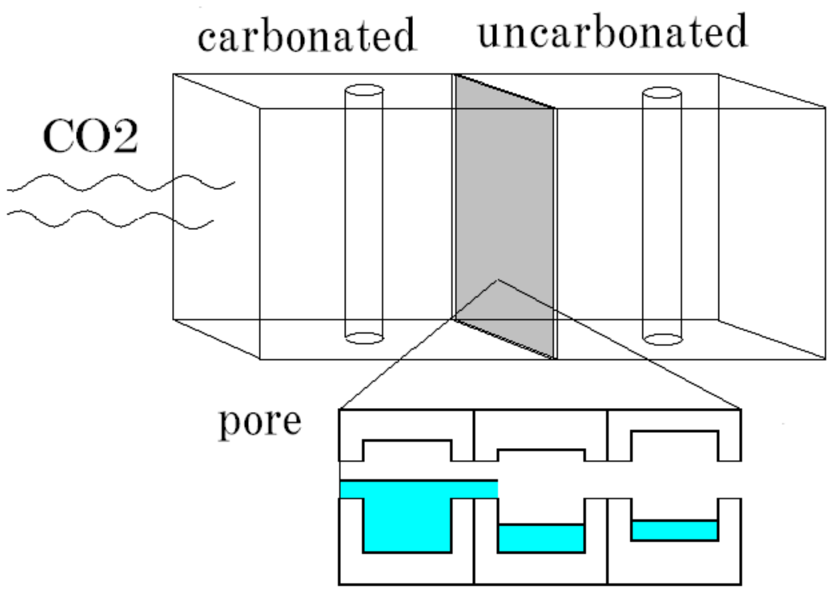
A multiscale model for moisture transport appearing in concrete carbonation process

Kota Kumazaki (Tomakomai National College of Technology)
Toyohiko Aiki (Japan Women's University)
Naoki Sato (Nagaoka National College of Technology)
Yusuke Murase (Meijo University)

KAAS seminar, 23 August, Karlstad University

Contents

1. Concrete Carbonation



$\cdots x \cdots$

- Chemical rection :

$$\underbrace{\mathrm{Ca(OH)_2}}_{\text{main ingradient}} + \underbrace{\mathrm{CO_2}}_{\text{external}} \Rightarrow \underbrace{\mathrm{CaCO_3}}_{\text{precipitation}} + \underbrace{\mathrm{H_2O}}_{\text{internal}}$$

- Speed : $x \propto \sqrt{t}$
  (x : position of carbonation, t : time)

Previous works (1D)

- Muntean-Böhm '07, '09
- Aiki-Muntean '09, '10
  - Free boundary problem for the front of carbonated zone
  - Large time behavior ($c\sqrt{t} \leq x \leq C\sqrt{t}$)

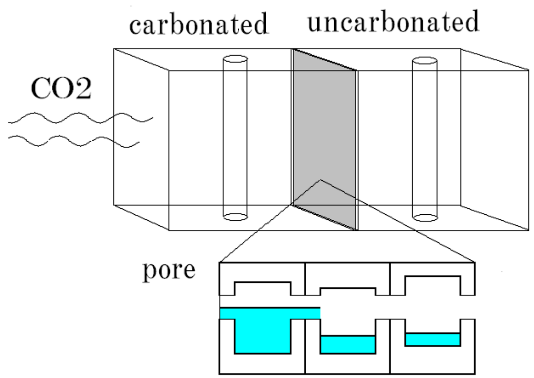
Previous works(3D)

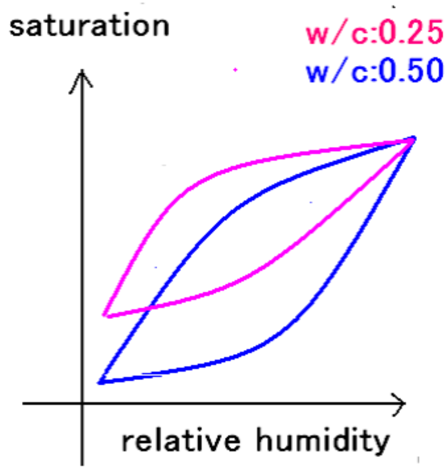
- K.-Aiki '11, '12, 14 (Moisture transport)
- K. '14 (Carbon dioxide transport)

2. Balanced law of moisture[Maekawa-Ishida-Kishi(J. Adv. Concr. Tech. (2003))]

$$\underbrace{\rho\frac{\partial}{\partial t}(\phi w)}_{\phi\frac{\partial w}{\partial t}+\frac{\partial \phi}{\partial t}w} - \text{div}(\underbrace{\phi[C_1K(h)+C_2(1-w)h]\nabla P}_{\text{water + vapor}}) = \underbrace{\phi w v^{q_1} z^{q_2}}_{\text{generation of water}}, \quad \underbrace{w=\mathcal{S}(h)}_{\text{hysteresis}}$$

- h : relative humidity
  (=water vapor/saturated water vapor)
  w : degree of saturation
- ρ : density of water , ϕ: porosity, $C_1, C_2 \geq 0$
- P : pore pressure $(= C\log h)$
- v : concentration of CO_2,
  z : concentration of $CaCO_3$





Previous works$(\nabla P = \nabla h/h,\ \phi = C_1 = C_2 = 1)$

$$\rho w_t - \text{div}(g(h)\nabla h) = wf,\ w = \mathcal{S}(h)$$

K. -Aiki : existence('12)、uniqueness('14)

2.1 Mathematical Treatment of Hysteresis

- M. A. Kranosel'skiǐ, A. V. Pokrovskiǐ "Systems with Hysteresis", Springer-Verlag
- M. Brokate, J. Sprekels, "Hysteresis and Phase Transitions", Springer
- A. Visintin, "Differential models of Hysteresis", Springer

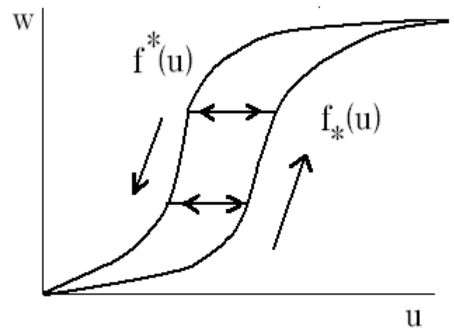
$$w = \mathcal{S}(u) \iff w_t + \partial I(u; w) \ni 0$$

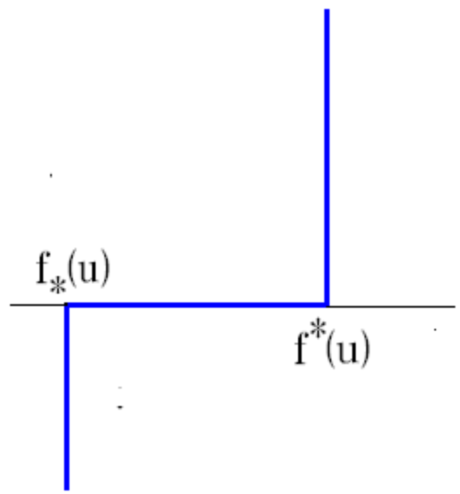
$$I(u; w) = \begin{cases} 0 & \text{if } f_*(u) \le w \le f^*(u) \\ +\infty & \text{otherwise} \end{cases}$$

$$\partial I(u; w) = \begin{cases} [0, \infty) & \text{if } w = f^*(u), \\ \{0\} & \text{if } f_*(u) < w < f^*(u), \\ (-\infty, 0] & \text{if } w = f_*(u). \end{cases}$$

$\Longrightarrow$

$$\rho u_t - \text{div}(g(u)\nabla u) = wf$$
$$w_t + \partial I(u; w) \ni 0$$

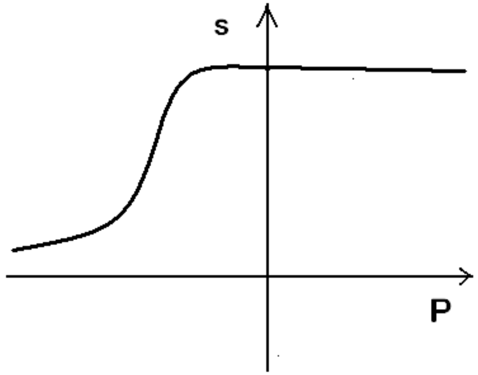


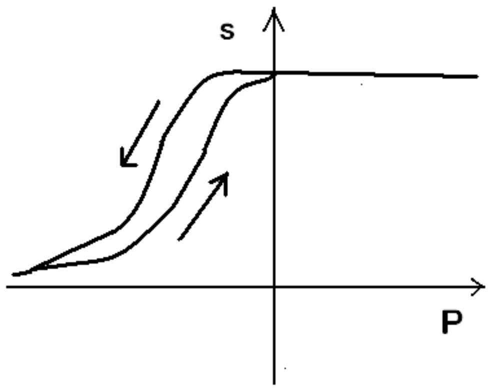


2.2 Flow in Porous Media

$$\frac{d}{dt}(\phi w) + \mathrm{div} J = f$$

- non hysteresis between P and w
  - $w = P^{\frac{1}{m}}$, $J = -K\nabla P$
  - $w = f(P)$, (f : non-decreasing)
    $J = -K(w)(\nabla P + \rho g)$
    - Alt(1979,1984),
    - Alt-Luckhaus-Visintin(1984)
    - Otto(1997) etc



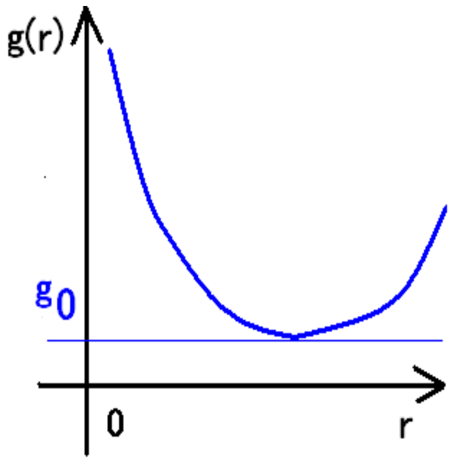


- Consider hysteresis between P and w
  - $w \in \mathcal{S}(P)$, $J = -K(w)(\nabla P + \rho g)$
    - Bagagiolo-Visintin(2000,2004)
    - Kordulová(2010) etc

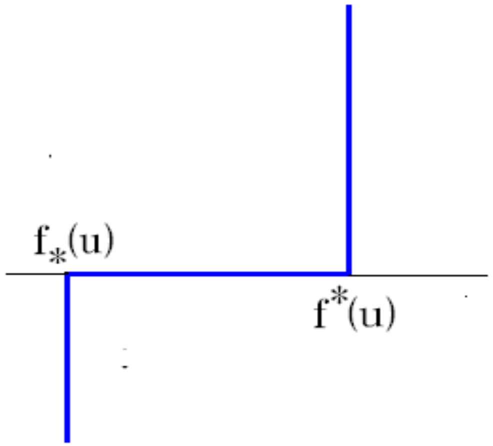
2.3 IBVPs for moisture transport

$$(P)_0 \begin{cases} \rho u_t - \mathrm{div}(g(u)\nabla u) = wf \text{ in } Q(T) \\ w_t + \partial I(u;w) \ni 0 \text{ in } Q(T) \\ u = u_b \text{ on } S(T) \\ u(0) = u_0,\ w(0) = w_0 \text{ in } \Omega \end{cases} \qquad (P)_{\nu\lambda m} \begin{cases} \rho u_t - \mathrm{div}(g_m(u)\nabla u) = wf \text{ in } Q(T) \\ w_t - \nu\Delta w + \partial I_\lambda(u;w) = 0 \text{ in } Q(T) \\ u = u_b, w = w_b \text{ on } S(T) \\ u(0) = u_0,\ w(0) = w_0 \text{ in } \Omega \end{cases}$$

- $\Omega \subset \mathbb{R}^3$: smooth, $Q(T) = [0,T] \times \Omega$
- $g \in C^2((0,\infty)) : \lim_{r\to+0} g(r) = +\infty$
  $g(r) \geq g_0 > 0$ for $r \in \mathbb{R}$
  $g_m = g$ for $\frac{1}{m} \leq r \leq m$, $g_m \geq g_0$ on $\mathbb{R}$
- $f \in L^\infty(Q(T))$ with $f \geq 0$ a.e. on $Q(T)$
- $\xi \in \partial I(u;w) \Longrightarrow$
  $\xi(\nu - w) \leq 0$ for $f_*(u) \leq \nu \leq f^*(u)$
- $\partial I_\lambda(w;u) = \frac{1}{\lambda}[w - f^*(u)]^+ - \frac{1}{\lambda}[f_*(u) - w]^+$

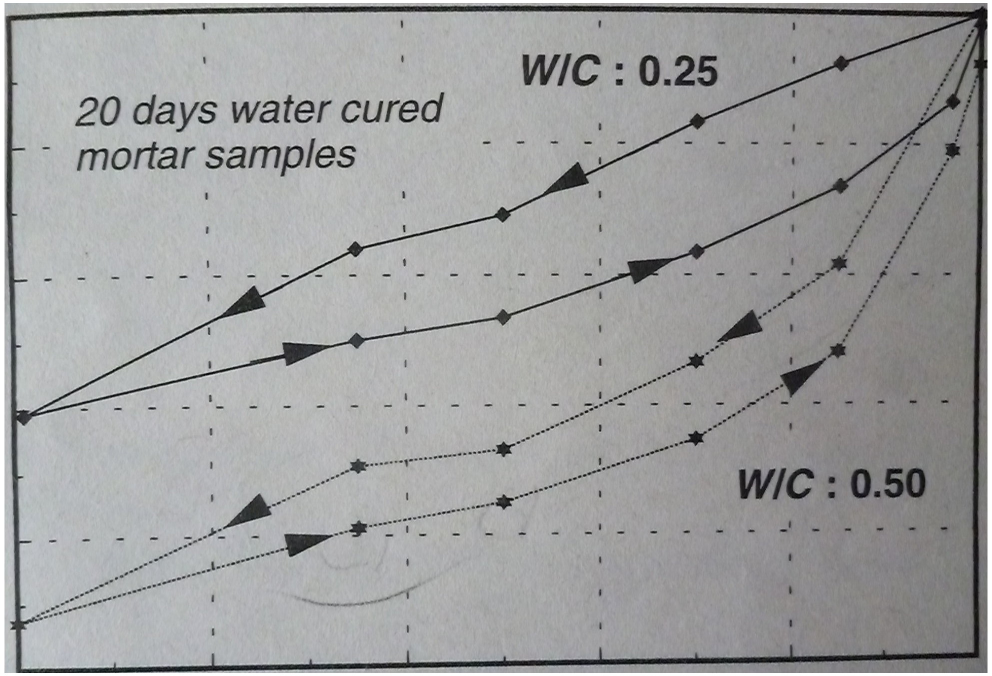


profile of g



f_*: lower
f^*: upper

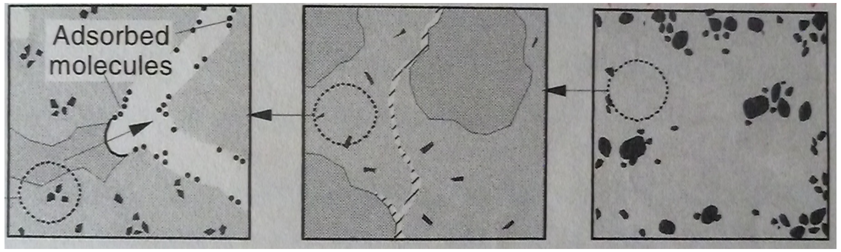
2.4 Relative humidity and Saturation

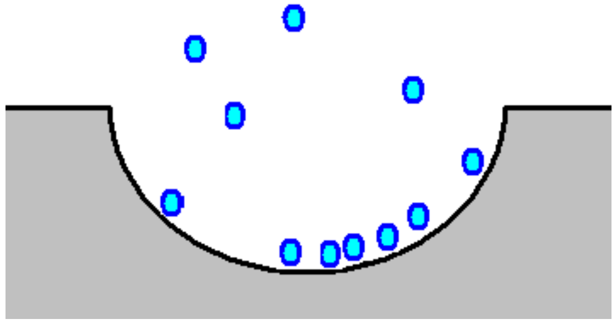


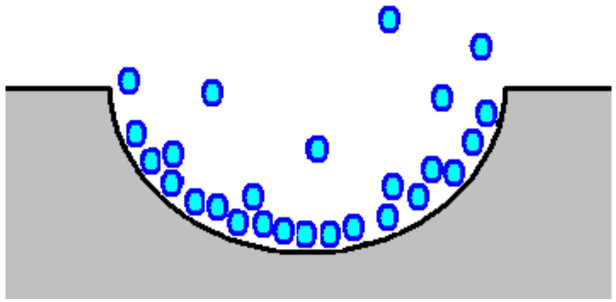
$$\mathrm{RH} = \frac{\text{water vapor}}{\text{saturated water vapor}}$$

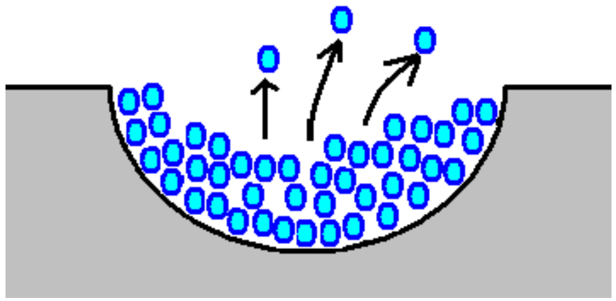
- vapor content increases (wetting process)
- vapor content decreases (drying process)

2.5 Adsorption phenomenon



(1)


(2)


(3)


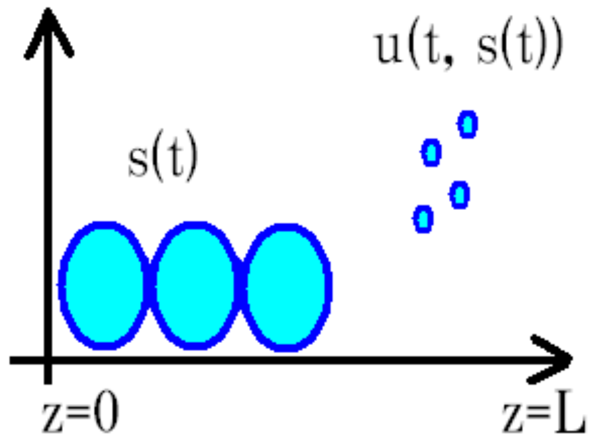
2.6 Model for adsorption phenomenon(Sato-Aiki-Murase-Shirakawa'13)

$$\rho_v u_t - k u_{zz} = 0 \text{ on}(s(t), L), \quad (1)$$

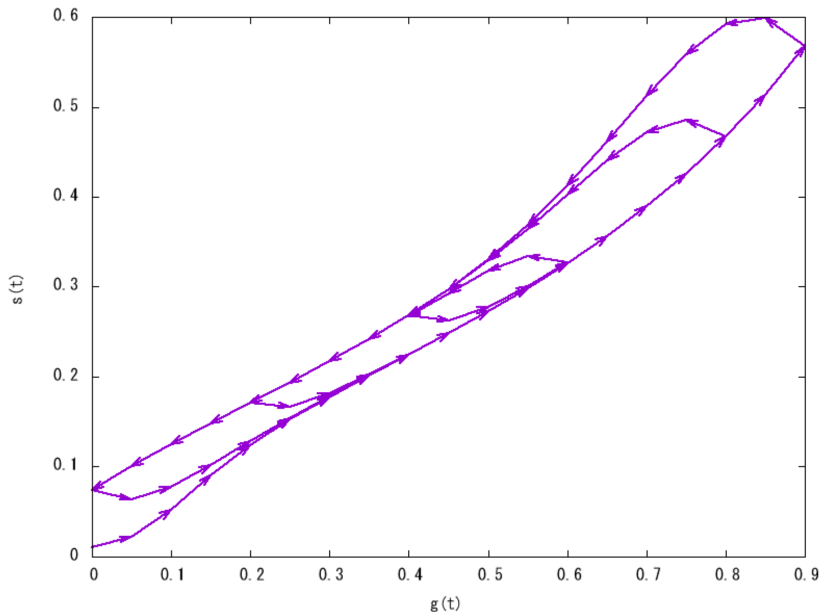
$$u(t, L) = h(t) \text{ for } 0 < t < T \quad (2)$$

$$\underbrace{k u_z(t, s(t))}_{\text{vapor to water}} = \underbrace{\rho_w s_t(t)}_{\text{liquid}} - \underbrace{\rho_v u(t, s(t)) s_t(t)}_{\text{vapor}} \quad (3)$$

$$s_t(t) = a\,(\underbrace{u(t, s(t))}_{\text{adsorp}} - \underbrace{\varphi(s(t))}_{\text{desorp}}) \text{ for } 0 < t < T, \quad (4)$$



- $[0, L]$: a hole in porous material
- $[0, s(t)]$: water drop region
- $z = 0$: wall, $z = L$: expose to air
- $u = u(t, z)$: RH in a hole
- ρ_v: density of water vapor
  ρ_w: density of water



(1): mass balanced law of RH
(3): balanced law of RH on the free boundary
(4): growth rate of the water drop region

3. Multiscale model for moisture transport

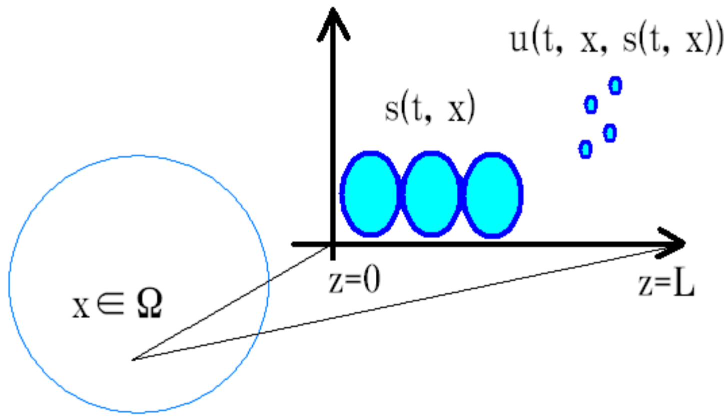
(moisture) macro

$$\begin{cases} \rho_v h_t - \text{div}(g(h)\nabla h) = sfv \text{ in } Q(T) := \Omega \times (0,T), \\ h = h_b \text{ on } S(T) := (0,T) \times \partial\Omega, \quad h(0,x) = h_0(x) \text{ in } \Omega, \end{cases}$$

(adsorption) micro

$$\begin{cases} \rho_v u_t - k u_{zz} = 0 \text{ for } (t,x,z) \in Q(T) \times (s(t,x), L), \\ u(t,x,L) = h(t,x) \text{ on } Q(T), \\ k u_z(t,x,s(t,x)) = (\rho_w - \rho_v u(t,x,s(t,x))) s_t(t,x) \text{ in } Q(T), \\ s_t(t,x) = a(u(t,x,s(t,x)) - \varphi(s(t,x)) \text{ in } Q(T), \\ s(0,x) = s_0(x) \text{ in } \Omega,\ u(0,x,z) = u_0(x,z) \text{ for } (x,z) \in \Omega \times [s_0(x), L] \end{cases}$$

- $\Omega \subset \mathbf{R}^3$: concrete
- h: relative humidity (macro)
- v: concentration of CO_2 in water (given)
- $g \in C^2(0,\infty)$: $\lim_{r \to +0} g(r) = \infty,\ g \geq g_0 > 0$
- ρ_v, ρ_w: density of water and vapor
- φ: the rate of water to vapor (given)



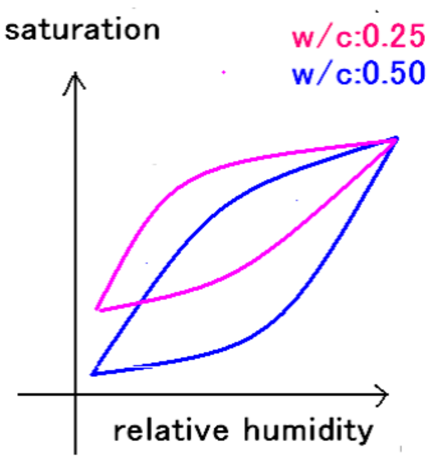
- A. Friedman-A. Travaras (1987)
- A. Muntean-M.N. Radu (2010)

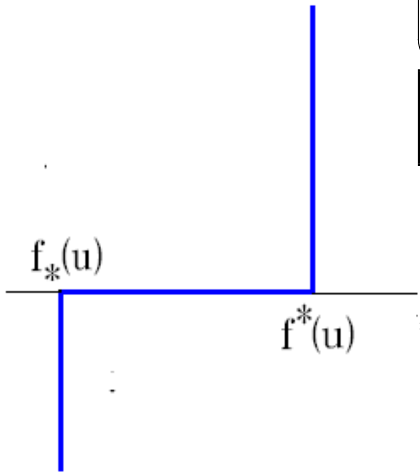
3.1 Compair to the previous model

Previous model

$$\rho_v h_t - \mathrm{div}(g(h)\nabla h) = w f(h) v \text{ in } Q(T)$$
$$w = \mathcal{S}(h) \text{ in } Q(T)$$
$$[l(w)v]_t - \mathrm{div}(l(w)\nabla v) = -w_0 w v$$

- v: concentration of CO_2 in air
- $w = \mathcal{S}(h) \Leftrightarrow w_t + \partial I(h; w) \ni 0$





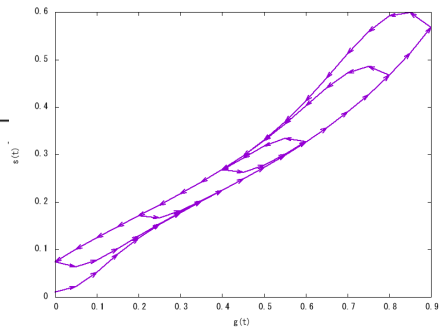
Multiscale model

$$\rho_v h_t - \mathrm{div}(g(h)\nabla h) = s f(h) v \text{ in } Q(T)$$

$$\begin{cases} \rho_v u_t - k u_{zz} = 0 \text{ on } (s(t,x), L), \\ u(t,x,L) = h(t,x) \text{ on } Q(T), \\ k u_z(t,x,s(t,x)) = \\ \qquad (\rho_w - \rho_v u(t,x,s(t,x))) s_t(t,x), \\ s_t(t,x) = a(u(t,x,s(t,x)) - \varphi(s(t,x))), \end{cases}$$

$$[(l(s)v]_t - \mathrm{div}(l(s)\nabla v) = -w_0 s v \text{ in } Q(T)$$

Previous work Aiki-Murase(13')



- hysteresis like behavior of s for given h
- differential possibility of s

3.2 Model for adsorption phenomenon for each $x \in \Omega$

$$
\text{(AP)}\begin{cases} \rho_v u_t - k u_{zz} = 0 \text{ on} (s(t), L) \\ u(t, L) = h(x, t) \text{ for } 0 < t < T \\ k u_z(t, s(t)) = \rho_w s_t(t) - \rho_v u(t, s(t)) s_t(t) \\ s_t(t) = a(u(t, s(t)) - \varphi(s(t)) \text{ for } 0 < t < T \end{cases}
$$

- $u = u(t, z) = u(x)(t, z)$: RH in each hole
- $s = s(t) = s(x)(t)$: saturation in each hole

$\Longrightarrow \tilde{u}(x)(t, y) = u(x)(t, (1 - y)s(t) + yL)$ for $y \in [0, 1]$

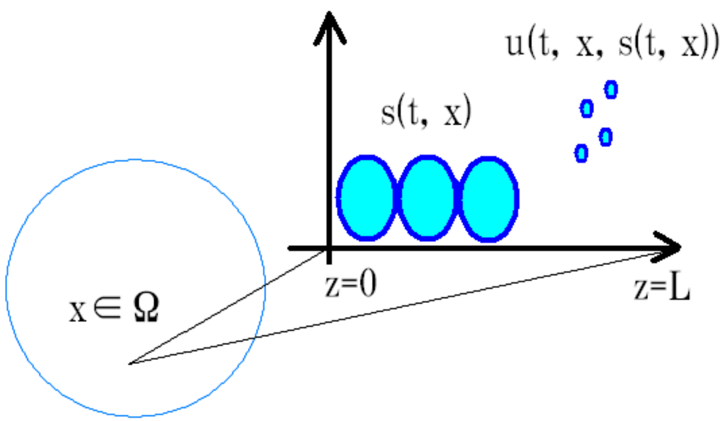
$$\rho_v \tilde{u}_t - \frac{k}{(L - s(t))^2} \tilde{u}_{yy} = \frac{\rho_v (1 - y) s_t}{L - s(t)} \tilde{u}_y$$

$$\tilde{u}(t, 1) = h(x, t)$$

$$\frac{k}{L - s(t)} \tilde{u}_y(t, 0) = (\rho_w - \rho_v \tilde{u}(t, 0)) s_t(t)$$

$$s_t(t) = a(\tilde{u}(t, 0) - \varphi(s(t)))$$

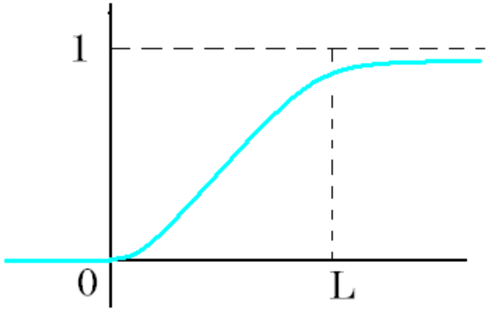
$$s(0) = s_0(x), \quad \tilde{u}(0, y) = u(0, (1 - y)s(0) + yL)$$



3.3 Assumptions for (AP)

- $\rho_w \geq \rho_v(\sup_{\mathbb{R}}\varphi + 2)$, $9aL\rho_v^2 \leq k\rho_w$
- $s_0 \in L^2(\Omega)$: $0 \leq s_0 \leq L - \delta$
  $x \to u_0(x)$: smooth
  $u_0(x, L) = h(x, 0)$ for $x \in \Omega$, $0 \leq u_0 \leq 1$
- h: smooth on $Q(T)$, $0 \leq h \leq h^* < 1$

Profile of φ:



3.4 Main results for (AP) (K. '16, '17, Adv. Math. Sci. Appl.)

(i) (Solvability) For a.e. $x \in \Omega$, (AP) has a solution $(\tilde{u}, s)$ on $[0, T]$

(ii) (Measurability) $\tilde{u} \in L^\infty(\Omega; W^{1,2}(0, T; L^2(0, 1))) \cap L^\infty(\Omega; L^\infty(0, T; H^1(0, 1))) \cap L^\infty(\Omega; L^2(0, T; H^2(0, 1)))$, $s \in L^\infty(\Omega; W^{1,\infty}(0, T))$ and $0 \leq s \leq L - \delta_*$ for $t \in [0, T]$ a.e. on Ω ($\delta_* = C(|\nabla\tilde{u}(x)|_{H^1(0,1)})$).

(ii) (Continuous Dependence)

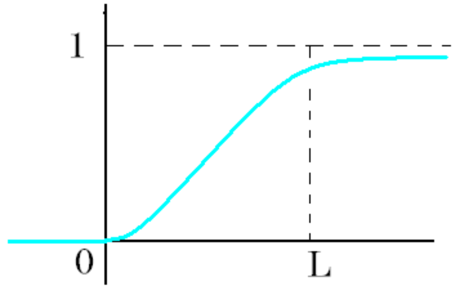
$$\int_\Omega |\tilde{u}_1(t) - \tilde{u}_2(t)|^2_{L^2(0,1)} dx + \int_\Omega \int_0^t |\tilde{u}_{1y}(t) - \tilde{u}_{2y}(t)|^2_{L^2(0,1)} dt dx$$
$$+|s_1 - s_2|^2_{L^\infty(0,t;L^2(\Omega))} \leq C|h_1 - h_2|^2_{W^{1,2}(0,t;L^2(\Omega))} \text{ for } t \in [0, T],$$

where $(\tilde{u}_1(x), s_1(x))$ and $(\tilde{u}_2(x), s_2(x))$ are solutions of (AP) on $[0, T]$ for given h_1 and h_2.

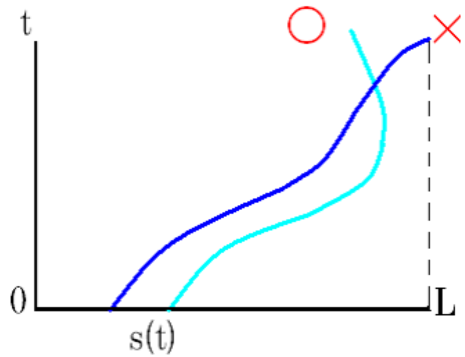
3.5 Assumptions ($H = L^2(\Omega)$)

- $f \in C^1(\mathbb{R})$ with $f \geq 0$, bdd
- h_b: smooth in $Q(T)$, $\kappa_0 \leq h_b < 1$
- h_0: smooth in Ω, $\kappa_0 \leq h_0 < 1$
  $h_0 = h_b(0)$ on $\partial\Omega$
- $\rho_w \geq \rho_v(\sup_{\mathbb{R}}\varphi + 2)$, $9aL\rho_v^2 \leq k\rho_w$
- $0 \leq s_0(x) < L$ on Ω
  $x \to |u_0(x)|_{H^1(s_0,L)}$: bdd
  $u_0(x, L) = h(x, 0)$ for $x \in \Omega$
  $0 \leq u_0 \leq 1$ on $\Omega \times [s_0, L]$

Profile of φ:



Find a solution $s(t)$:



3.6 Main result (K.-Aiki-Sato-Murase '17 Applicable Analysis)

Under the assumptions, (P) has a unique solution (h, s, u) on $[0, T'](T' < T)$.

(Regularity) $h \in W^{1,2}(0, T; H) \cap L^\infty(0, T; H^1) \cap L^2(0, T; H^2)$, $s \in W^{1,\infty}(Q(T))$
u_t, $u_{zz} \in L^2(0, T; L^2(\Omega, L^2(s(\cdot), L)))$, $|u_z(\cdot)|_{L^2(s(\cdot,\cdot),L)} \in L^\infty(Q(T))$

(Boundedness) $\kappa_0 \leq h \leq 1$ a.e. on $Q(T')$, $0 \leq s \leq L - \delta*$ a.e. on $Q(T')$

(Proof) Banach's fixed point theorem

3.7 Outline of the proof

(Step 1) s : given on $[0,T']$

$$\begin{cases} h_t - \text{ div } (g(h)\nabla h) = sf \\ h = h_b \text{ on } S(T) \\ h(0) = h_0 \text{ on } \Omega \end{cases}$$

(i) $\kappa_0 \le h < 1$ a.e. on $Q(T')$
(ii) $|\nabla h|_{L^\infty(Q(T))} \le C$
(Ladyzenskaja et al)
(iii) $|h_t|_{L^\infty(Q(T))} \le C$

(Step 2) h : solution of (Step 1) on $[0,T']$

$\tilde{u}(t,x,y) = u(t,x,(1-y)s(t,x)+yL)$ for $(t,x,y) \in Q(T') \times (0,1)$

$$\begin{cases} \rho_v \tilde{u}_t - \frac{k}{(L-s(t,x))^2}\tilde{u}_{yy} = \frac{\rho_v(1-y)s_t}{L-s(t,x)}\tilde{u}_y \text{ on } Q(T) \times (0,1) \\ \tilde{u}(t,x,1) = h(t,x) \text{ on } Q(T'), \\ \frac{k}{L-s(t,x)}\tilde{u}_y(t,x,0) = (\rho_w - \rho_v \tilde{u}(t,x,0))s_t(t,x) \text{ on } Q(T'), \\ s_t(t,x) = a(\tilde{u}(t,x,0) - \varphi(s(t,x))) \text{ on } Q(T'), \\ s(0,x) = s_0(x) \text{ in } \Omega, \tilde{u}(0,x,y) = u_0(x,(1-y)s_0 + yL) \text{ on } \Omega \times [0,1] \end{cases}$$

$(s,\tilde{u})$: solution on $[0,T']$:
$s \in W^{1,\infty}(Q(T')), 0 \le s < L$ on $Q(T')$, $\tilde{u} \in W^{1,2}(0,T';L^2(\Omega \times (0,1))$
$\cap L^\infty(0,T';L^2(\Omega,H^1(0,1))) \cap L^2(0,T';L^2(\Omega,H^2(0,1)))$

(Step 3) $s \to h$(Step 1) $\to (s,\tilde{u})$(Step 2):
Banach's fixed point theorem ($\exists T_0 < T'$ s.t. $s = \mathcal{S}(s)$ on $[0,T']$)

4. Future works

- Time global solution and large time behavior of a solution of (P)

- Multiscale model for concrete carbonation

$$(\text{moisture})\ \rho_v h_t - \text{div}(g(h)\nabla h) = sf(h)v \text{ in } Q(T),$$

$$(\text{adsorption}) \begin{cases} \rho_v u_t - k u_{zz} = 0 \text{ on } (s(t,x),L), \\ u(t,x,L) = h(t,x) \text{ on } Q(T), \\ k u_z(t,x,s(t,x)) = (\rho_w - \rho_v u(t,x,s(t,x)))s_t(t,x) \text{ in } Q(T), \\ s_t(t,x) = a(u(t,x,s(t,x)) - \varphi(s(t,x)) \text{ in } Q(T). \end{cases}$$

$$(\text{carbon dioxide})[(l(s)v]_t - \text{div}(l(s)\nabla v) = -w_0 sv \text{ in } Q(T)$$

- Multiscale model for concrete carbonation with non-constant porosity
- Improvement (effect of temperature etc)
- Numerical calculation