla_\xi s|_{W^{1,2}(0,T)} \le C(1 + |\nabla_\xi h|_{L^2(0,T)} + |\nabla_\xi h_t|_{L^2(0,T)} + |\nabla_\xi s_0| + |\nabla_\xi u_0|_{W^{1,2}(s_0,1)}).$$

5. Summary, future works (4): Future works

The above estimate may not be enough to deal with the system of moisture transport and CO_2 diffusion.

1. **To solve the system we need to modify:**
   - FBP, particularly, $u(t, 1) = h(t)$.
   - Equation for moisture transport.
   - Diffusion equation for CO_2.
2. Uniqueness of periodic solutions of 1D FBP
3. Construction of a weak solution of 1D FBP