MULTI-SCALE MODELING OF CONCRETE PERFORMANCE

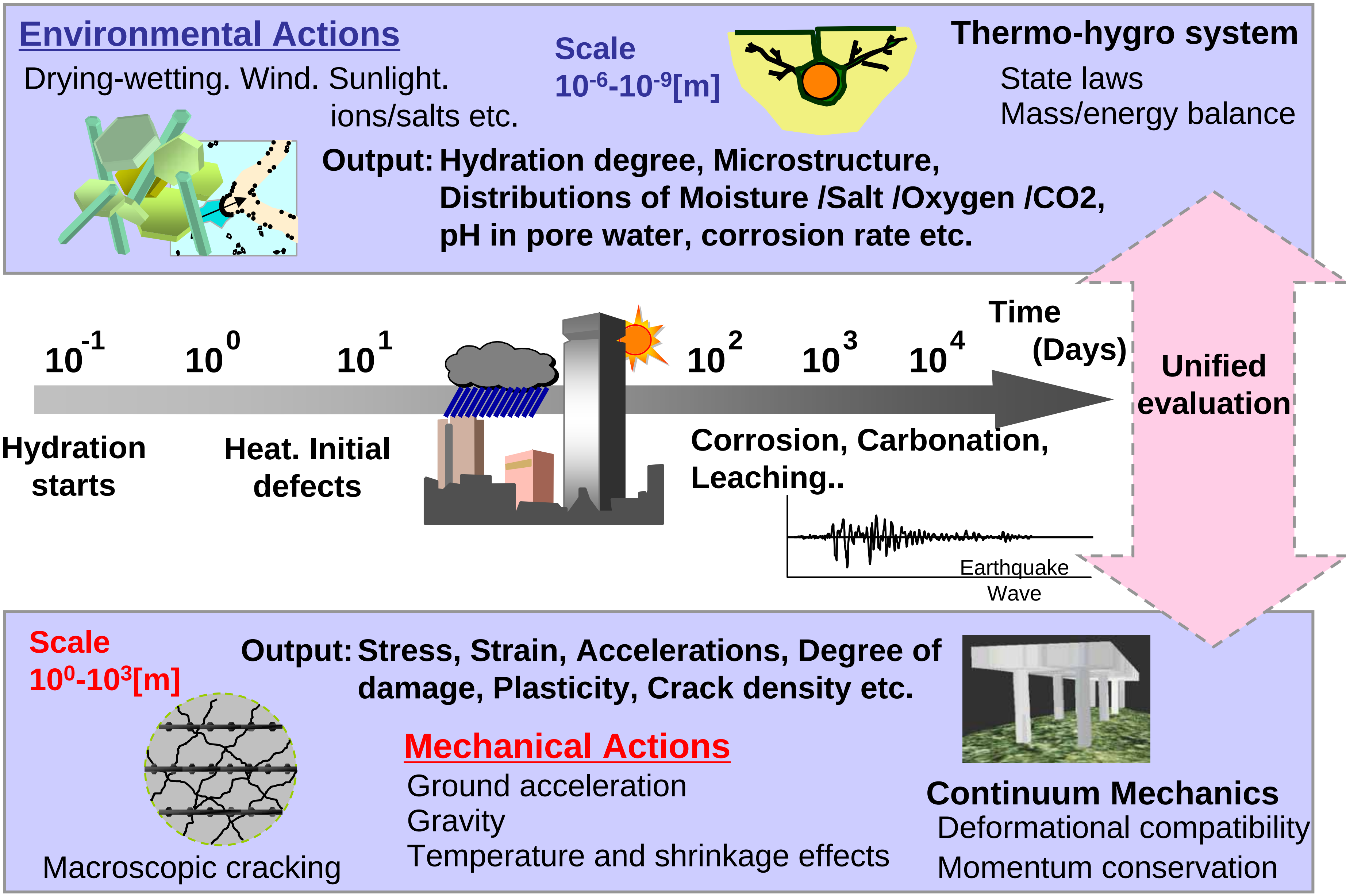
Tetsuya ISHIDA

The University of Tokyo

The COE Workshop on Material Science in 21st Century for the Construction Industry - Durability, Repair and Recycling of Concrete Structures

11/Aug/2005 Hokkaido University

Lifespan simulation for materials and structures



Our concern and target

Not only….	But also….
Small specimen (laboratory scale, homogenous)	Large-scale structure (MQ differ with space)
Standard curing	Various curing conditions
Saturated porous media	Unsaturated porous media
Constant env. condition	Variable env. condition (temp., RH, Cl, CO2…)

for engineering and practical use

Based on multi-scale modeling and coupled analytical system

DuCOM Coupled Computational Scheme

-Thermo-hygro physics for materials-

Basic Equation

$$\frac{\partial S(\theta_i)}{\partial t} + div\mathbf{J}_i(\theta_i, \nabla\theta_i) - Q_i(\theta_i) = 0$$

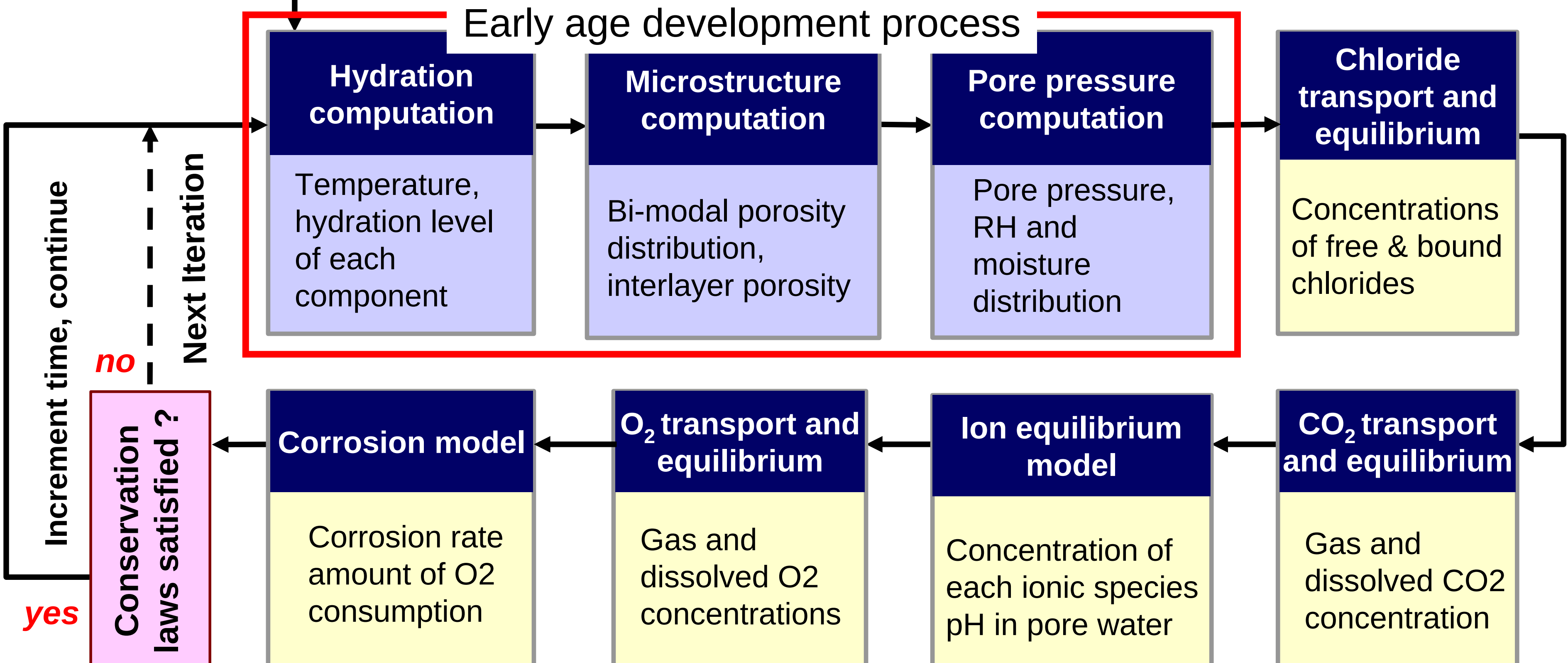
Potential term　　Flux term　　Sink term

θ_i; Degree of freedom

Temperature, Pore pressure, Chlorides, CO_2, and O_2

START

Size, shape, mix proportions, initial and boundary conditions



Each term has been formulated based on thermodynamics , chemical equilibrium and electrochemistry

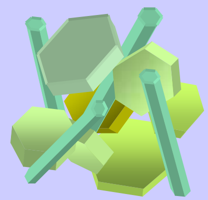
Coupled Simulation for Early Age Development Process

Our concern is… not to predict hydration process under ideal conditions
but to predict early age development process
under various temperature, wetting & drying conditions

For that purpose, non-linear interactive phenomena should be taken into account

Coupling processes among hydration, moisture transport, and micro-pore structure development

Hydration process



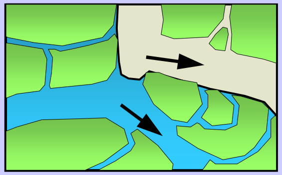
Heat generation
→ Acceleration of reaction
(Coupled with thermal conduction analysis)

Free water for hydration

C-S-H gel precipitation

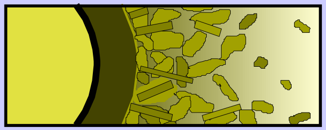
Water consumption

Moisture equilibrium and transport



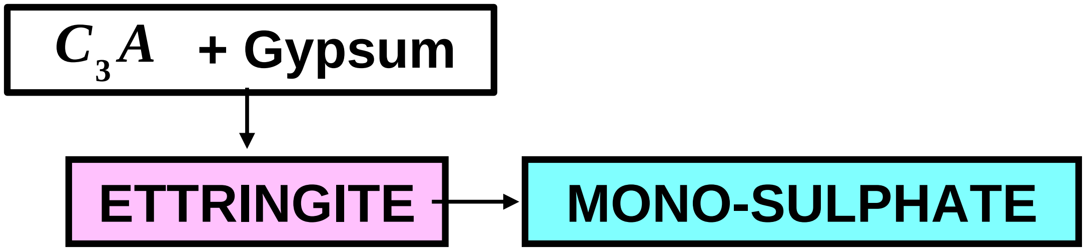
Governed by mass balance law for moisture

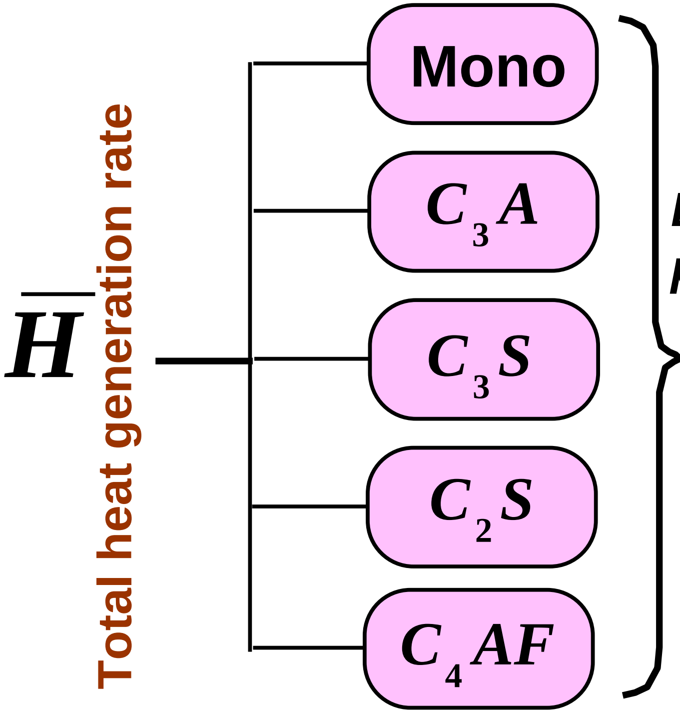
Micro-pore struc. development



Vapor diffusivity
Liquid permeability
Condensed water
Adsorbed water on pore wall

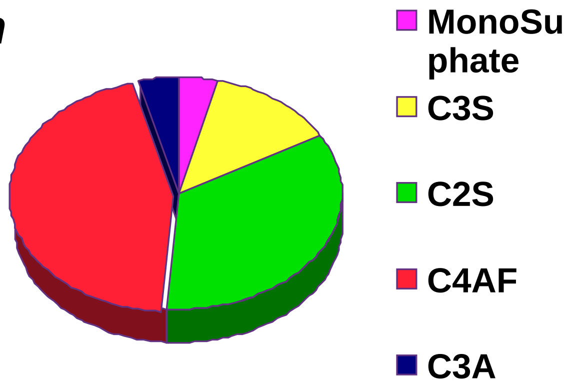
Multi-component cement hydration model





Each component hydration progress dependent on

- ***Temperature***
- ***Moisture content***
- ***Degree of hydration***



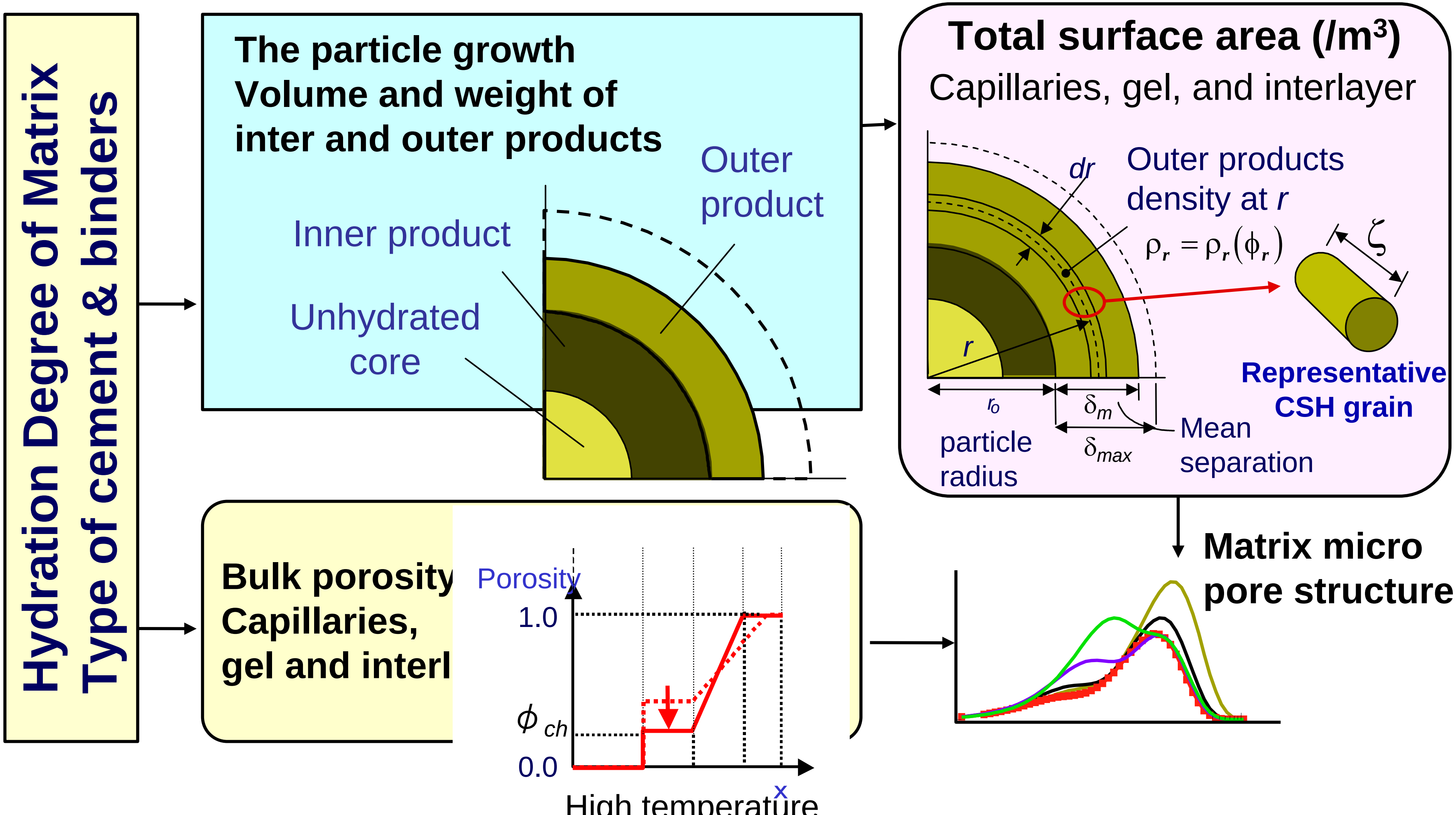
Typical component composition of cement

Hydration heat rate $\overline{H}_i$ of each component at T_o

$$\overline{H}_i = \overline{H}_{i,T_o} \exp\left[-\frac{E_i}{R}\left(\frac{1}{T}-\frac{1}{T_o}\right)\right]$$

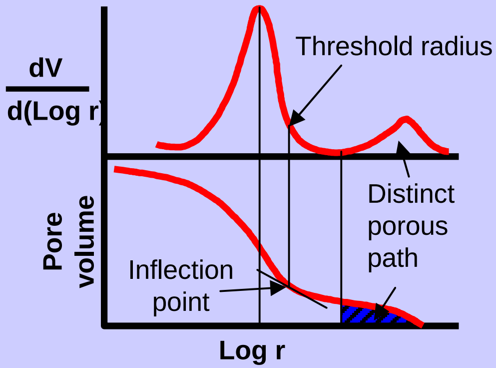
Outline of the pore structure development computation

Two important functions →
- Path for Mass transport (gas, liquid, ion)
- Moisture reservoir (as solvent, reaction field, etc)



Mass balance equation for vapor and liquid

Flux term



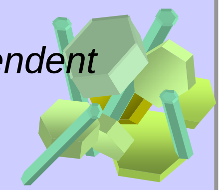
Moisture conductivity

- *Liquid + vapor*
- *Computed from pore structure directly*
- *Random pore model*

Sink term

Moisture loss due to hydration

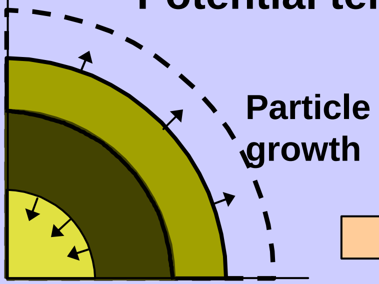
- *Obtained directly from hydration model. Based on reaction pattern of each clinker component*
- *Cement composition dependent*



Governing equation

$$\frac{\partial(\rho_l \phi S)}{\partial t} - div\{\mathbf{J}(P_l, \nabla P, \nabla T)\} - Q_{hyd} = 0$$

Potential term



Pore-structure development model

Pore distribution, surface area

- **Equilibrium of gas and liquid**

  Kelvin's equation (Under isothermal)
  Laplace's equation
  Clausius-Clapeyron equaition

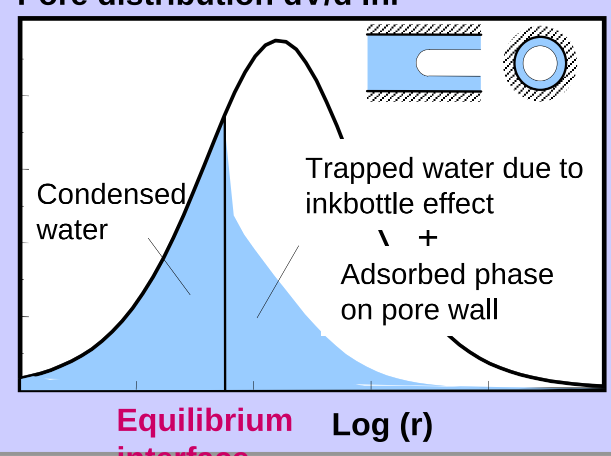
- **Adsorbed phase on pore wall**

  B.E.T Theory

- **Ink bottle effect**

  Statistical approach based on geometric characteristics of pores

Pore distribution dV/d lnr



Modeling of Moisture Equilibrium and Micro-pore Structure

Moisture equilibrium model

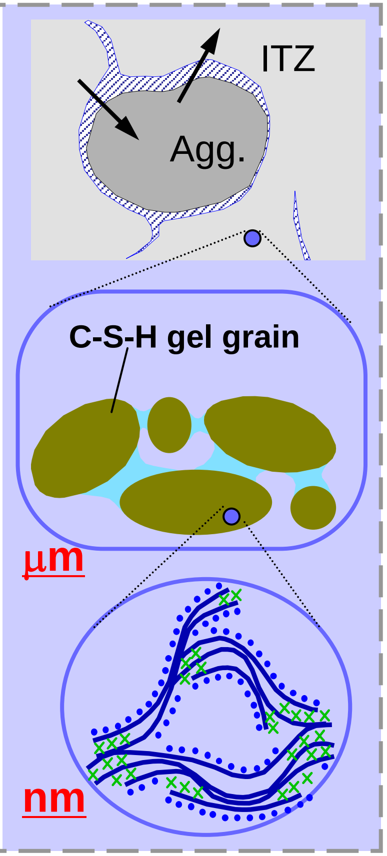
Local moisture transfer
between agg. and HCP
Connection of ITZ

Condensed & adsorbed water

- Kelvin's eq. (Isothermal)
- Clausius-Clapeyron eq.
  (for arbitrary temp.)
- Inkbottle effect (Hysteresis)
- B.E.T. Theory

Interlayer water

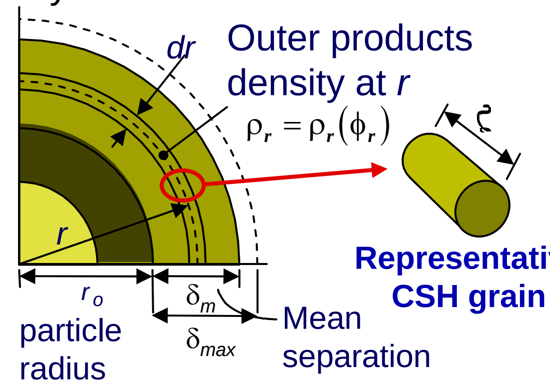
- Simplified empirical formula base on past researches

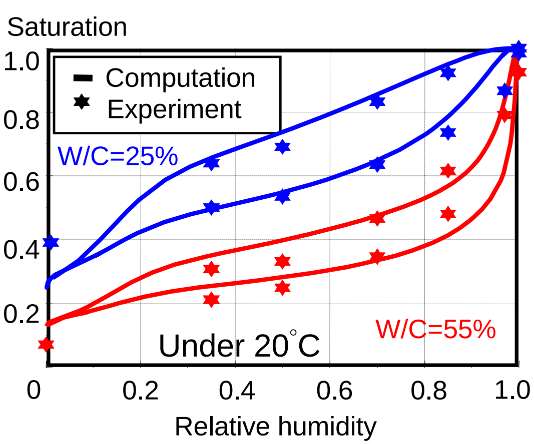


Hydration degree of matrix

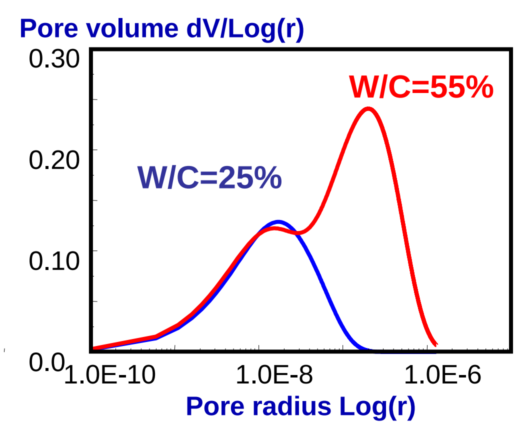
Pore structure development model

- The particle growth volume and weight of inter and outer products
- Bulk porosity of capillaries, gel and interlayer
- Total surface area of capillaries, gel and interlayer



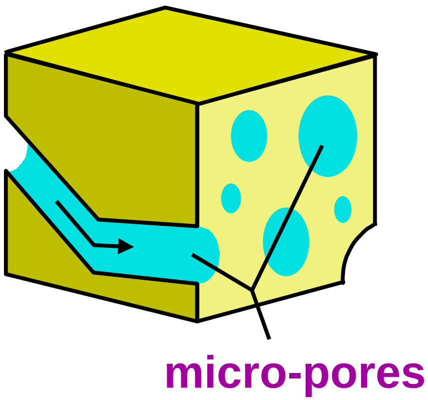


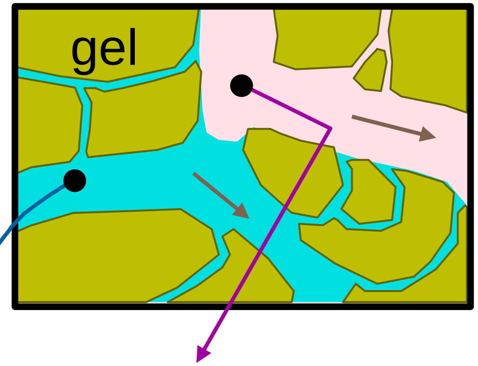
Calculated
pore structure

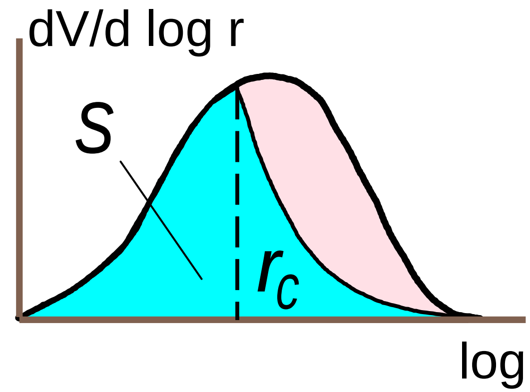


Porosity of capillary, gel and interlayer

Moisture Conductivity of Concrete







Model assumptions

- Random spatial pore distribution
- Cylindrical shape of micro-pores
- Thermodynamic equilibrium of phases

Vapor Transport

$$K_V = \frac{\phi \rho_v D_o}{2.5}\left[(1-S)\,K(h)\right]\left[Mh/\rho_l RT\right]$$

Knudsen diffusion factor

Liquid Transport

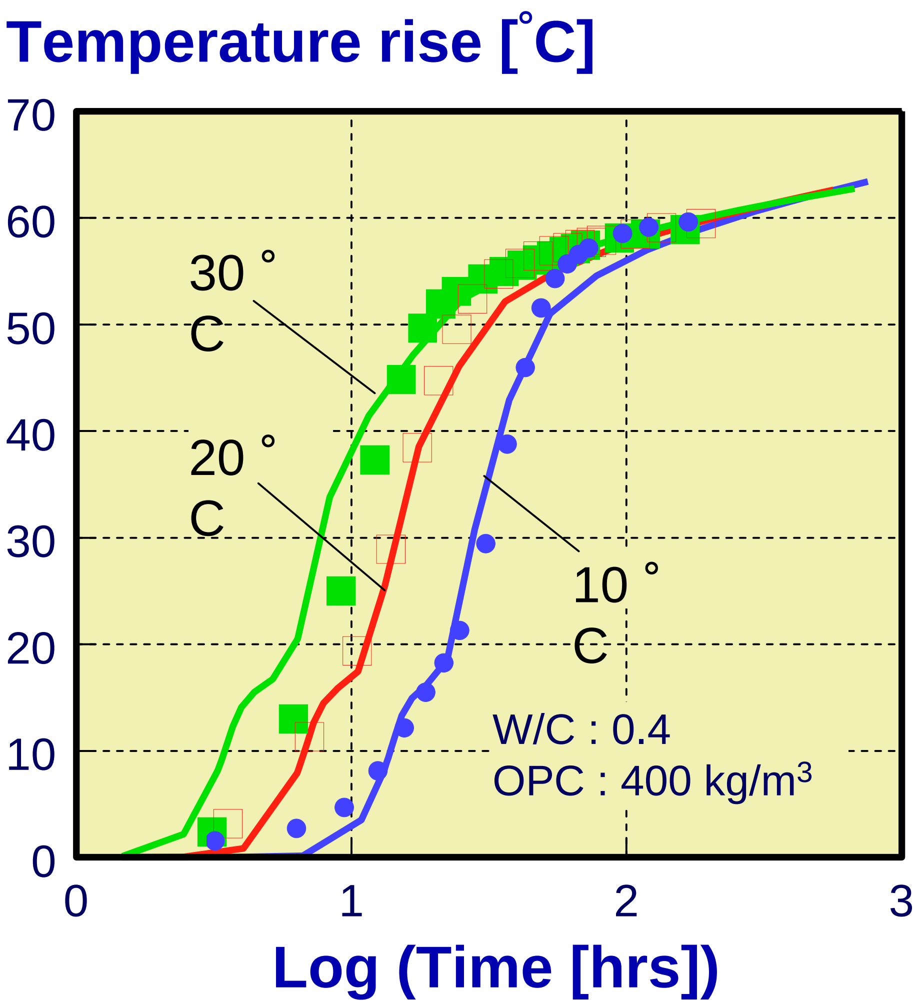
$$K_L = \frac{\phi^2 \rho_l}{50\eta}\left[\int_0^{r_c} r\,dV\right]^2$$

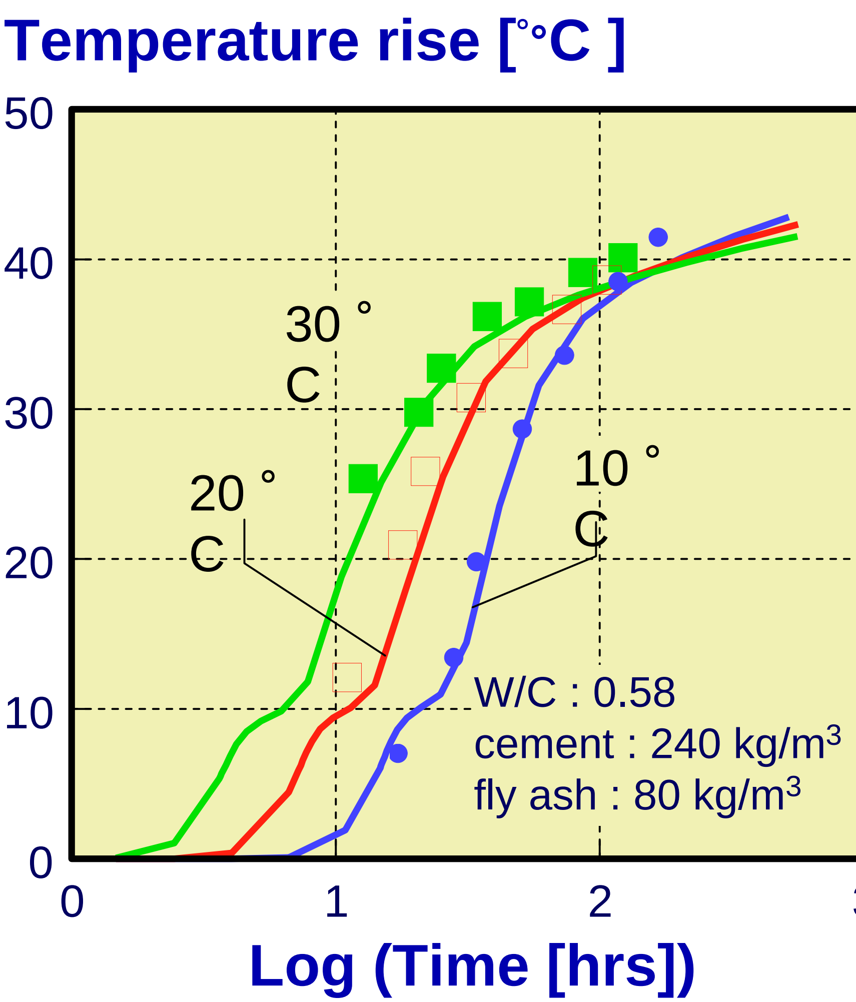
History dependent liquid viscosity

Total Conductivity K = Liquid Conductivity K_L + Vapor Conductivity K_V

Influence of Casting Temperature

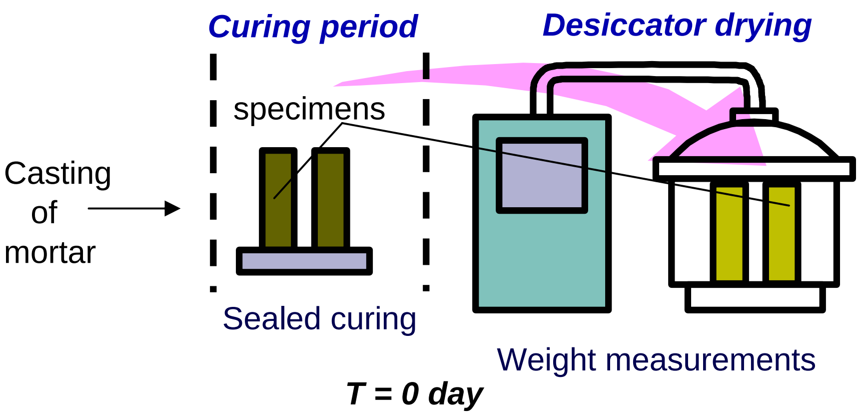
Comparison of predicted and measured temperature rise for different casting temperatures and various cement types.





Prediction of moisture loss behavior for early age under severe conditions

EXPERIMENTAL PROCEDURE :



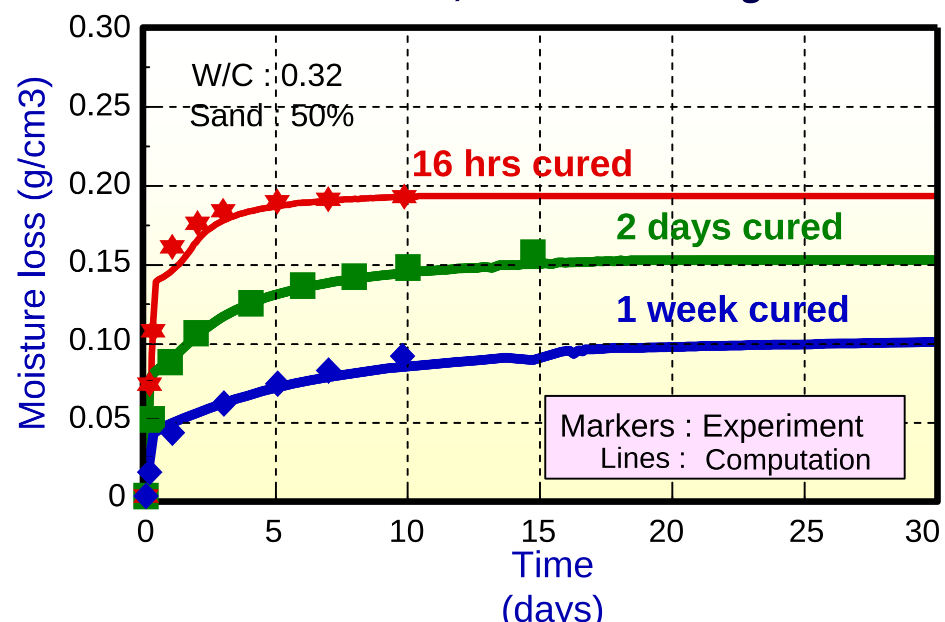
FEM ANALYSIS :

BC = Boundary Condition

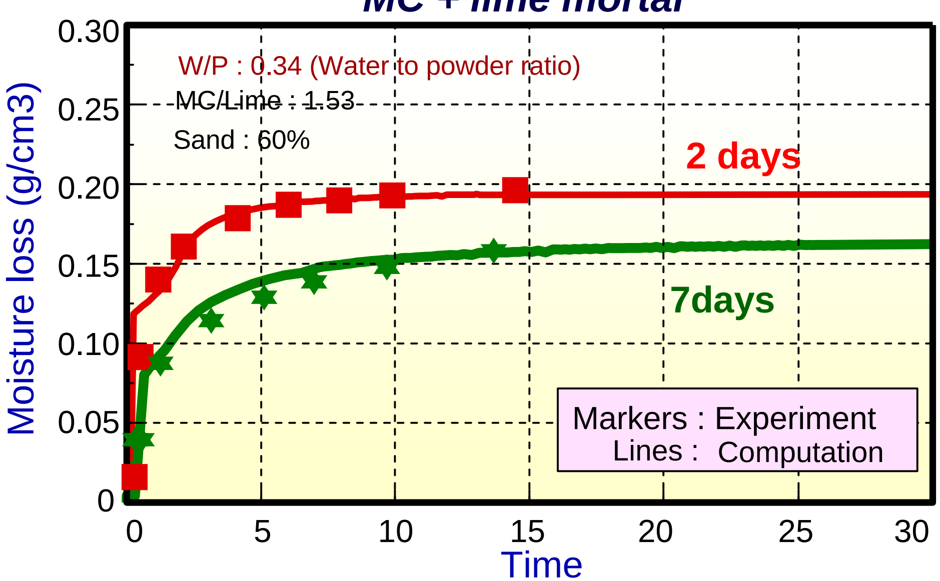
Input ; → Sealed BC → BC : 0.001 RH

Mix proportions — Hydration dominant — Moisture transport dominant

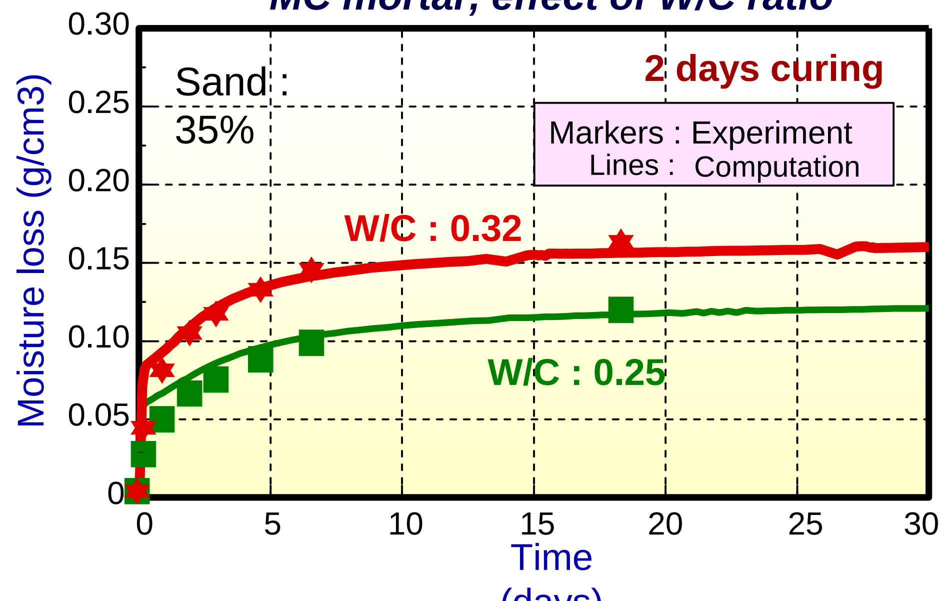
MC mortar, effect of curing time



MC + lime mortar



MC mortar, effect of W/C ratio



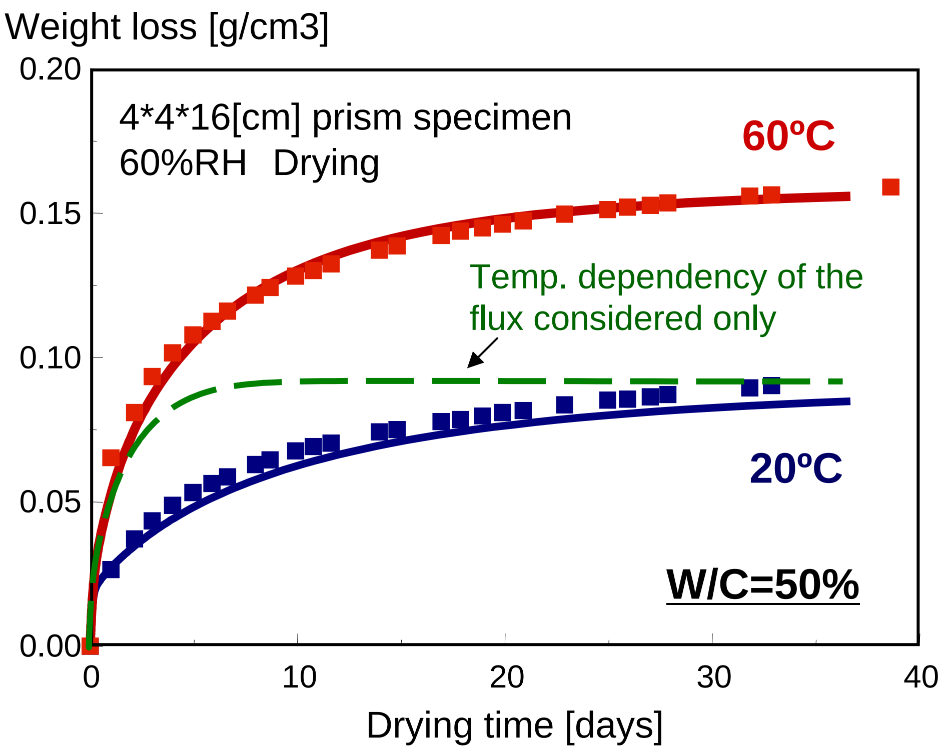
Moisture loss behaviors under different temperature

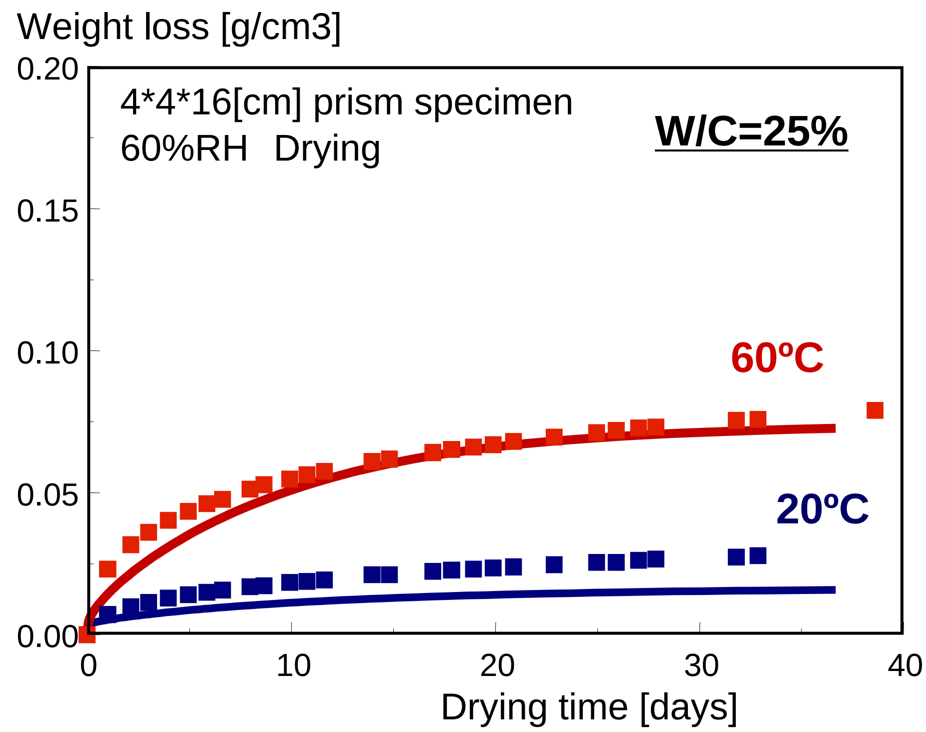
Temperature-dependent moisture isotherm model

- Two phase equilbrium (Clausius-Clapeyron eq.)
- Temp. dependency of surface tension
- Time-dependency of inkbottle water
- Temp-dependency of interlayer water

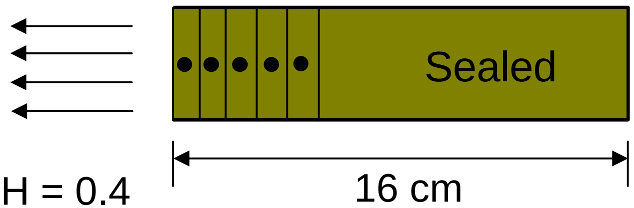
Moisture flux under arbitrary pressure & temperature gradient

- Mass flux potential based on partial pressure of vapor
- Temp. dependency of vapor diffusivity
- Temp. dependency of liquid viscosity





Verification of the influence of early age drying on microstructure development



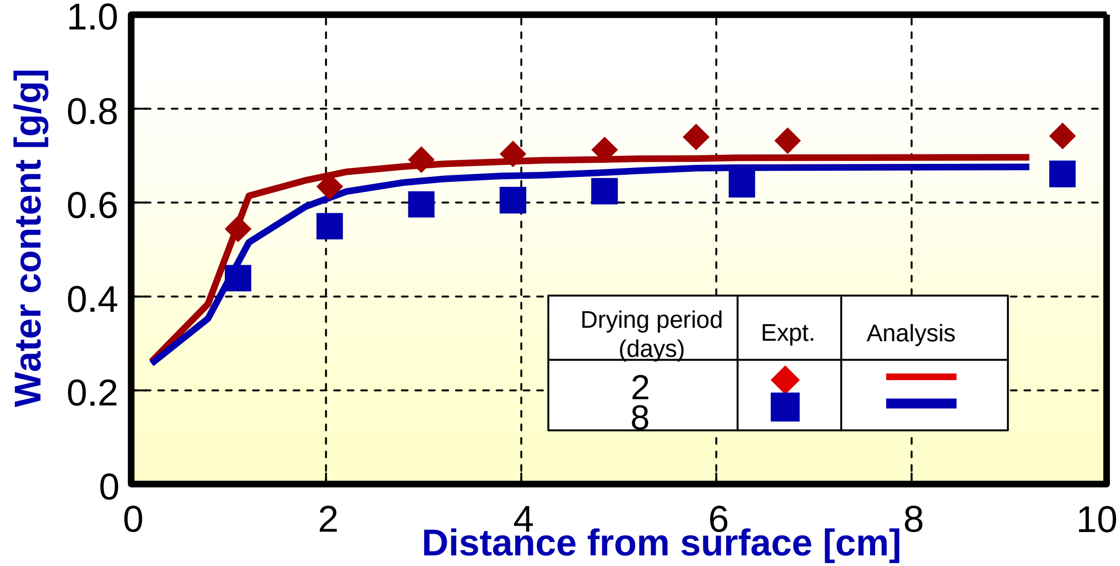
RH = 0.4

T = 20 C

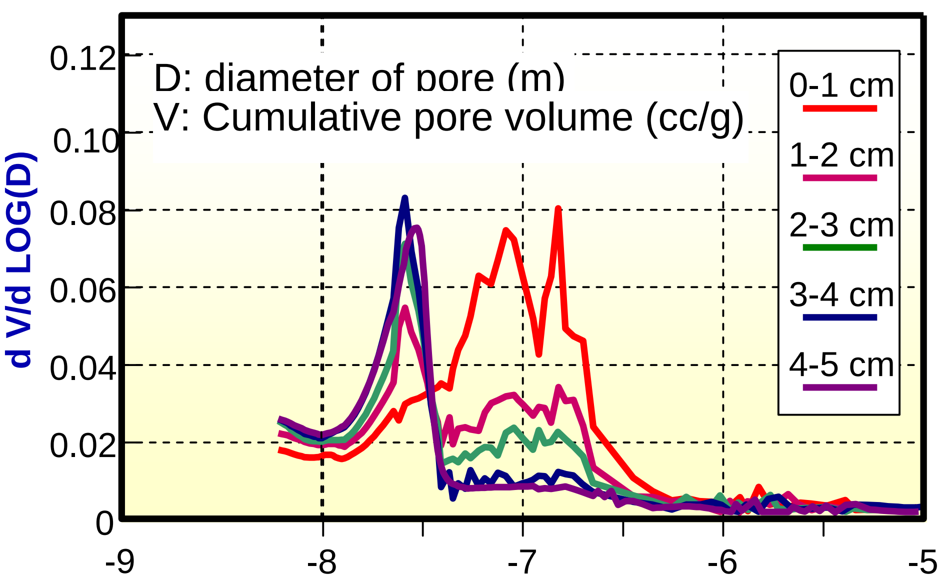
One day sealed cured; 8 days dried in 0.4 RH

W/C = 0.265

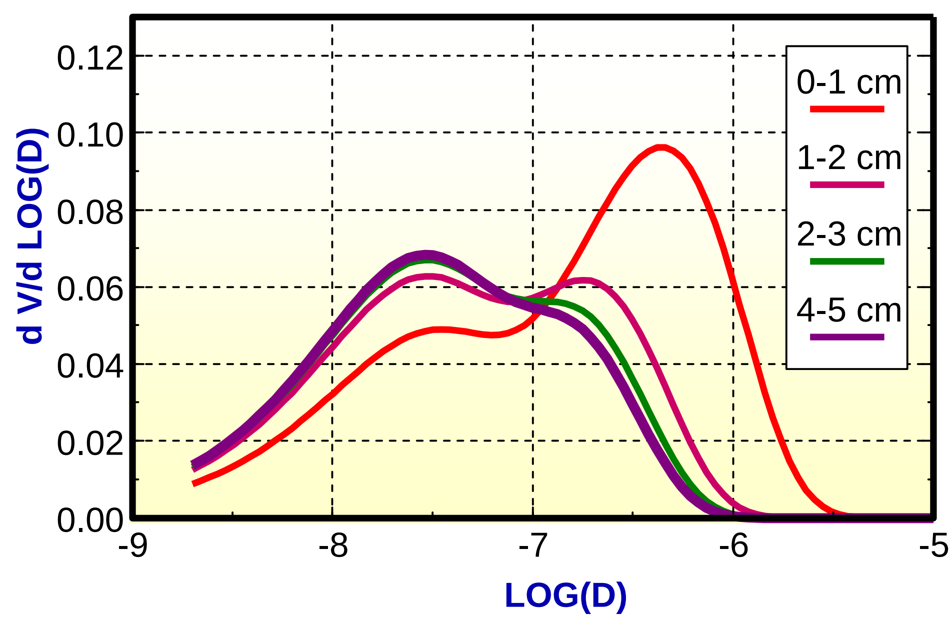
Computed and measured moisture profiles



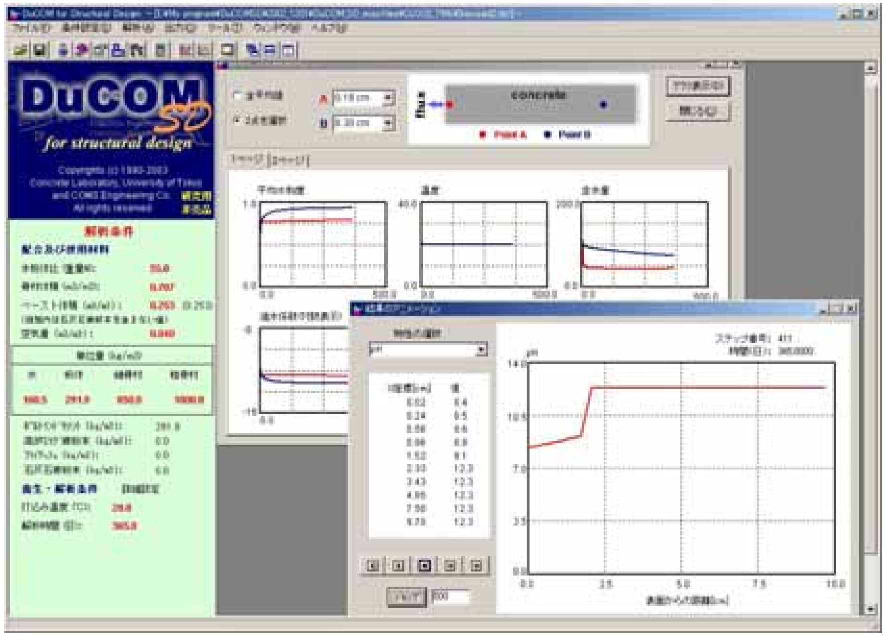
Measured pore distribution



Computed pore distribution



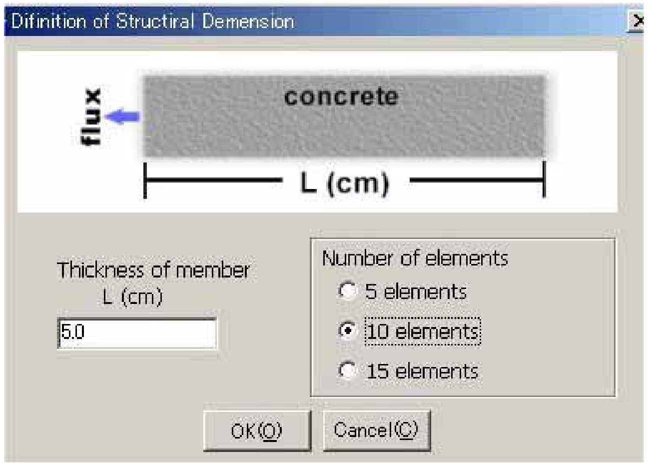
Durability Simulation Tool on Windows Environment
- DuCOM for Structural Design -



■The system covers 1-D mass/energy transport (heat generation/transport, moisture loss, chloride penetration, carbonation, corrosion, etc.)
■1-D simulation can represent most deterioration phenomenon
(full 3-D analysis is not always necessary for typical durability assessments)
■1~2 hours computation for several decades~ a hundred years (in case of cyclic drying-wetting)

http://www.comse.co.jp

Definition of structural dimension

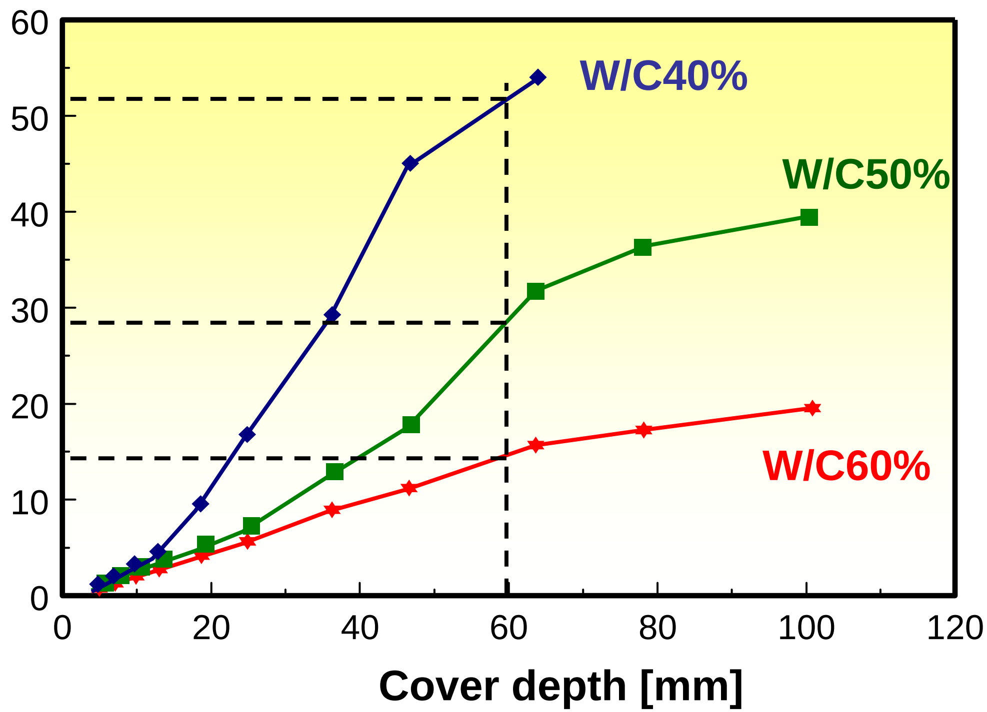


Definition of reinforcements

Performance evaluation of RC structures under environmental actions

-- Simulation of steel corrosion in RC guarder bridge exposed to marine environment --

Structural age until cracking due to corrosion [year]

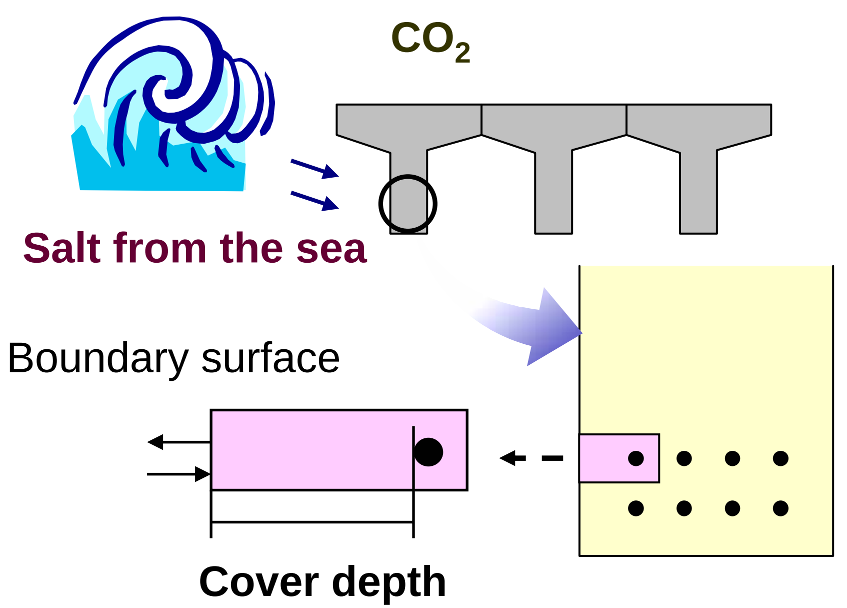


Target structure

RC T shaped guarder bridge

Environmental conditions

Marine environment
CO_2 concentration: 0.07%
O_2 concentration : 20%
Concentration of Cl^-: 0.51[mol/l]
Cyclic drying-wetting conditions
60%RH (10days) ↔ 99%RH (10days)



If cover depth is 60mm ..

W/C40%: After 52 years, repair needed.

W/C50%: After 28 years, repair needed.

W/C60%: After 15 years, repair needed.

DuCOM Coupled Computational Scheme

-Thermo-hygro physics for materials-

START

Size, shape, mix proportions, initial and boundary conditions

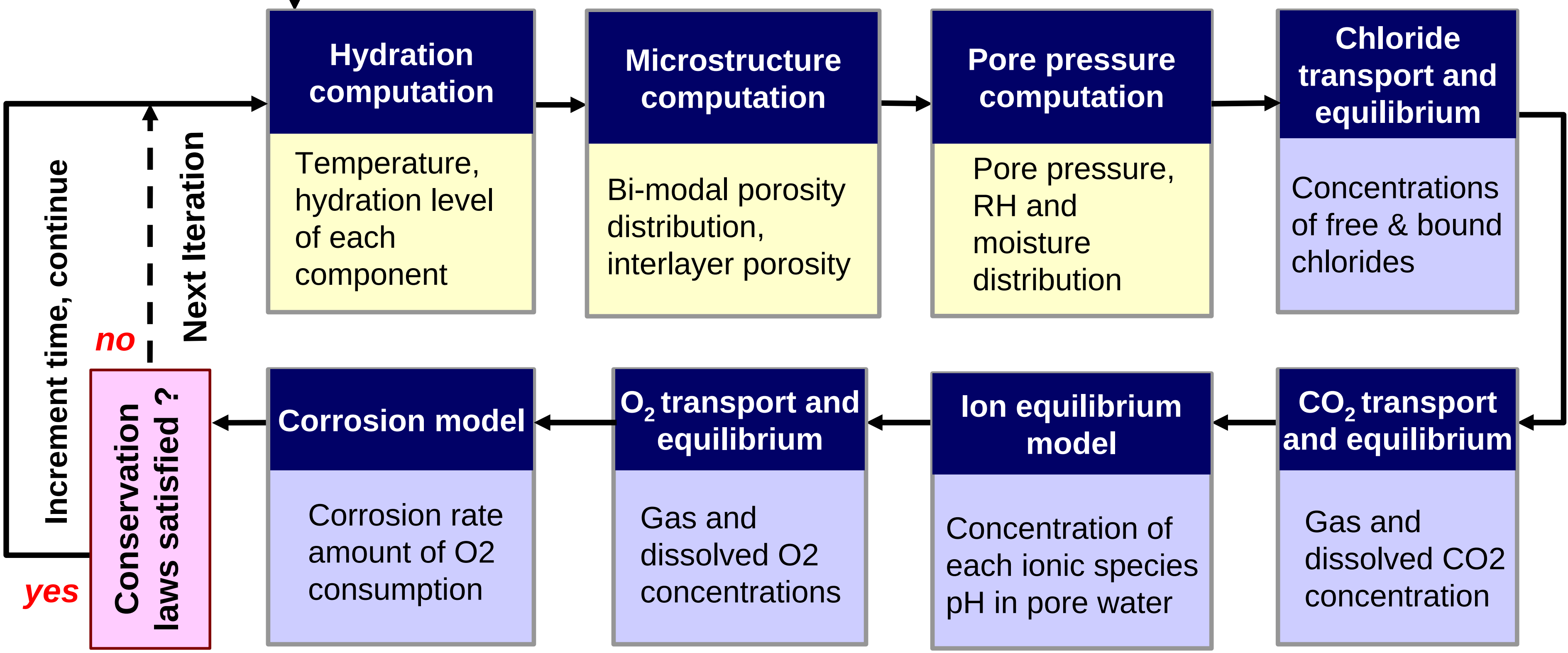
Basic Equation

$$\frac{\partial S(\theta_i)}{\partial t} + div\mathbf{J}_i(\theta_i, \nabla\theta_i) - Q_i(\theta_i) = 0$$

Potential term   Flux term   Sink term

θ_i; **Degree of freedom**

Temperature, Pore pressure, Chlorides, CO_2, and O_2

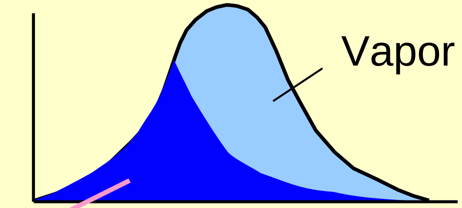


Each term has been formulated based on thermodynamics , chemical equilibrium and electrochemistry

Mass balance condition for free chlorides

Potential term

Porosity and saturation directly obtained by thermo-hygro physics



Liquid
(path for transport, ionic capacity)

Sink term

Rate of binding of free chloride to bound chloride per unit volume

↓

Chloride equilibrium model
（Model describing the relationship between free and bound chloride)

Governing equation $$\frac{\partial}{\partial t}\left(\phi S C_{Cl}\right) + div\mathbf{J}_{Cl} - Q_{Cl} = 0$$

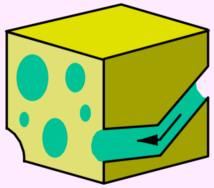
Flux term

$$\mathbf{J}_{Cl} = -\frac{\phi S}{\Omega}\delta \cdot D_{Cl}\nabla C_{Cl} + \phi S\mathbf{u}C_{Cl}$$

u; Velocity vector of pore water
→Obtained by liquid transport model

Diffusion due to ionic concentration difference

Convective term



2. Chloride ion transport

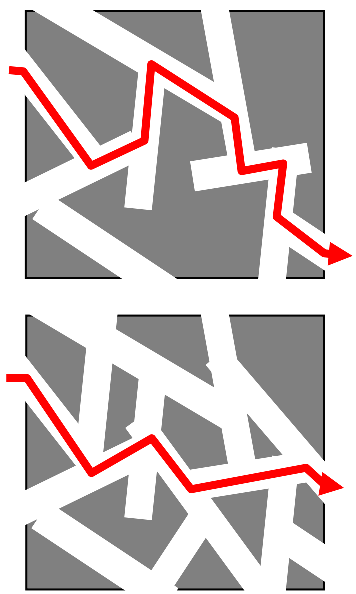
$$J_{ion} = -\left(\frac{\phi \cdot S}{\Omega} \cdot \delta \cdot D_{ion} \right) \cdot \nabla C_{ion} + \phi \cdot S \cdot \mathbf{u} \cdot C_{ion}$$

Ionic diffusion
due to concentration gradients

Advective transport
due to bulk movement

Reduction factor of ion diffusion due to property of pore structure

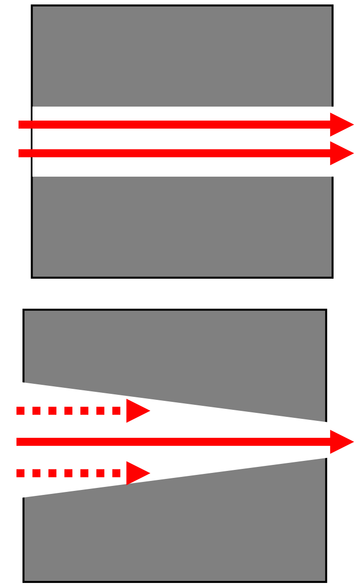
Tortuosity Ω



ϕ small
Ω large

ϕ large
Ω small

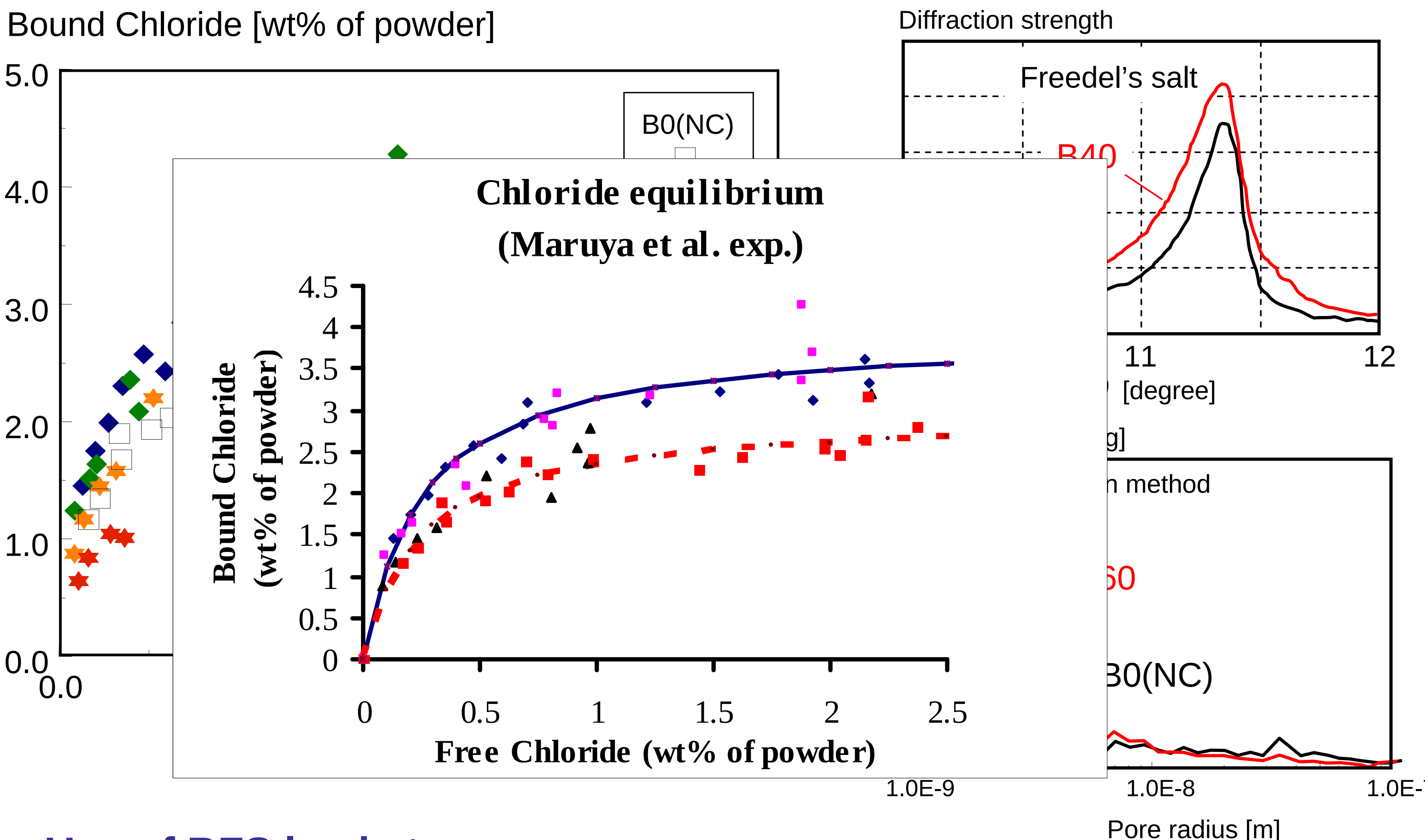
Constrictivity δ



$\delta = 1.0$

$\delta < 1.0$

Effect of BFS Use on Chloride Binding Capacity



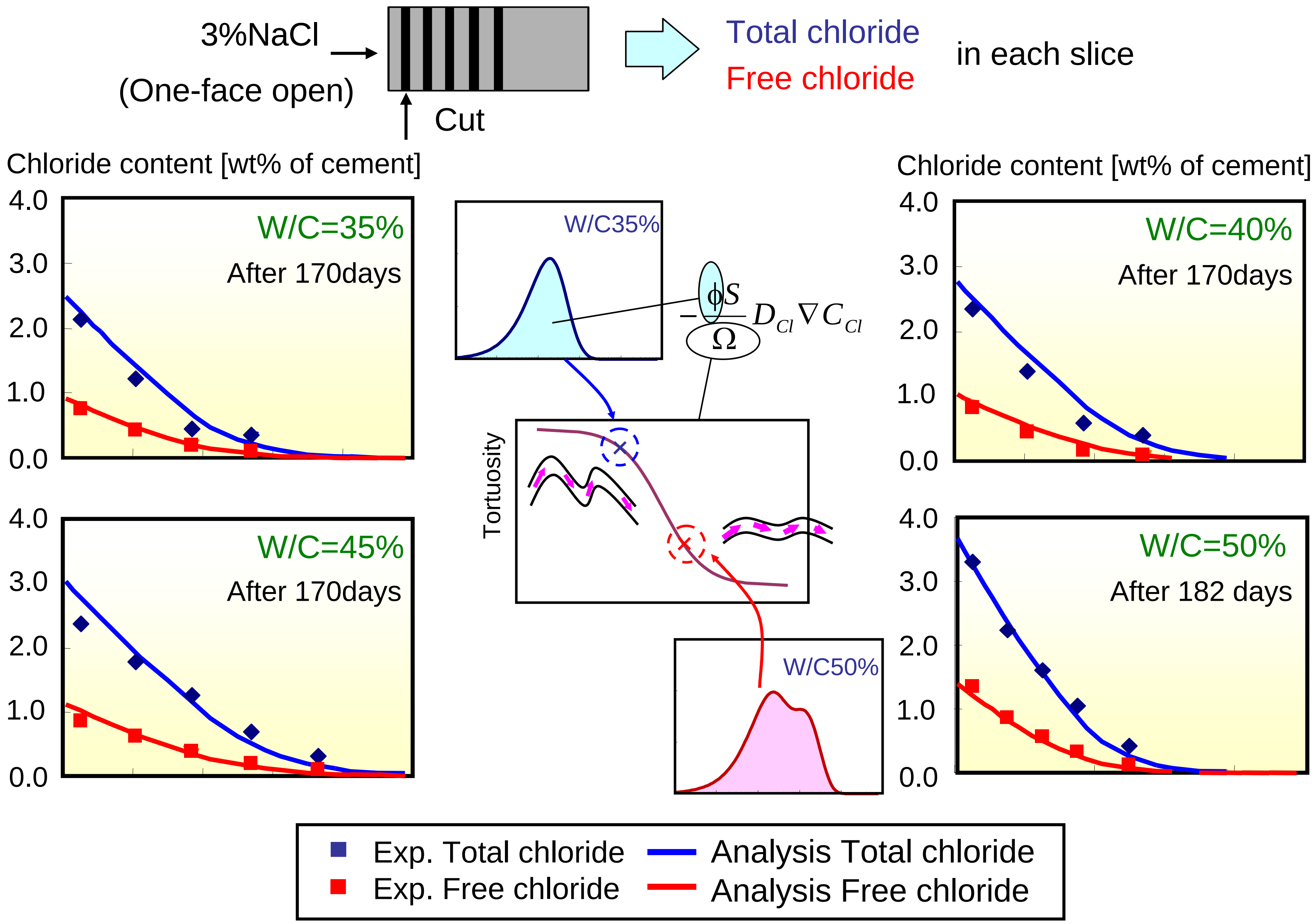
Use of BFS leads to

- Change of Pore Structure（Ads. Cl change）
- Al_2O_3 Increase (Bound Cl change）

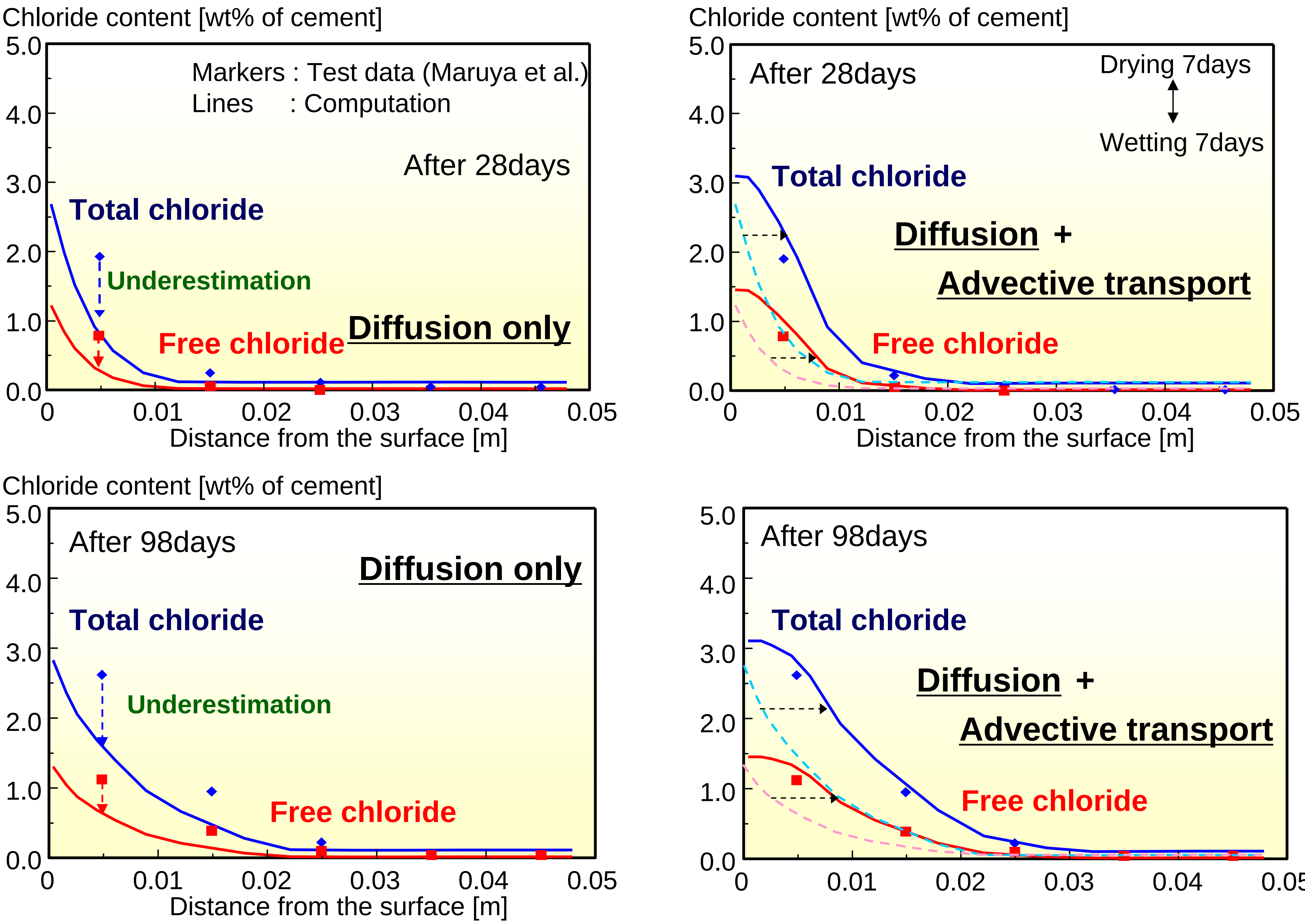
→ How much ?

Chloride distribution under submerged condition

ーW/C35%～50%　OPC mortar ー



Chloride content profile in concrete exposed to cyclic wetting and drying



Conventional approach to carbonation phenomena & Features of this research

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \longrightarrow X_c = b\sqrt{t}$$

Linear diffusion equation

Square root t equation

X_c ; Carbonation depth

b ; Carbonation rate coefficient

↳ Water to cement ratio, strength, environmental conditions…

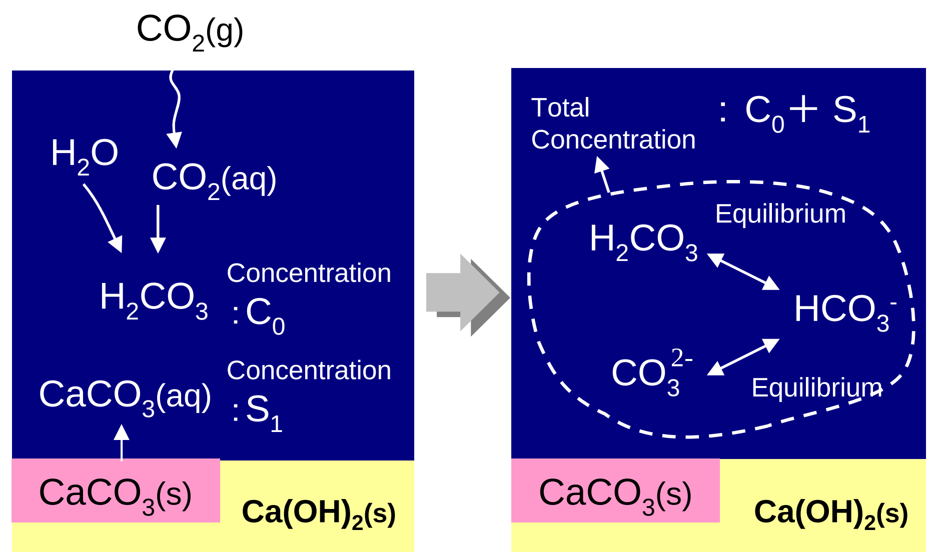
Features of this research

■Strict consideration of ions equilibrium

- Dissolution of carbon dioxide
- Dissolution and re-dissolution of precipitations depending on pH
- Dissociation of reactive mass
- Common ion effect

■Modeling of carbon dioxide transport

- Hindered diffusion in both the dissolved and gaseous phases.
- Nonlinear diffusion process depending on pore structures and moisture profile



Before ion dissociation

After ion dissociation

→ **pH profile in pore water can be obtained for arbitrary conditions**

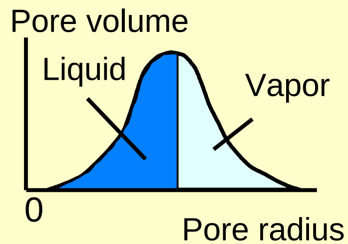
Mass balance condition for gas and dissolved carbon dioxide

Potential term

Gas ⟷ Dissolved CO_2

Based on Henry's law

Porosity and Saturation directly obtained by thermo-hygro physics



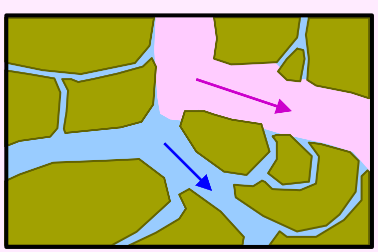
Sink term

Consumption rate of CO_2 due to carbonation

- Modeling of carbonation reaction
- Modeling of ion equilibriums

$$\frac{\partial}{\partial t}\{\phi[(1-S)\cdot\rho_{gCO_2} + S\cdot\rho_{dCO_2}]\} + divJ_{CO_2} - Q_{CO_2} = 0$$

Flux term



Porosity and Saturation

Gas **Dissolved**

$$J_{CO_2} = -\left(D_{gCO_2}\nabla\rho_g + D_{dCO_2}\nabla\rho_d\right)$$

$$\frac{\phi D_0^g (1-S)^4}{\Omega} N_k(h) \qquad \frac{\phi S}{\Omega} D_0^d$$

- **Knudsen diffusion factor**
- **Effect of tortuosity and connectivity of pores**

Modeling of carbonation reaction

Carbonation reaction

$$Ca^{2+} + CO_3^{2-} \rightarrow CaCO_3$$

Reaction of silicic acid calcium hydroxide (C-S-H) is not considered

→ Its solubility is quite law compared with calcium hydroxide

Rate of carbonation reaction

$$Q_{CO_2} = \frac{\partial\left(C_{CaCO_3}\right)}{\partial t} = k[Ca^{2+}][CO_3^{2-}]$$

↑ Reaction velocity coefficient

Modeling of ions equilibrium

$$H_2O \leftrightarrow H^+ + OH^-$$

$$H_2CO_3 \leftrightarrow H^+ + HCO_3^- \leftrightarrow 2H^+ + CO_3^{2-}$$

$$Ca(OH)_2 \leftrightarrow Ca^{2+} + 2OH^-$$

$$CaCO_3 \leftrightarrow Ca^{2+} + CO_3^{2-}$$

Ion dissociation, Solubility of precipitations

→ Depending on pH in pore solutions

- **Law of mass action**
- **Mass conservation law**
- **Proton balance**

↓

- **Each acid-base reaction**
- **Solubility of each product**
- **Common ion effect**

Concentration of proton

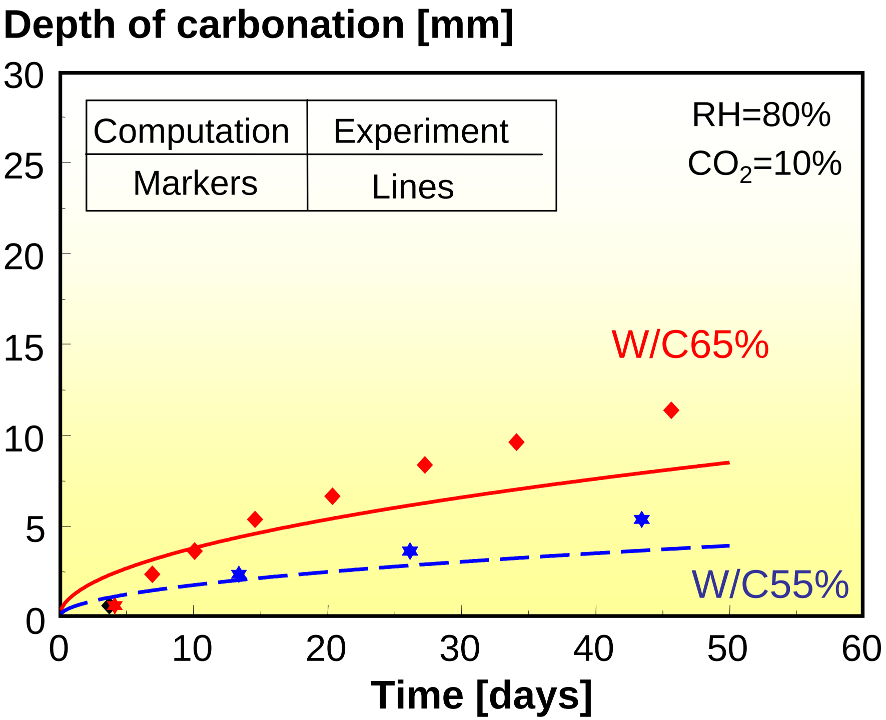
↓

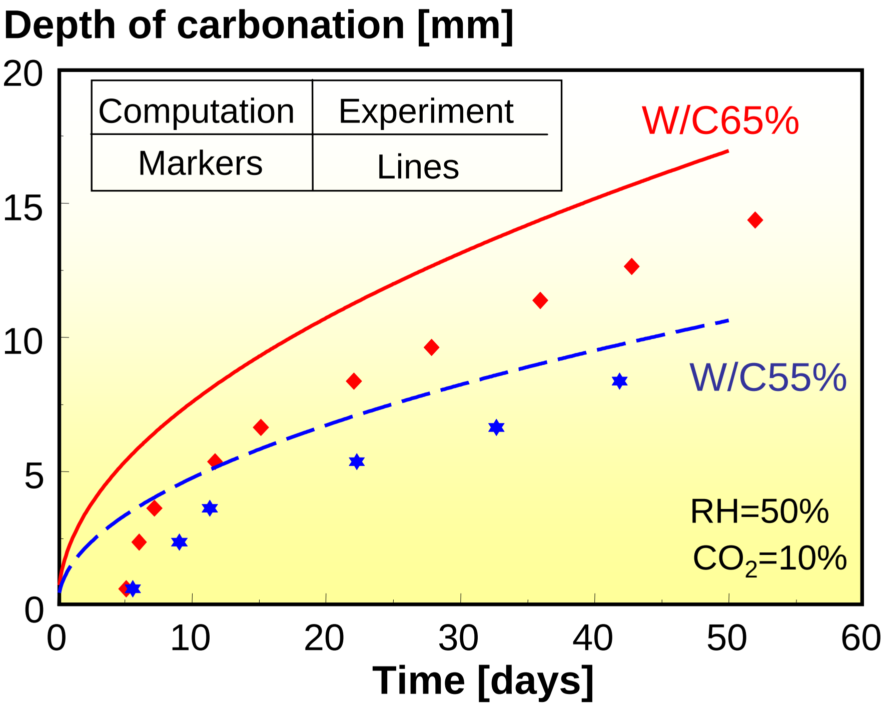
Concentration of each ion at arbitrary stage

Simulation of carbonation progress I

- Verification with accelerated carbonation tests-

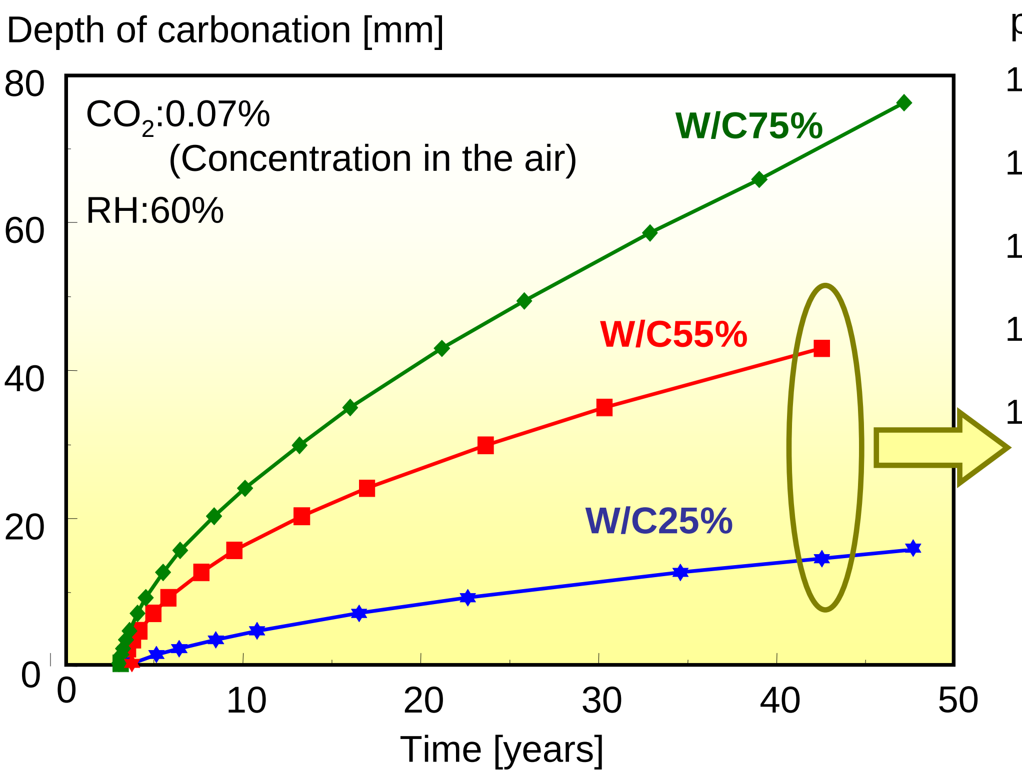
Input				*Output*
Mix proportion (W/C) Relative humidity CO_2 Concentration	→	Profile of Pore structure Moisture distribution Amount of $Ca(OH)_2$	→	pH value in pore water Reacted $Ca(OH)_2$

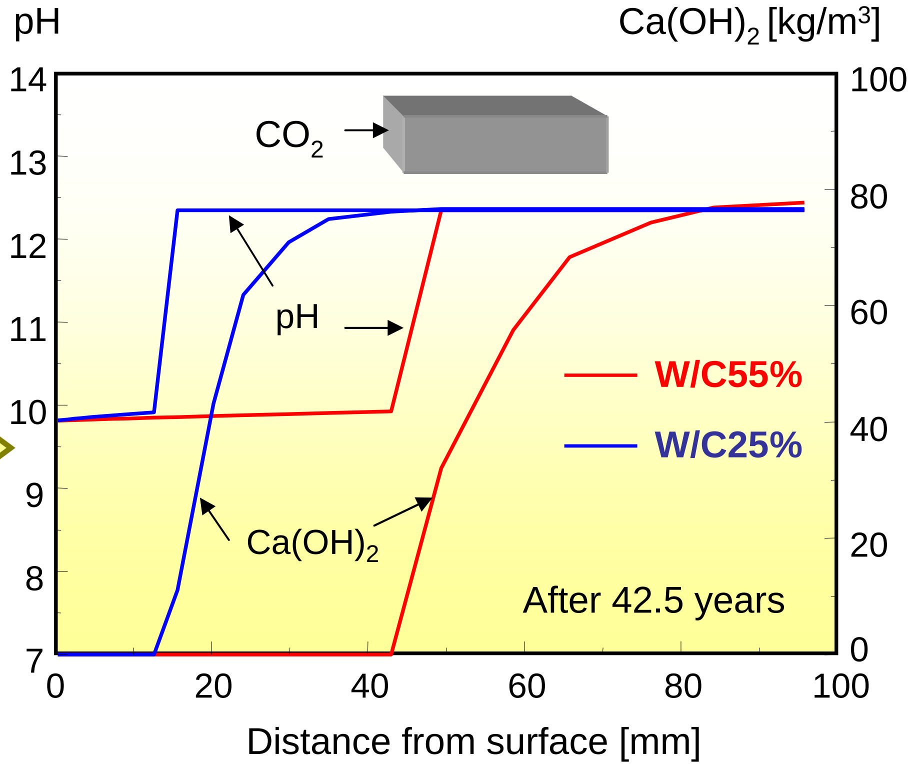




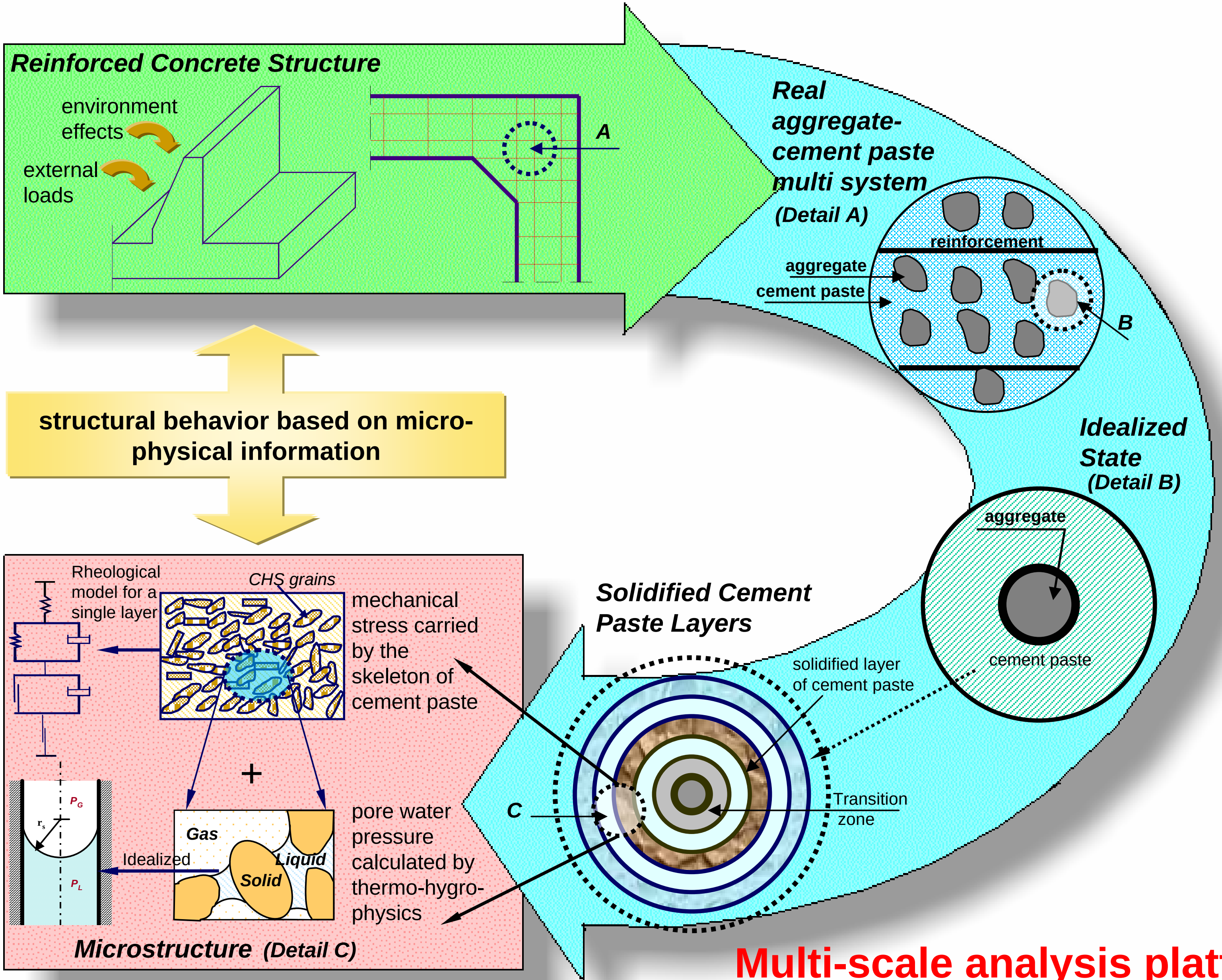
Simulation of carbonation progress II

- pH fluctuation for different W/C cases under normal environmental condition-





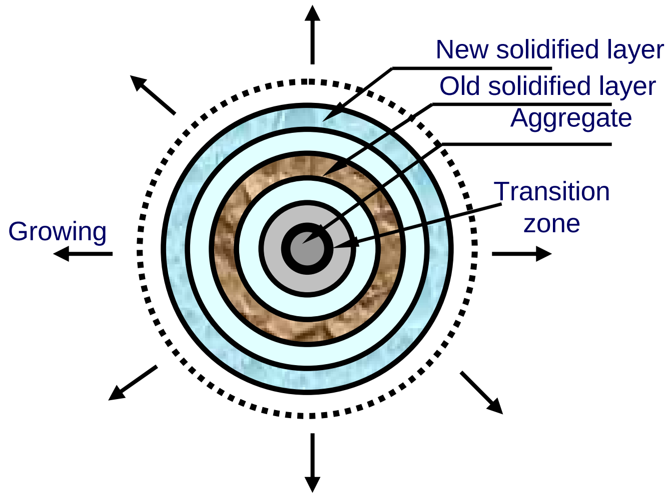
Macrostructure Microstructure Correlation

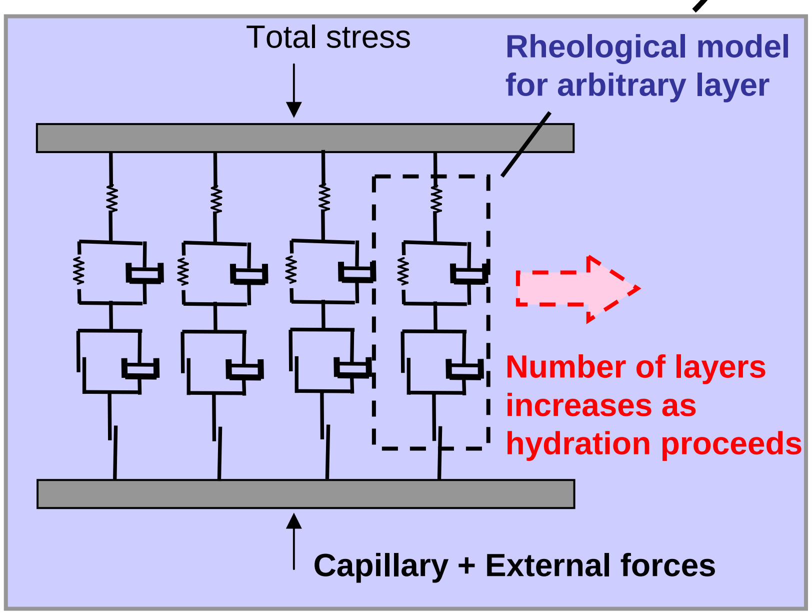


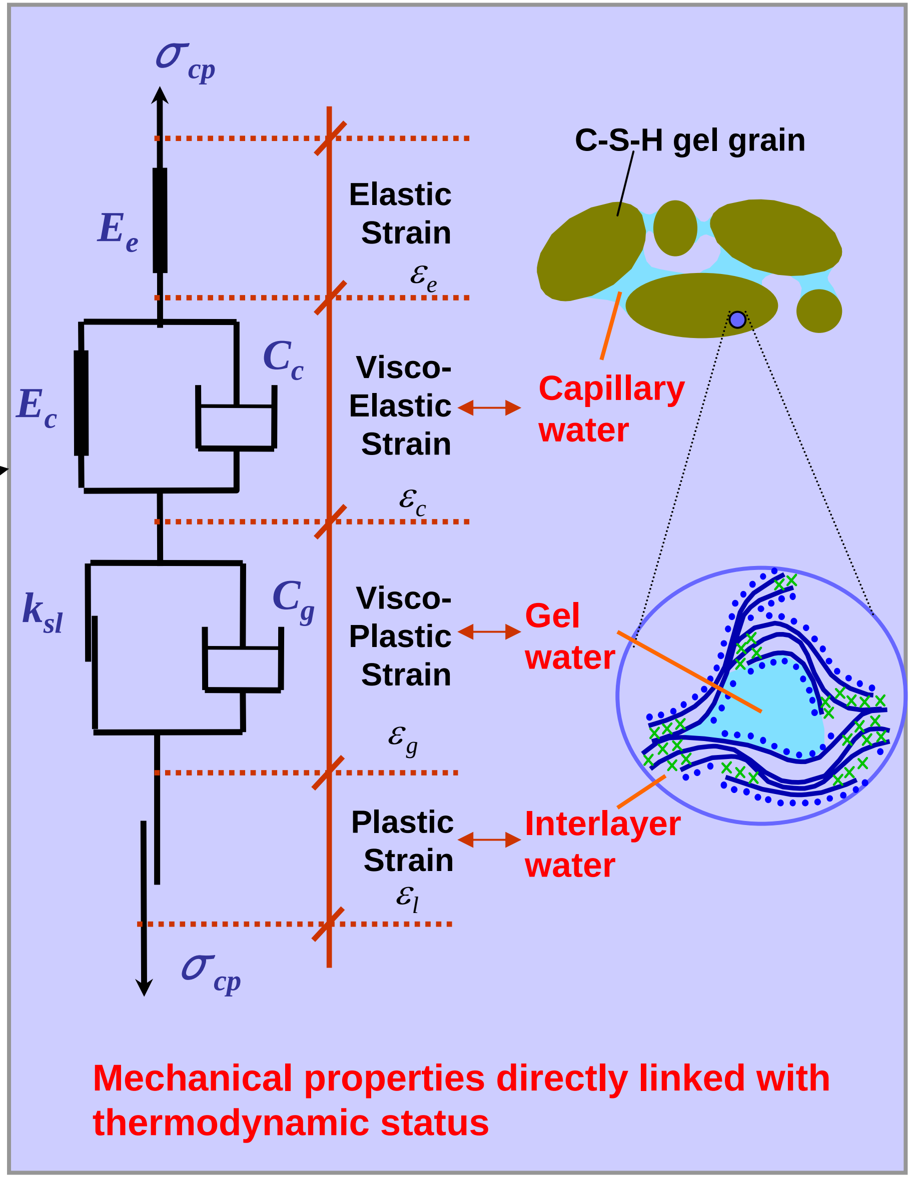
Multi-scale analysis platform: DuCOM+COM3

Solidification Model of Hardening Concrete Composite

Proposed by Maekawa, Rasha, Zhu, and Ishida



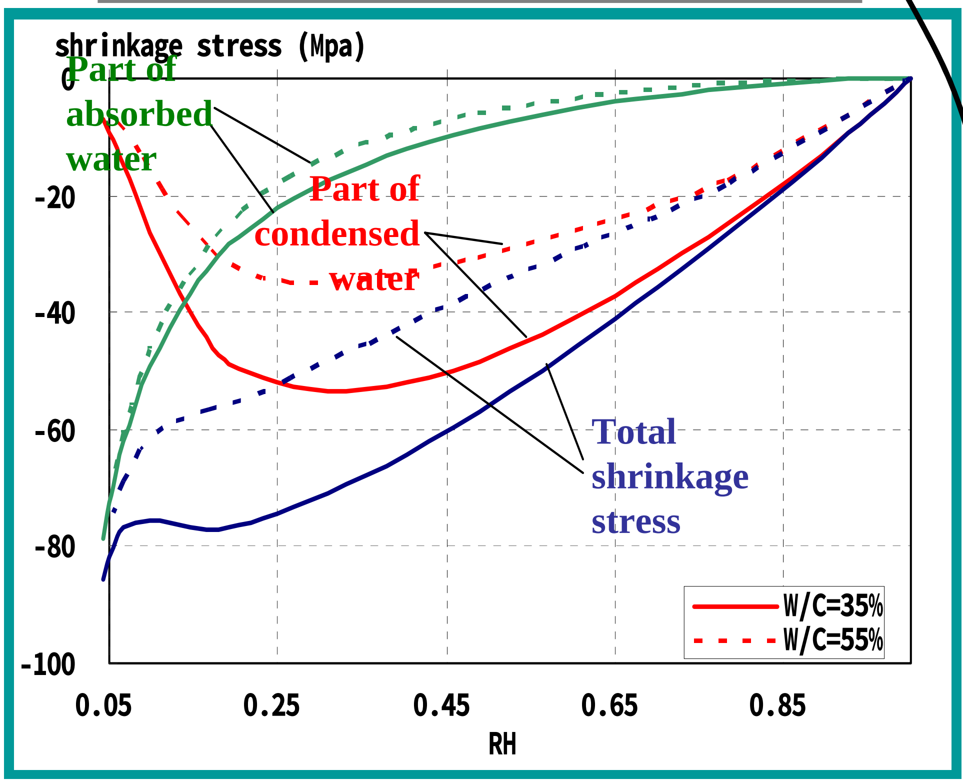




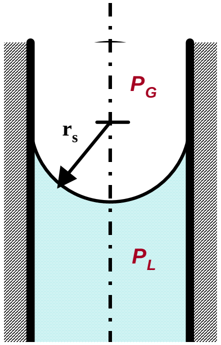
Constitutive Model of Concrete － Modeling of shrinkage stress, 1

$$\sigma_s = \sigma_{sd} + \sigma_{sc}$$

Inherent driving forces in terms of RH



Theory of capillary tension



$$\sigma_{sc} = \beta \cdot P$$

$$P = -\frac{\rho RT}{M}\ln h$$

$$\beta = \frac{\phi_{cap} \cdot S_{cap} + \phi_{gel} \cdot S_{gel}}{\phi_{cap} + \phi_{gel}}$$

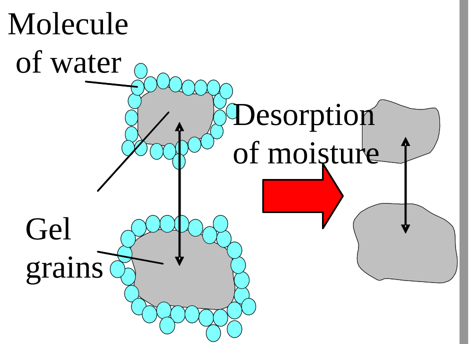
- Kelvin & Laplace equations
- Content of condensed water

Theory of surface energy

$$\sigma_{sd} = S_{sd} \cdot \gamma$$

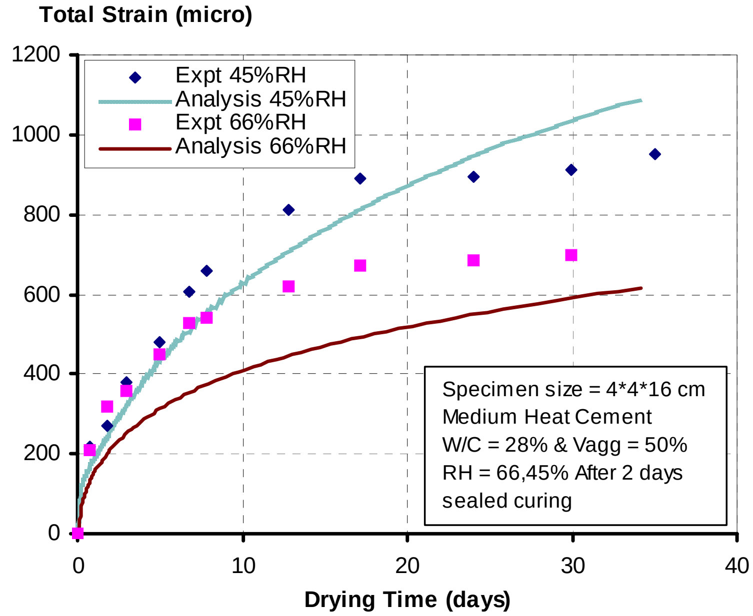
$$S_{sd} = f(h) S_{gel}$$

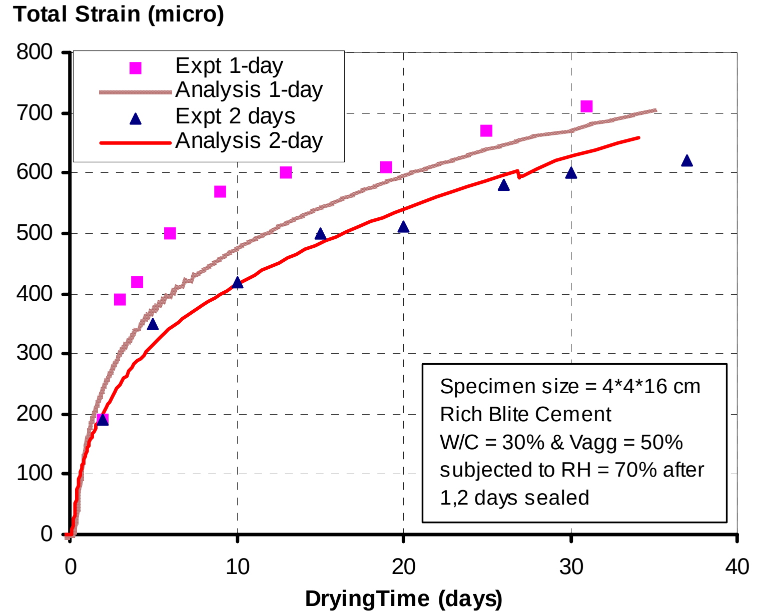
$$f(h) = \frac{1 - k_2 h}{1 - k_2 h + k_1 h}$$

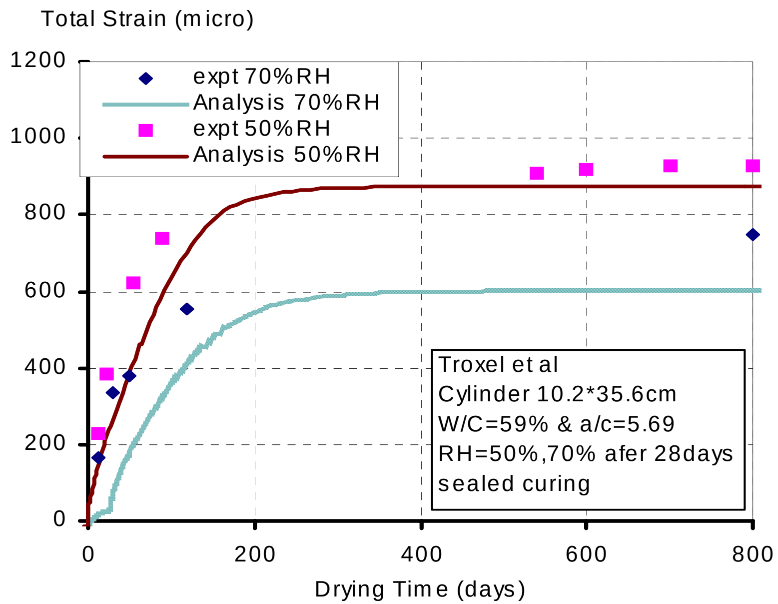


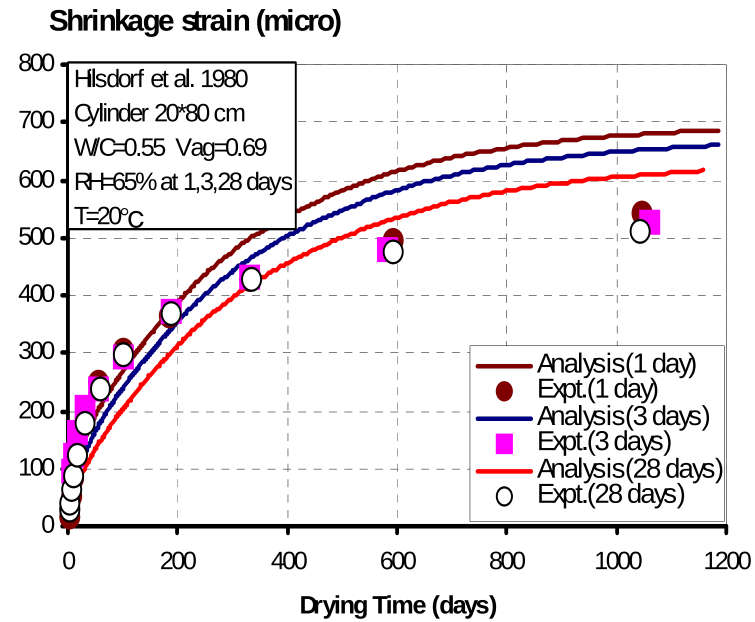
- Thickness of absorbed water by B.E.T theory
- Surface area of gel

Verification (Drying shrinkage)

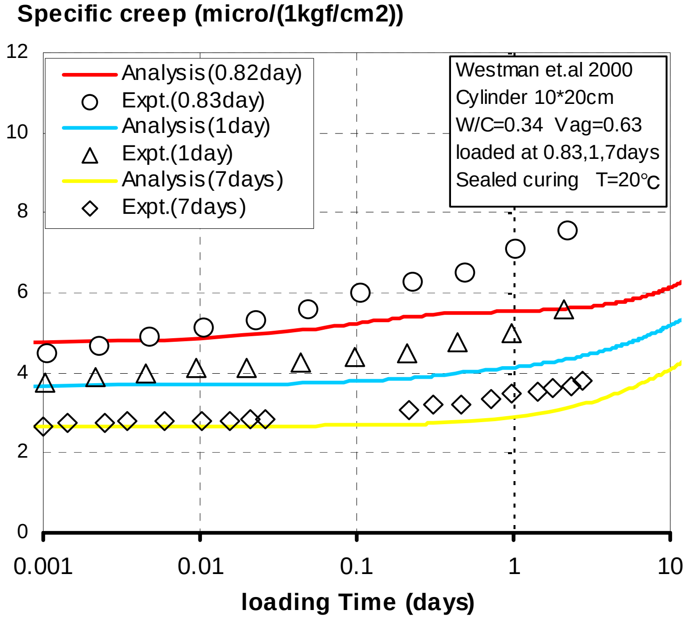


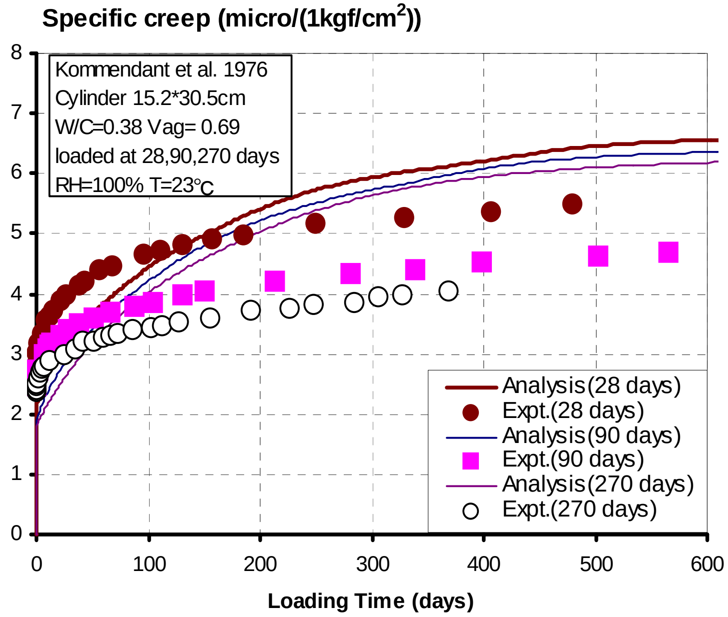


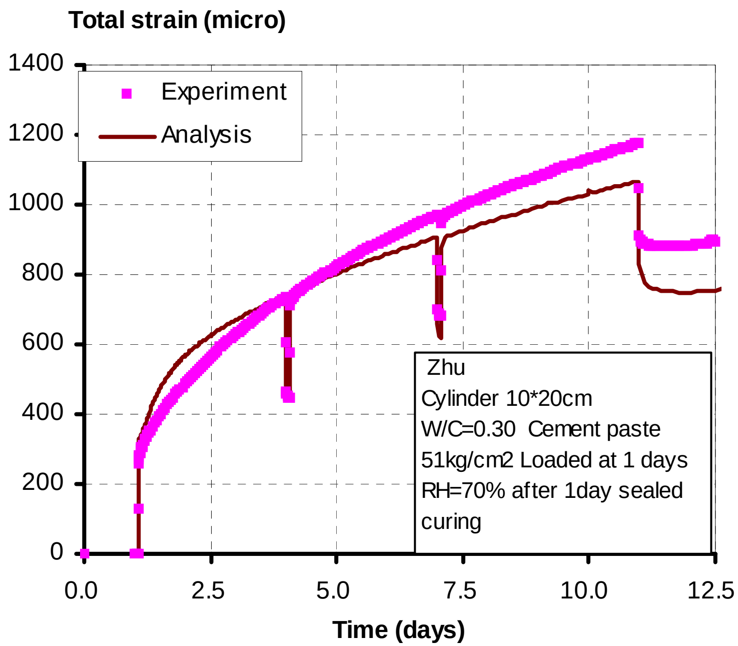


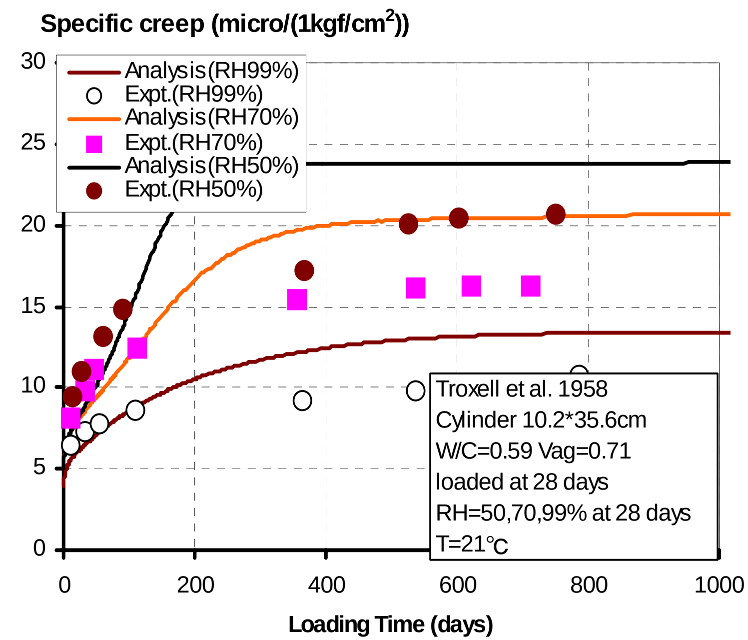


Verification (Creep)









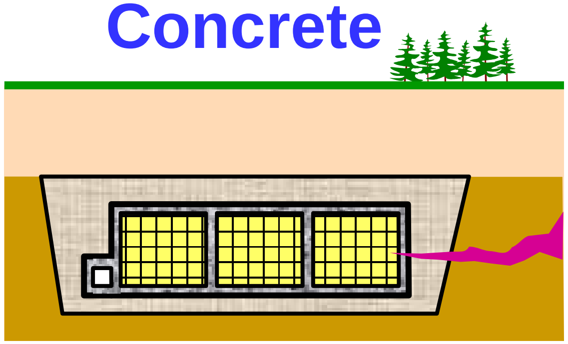
Durability problem (Calcium leaching)

Past : Since rate of leaching is very slow, it is not so important.

Present : Calcium leaching is one of the most important problems.

Extended application

Concrete

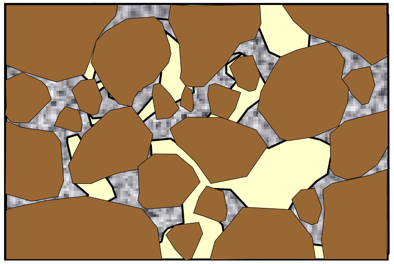


Low-level radioactive waste (Now) ->

Mid and High-level waste should be treated in very near future

New material

Cemented soil



Isolation of radioactivity	Purpose	Ground improvement
Deep underground	Environment	Underground
$10^3 – 10^4$ [year]	Time scale	$10^1 – 10^2$ [year]

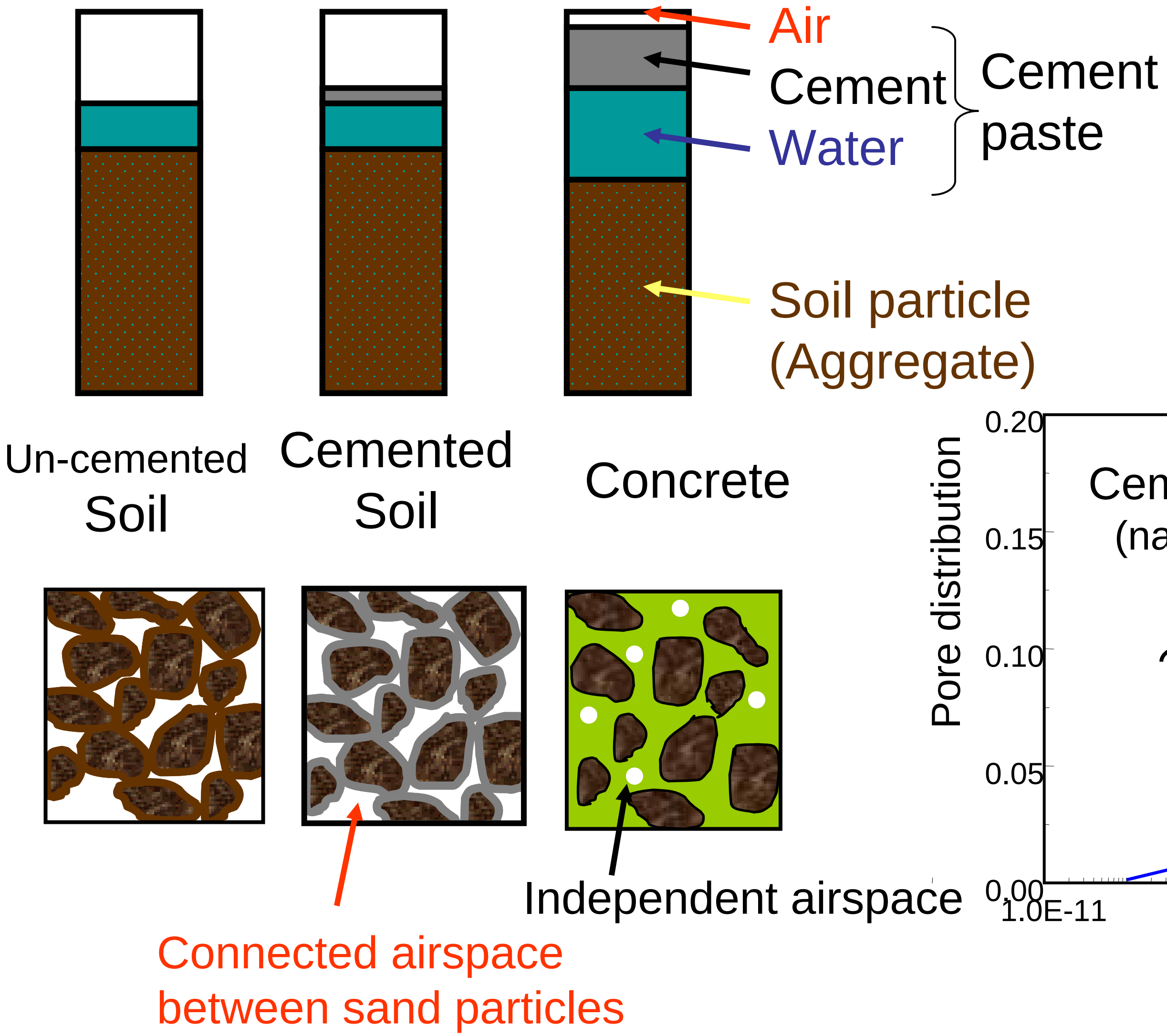
Very long-term
Diffusion of ions from Concrete to soil

High W/C, large voids
Property between soil and concrete

Modeling of micro-pore structure for cemented soil

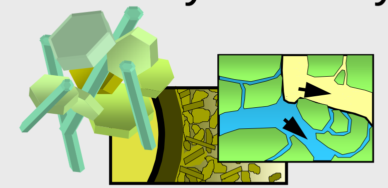
Extend to cemented soil

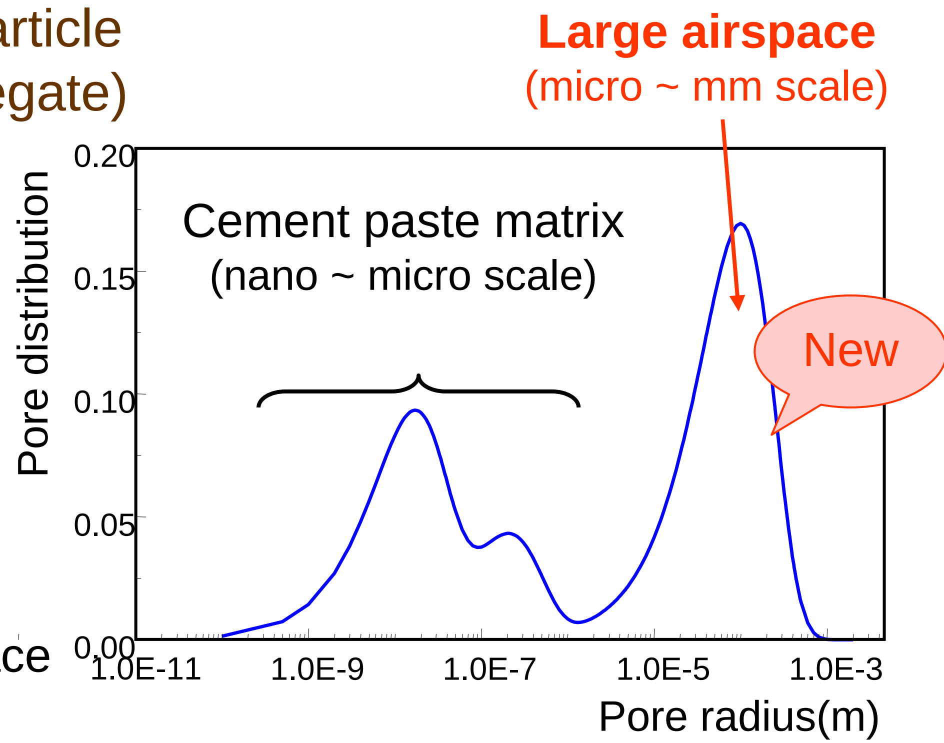
Mix proportions (in volume)



DuCOM

Thermodynamic system





Pore distribution

Mass balance condition for calcium ion in cementitious materials

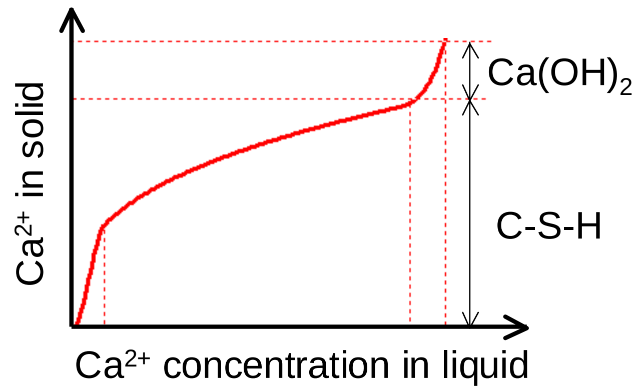
Basic Equation for total calcium

$$\frac{\partial}{\partial t}(\phi \cdot S \cdot C_{ion}) + \frac{\partial C_{solid}}{\partial t} - divJ_{ion} = 0$$

Liquid-phase Solid-phase Transport

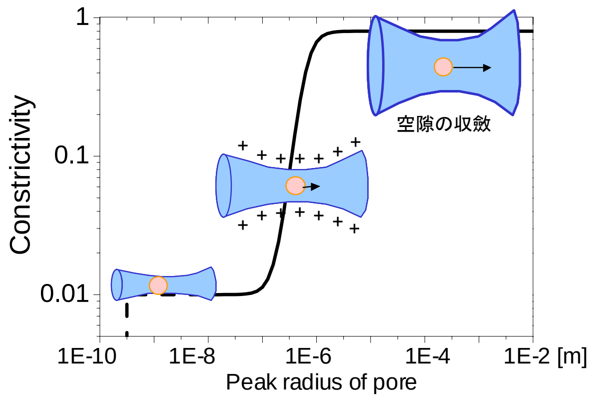
1. Ca liquid/solid equilibrium

$$C_{Solid} = f(C_{ion})$$



2. Ca^{2+} ion transport

$$J_{ion} = -\left(\frac{\phi \cdot S}{\Omega} \cdot \delta \cdot D_{ion}\right) \cdot \nabla C_{ion} + \phi \cdot S \cdot \mathbf{u} \cdot C_{ion}$$



solubility product

Saturated concentration

Transport route

Increase of pore space (CH&CSH)

Chloride model

Free chloride ion

Hydration model

Temperature, Hydration degree, Amount of Ca(OH)2 and C-S-H

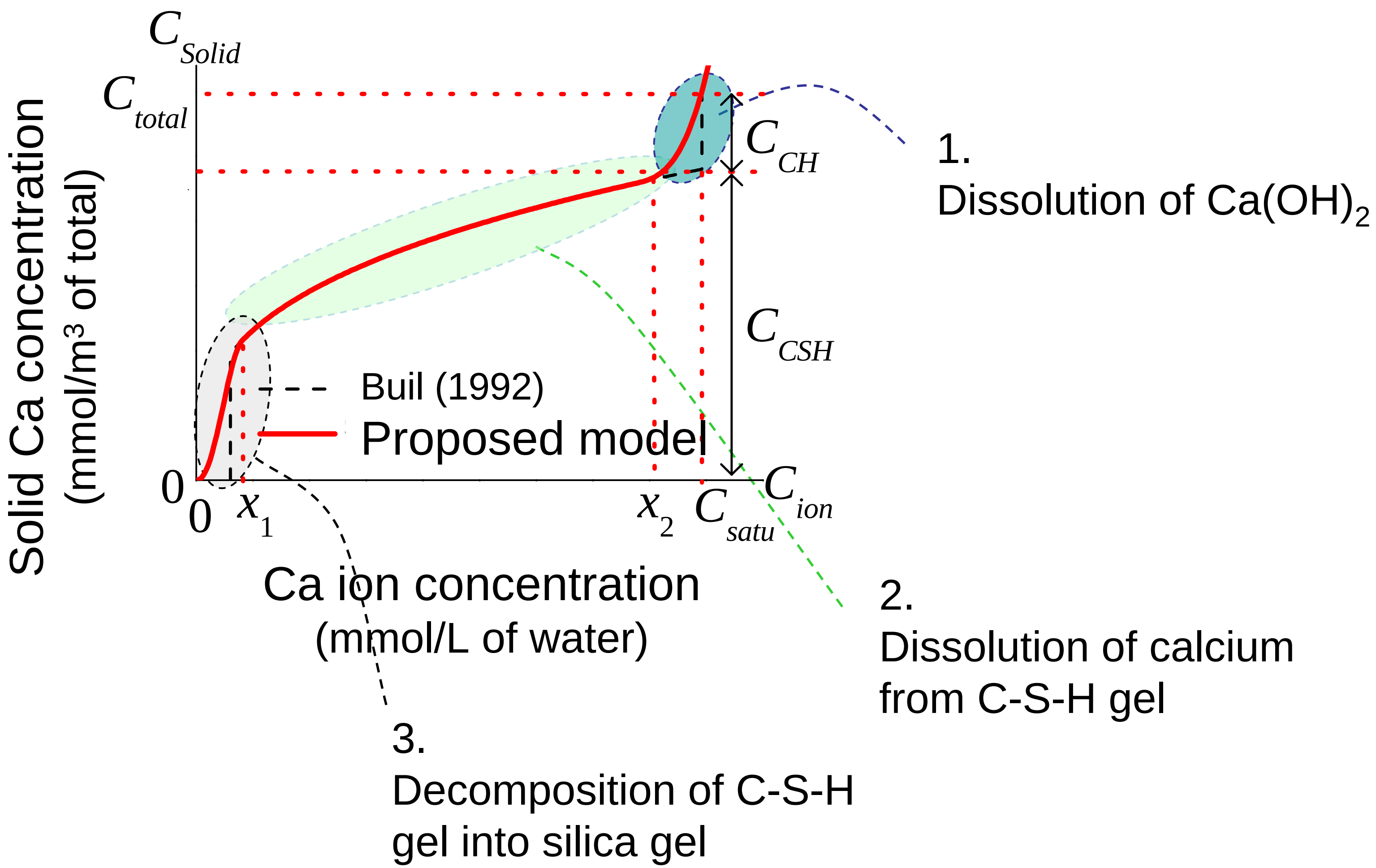
Pore structure model
Moisture model

Pore distribution, moisture distribution

Modeling of Calcium liquid-solid equilibrium

1. Ca liquid/solid equilibrium

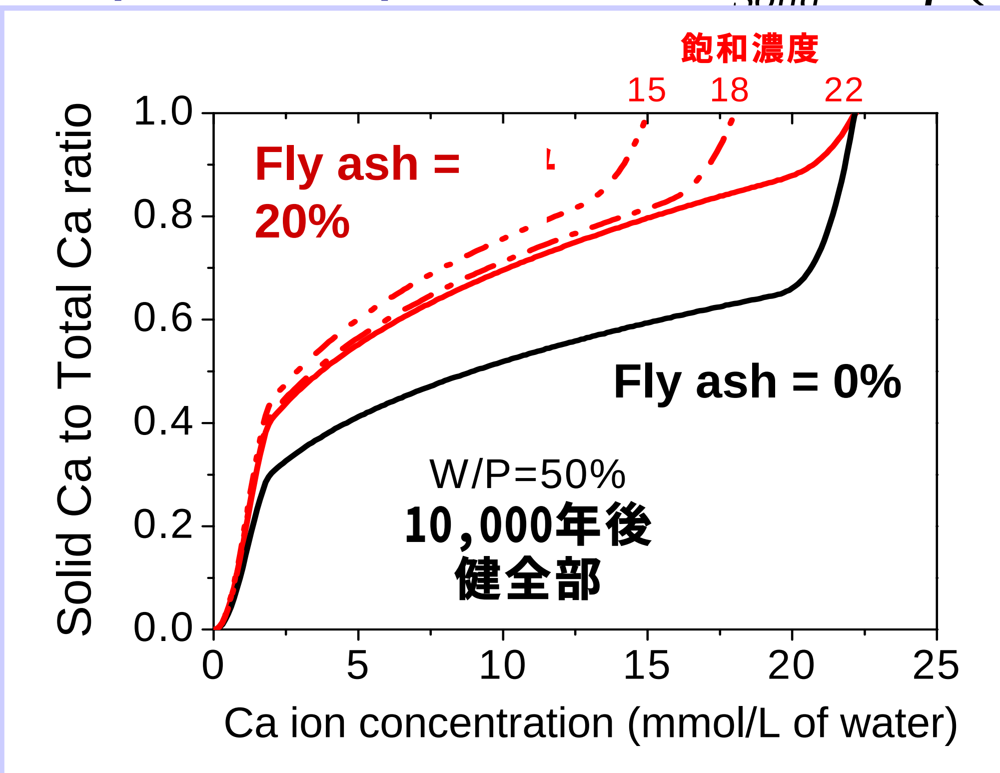
$$C_{Solid} = f(C_{ion})$$



Equilibrium model of calcium

1. Ca liquid/solid equilibrium

$$C_{Solid} = f(C_{ion})$$



Total Ca (constant)

Mix proportion

Ca in generated $Ca(OH)_2$

Hydration model

Ca in C-S-H gel

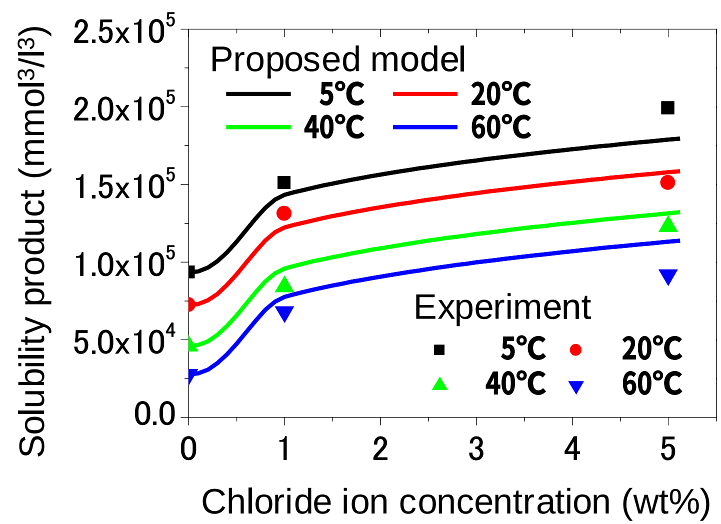
$$C_{CSH} = C_{Total} - C_{CH}$$

Saturated concentration

$$C_{satu} = \frac{1}{2}\sqrt[3]{2K_{sp}}$$

solubility product of $Ca(OH)_2$

-Temperature
-Chloride ion concentration



Modeling of Calcium transport

2. Ca^{2+} ion transport

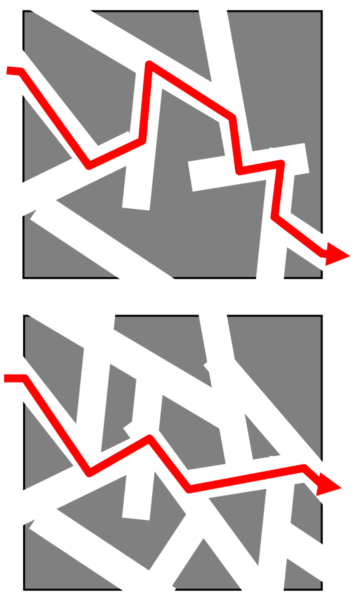
$$J_{ion} = -\left(\frac{\phi \cdot S}{\Omega} \cdot \delta \cdot D_{ion} \right) \cdot \nabla C_{ion} + \phi \cdot S \cdot \mathbf{u} \cdot C_{ion}$$

Ionic diffusion
due to concentration gradients

Advective transport
due to bulk movement

Reduction factor of ion diffusion due to property of pore structure

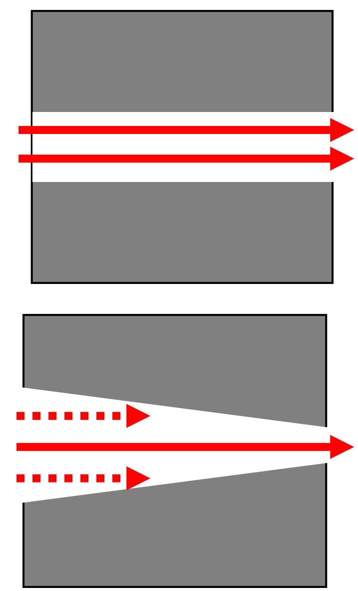
Tortuosity Ω



ϕ small
Ω large

ϕ large
Ω small

Constrictivity δ



$\delta = 1.0$

$\delta < 1.0$

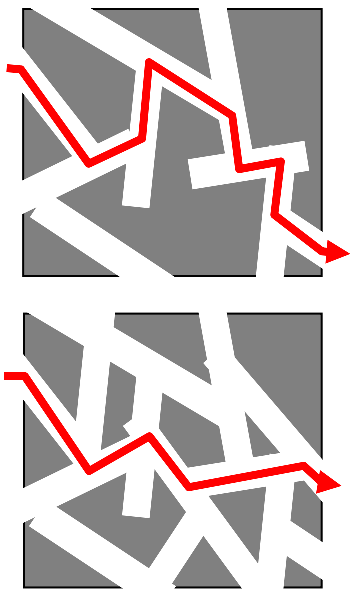
2. Ca^{2+} ion transport

$$J_{ion} = -\left(\frac{\phi \cdot S}{\Omega} \cdot \delta \cdot D_{ion}\right) \cdot \nabla C_{ion} + \phi \cdot S \cdot \mathbf{u} \cdot C_{ion}$$

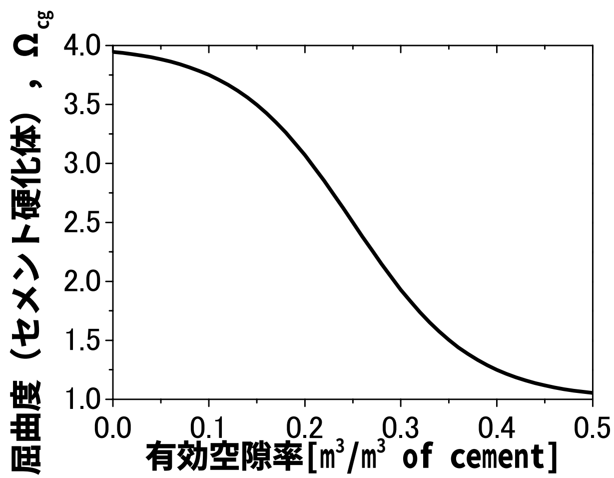
Ionic diffusion
due to concentration gradients

Advective transport
due to bulk movement

Tortuosity Ω

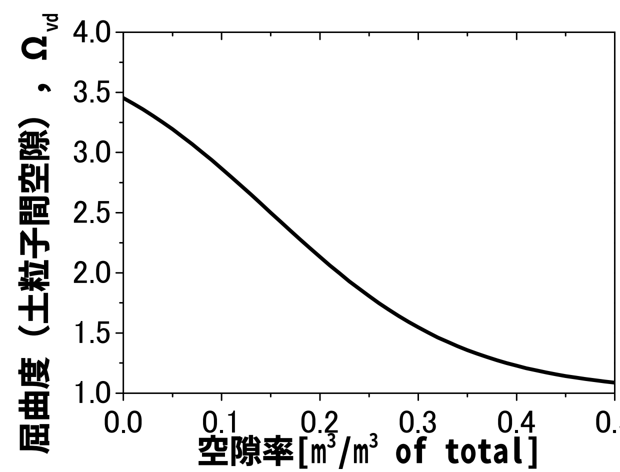


Tortuosity of cement paste



Effective porosity rate

Tortuosity of soil



Porosity rate of void

Tortuosity is defined as a function of porosity.

Modeling of transport of calcium ion

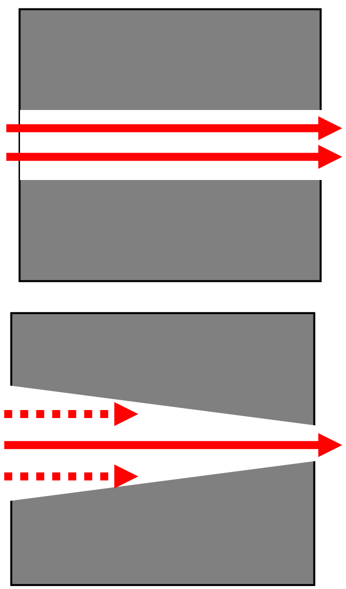
2. Ca^{2+} ion transport

$$J_{ion} = -\left(\frac{\phi \cdot S}{\Omega} \cdot \delta \cdot D_{ion}\right) \cdot \nabla C_{ion} + \phi \cdot S \cdot \mathbf{u} \cdot C_{ion}$$

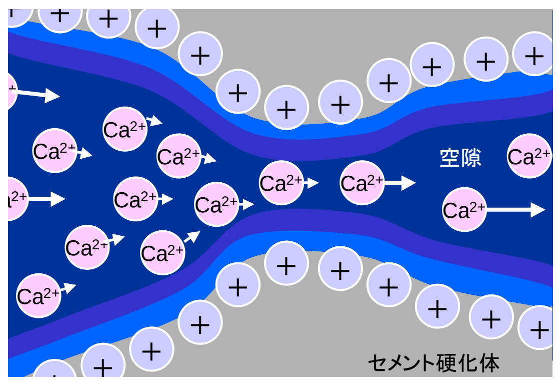
Ionic diffusion
due to concentration gradients

Advective transport
due to bulk movement

Constrictivity δ

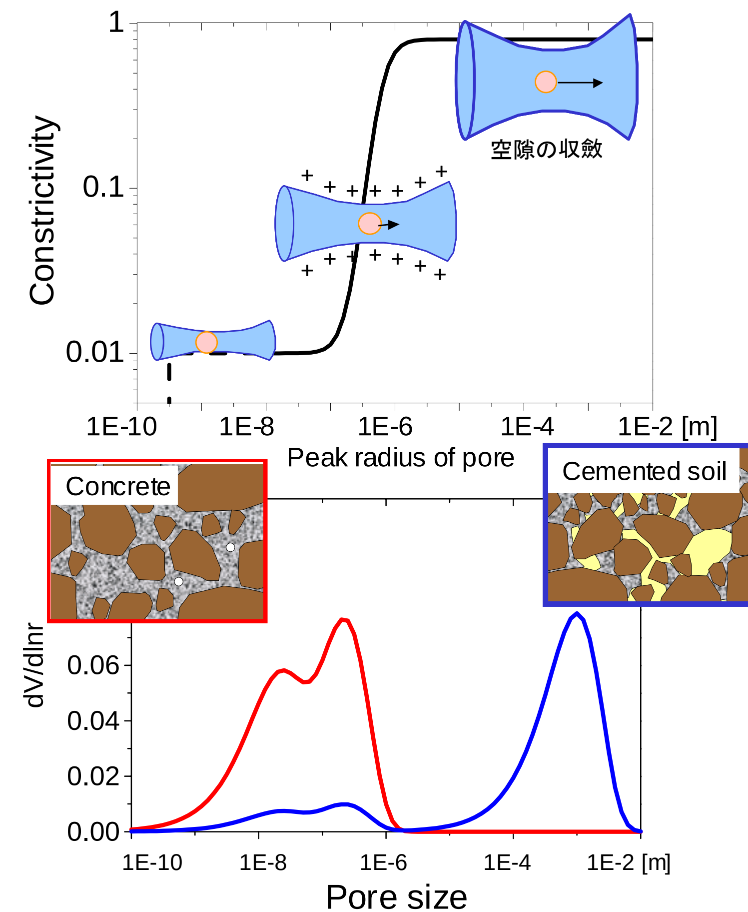


In cement paste

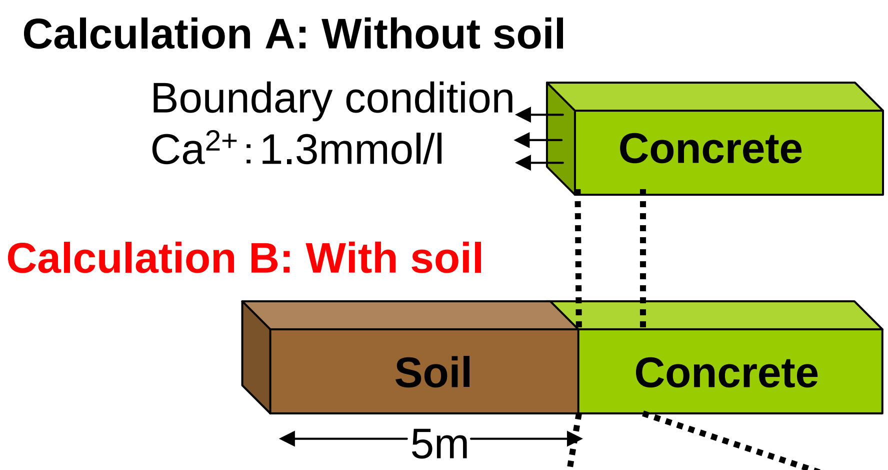


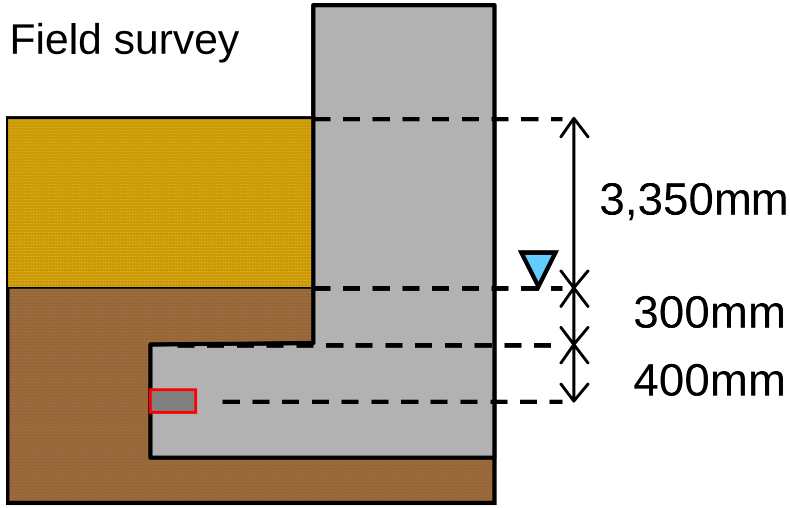
Strong interaction between ion and wall of micro-pore

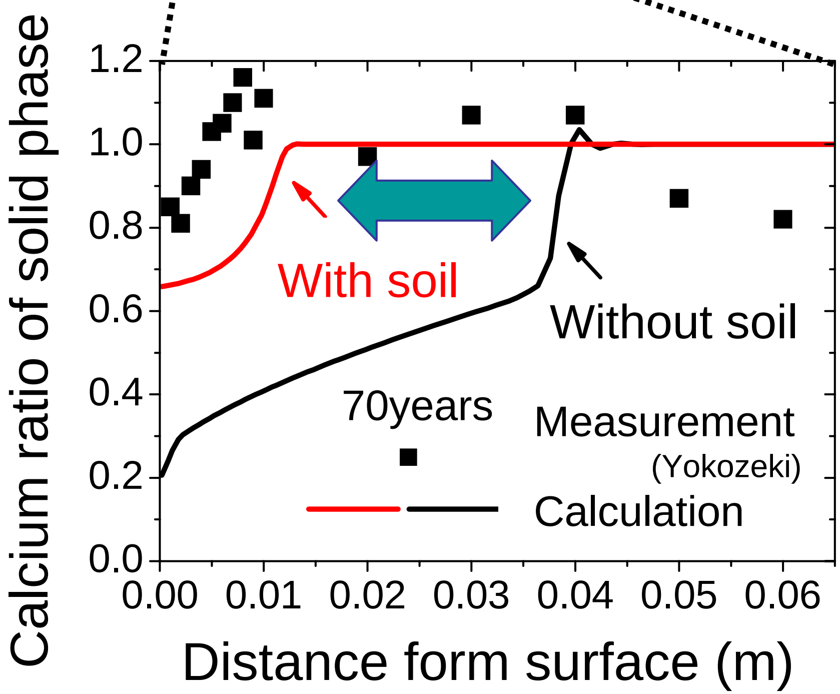
Constrictivity is defined as a function of pore size.



1. Leaching from concrete to soil foundation



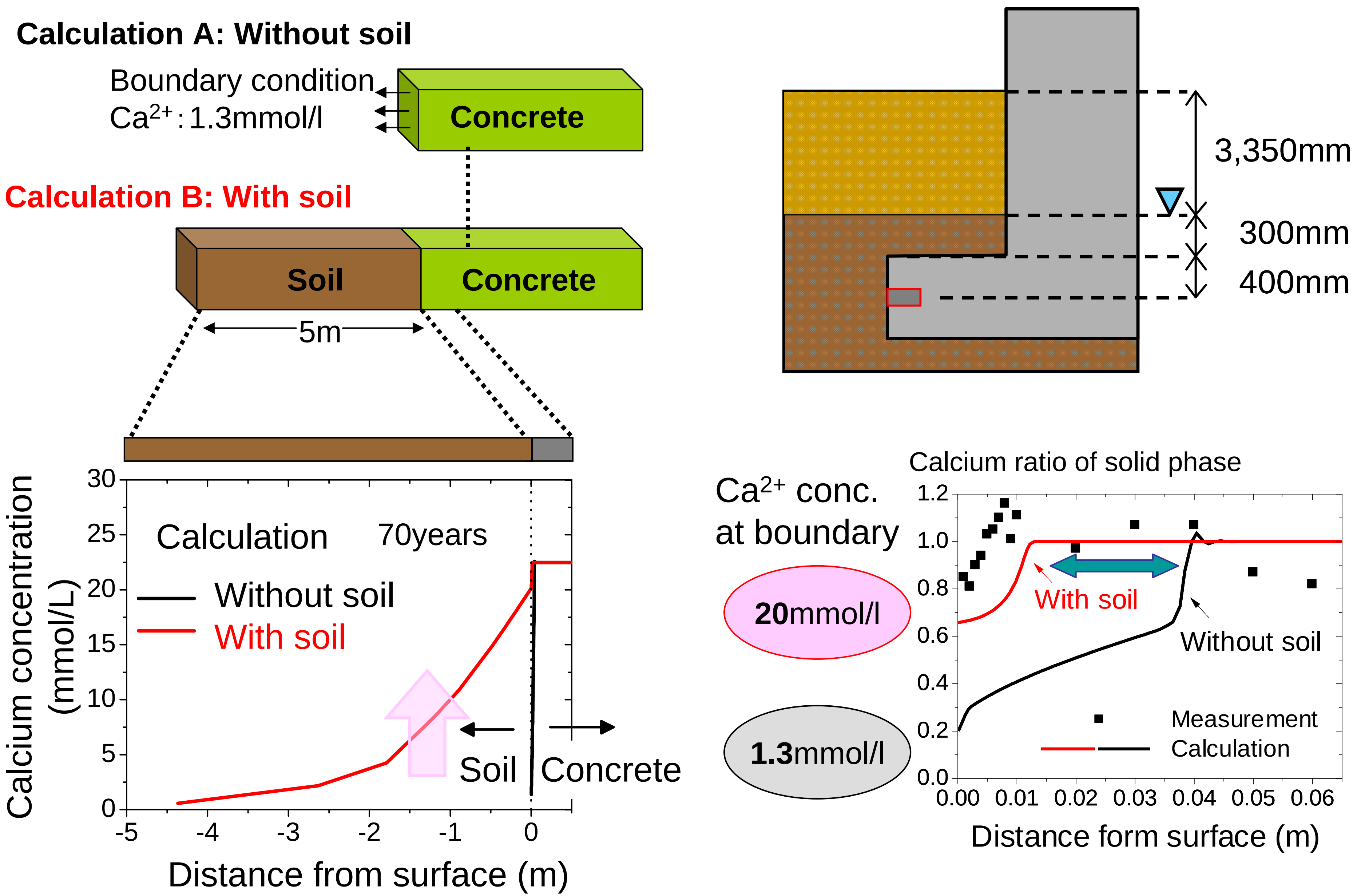




Footing

Concrete (W/C=55%)

70years after construction

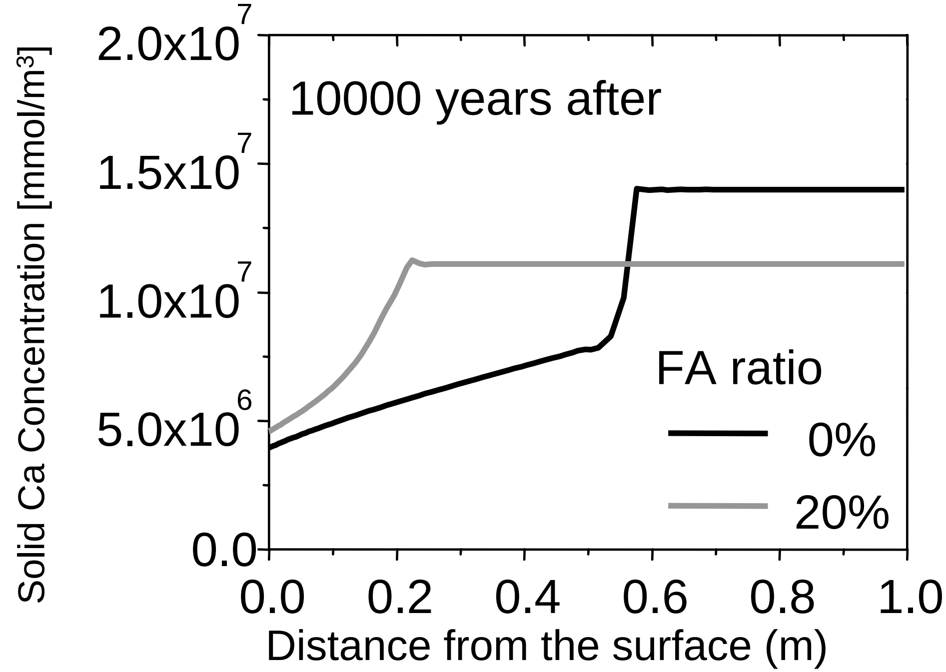


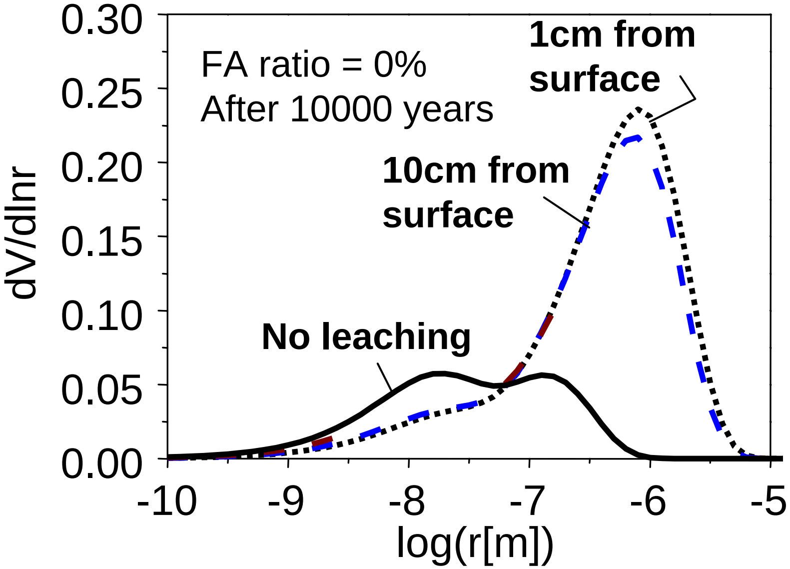
Calculation A: Without soil
Boundary condition
Ca2+ : 1.3mmol/l
Concrete
Calculation B: With soil
Soil
Concrete
5m
3,350mm
300mm
400mm
Calculation
70years
Without soil
With soil
Soil
Concrete
Calcium concentration (mmol/L)
Distance from surface (m)
Ca2+ conc. at boundary
20mmol/l
1.3mmol/l
Calcium ratio of solid phase
With soil
Without soil
Measurement
Calculation
Distance form surface (m)

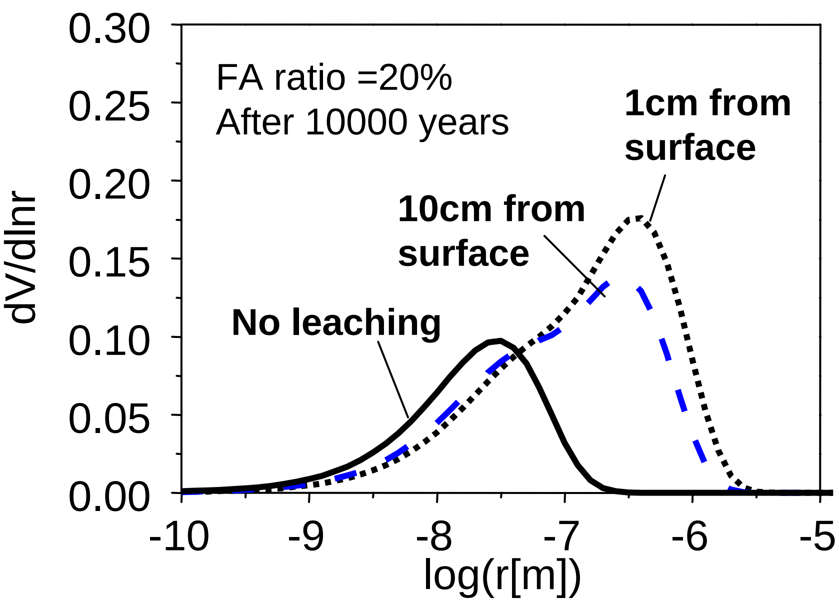
Boundary condition
Ca^{2+} : 2mmol/l

Concrete
(W/P=50%)

Fly ash (FA): 0%, 20%



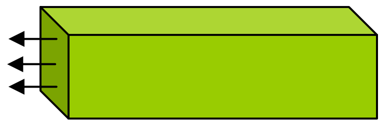




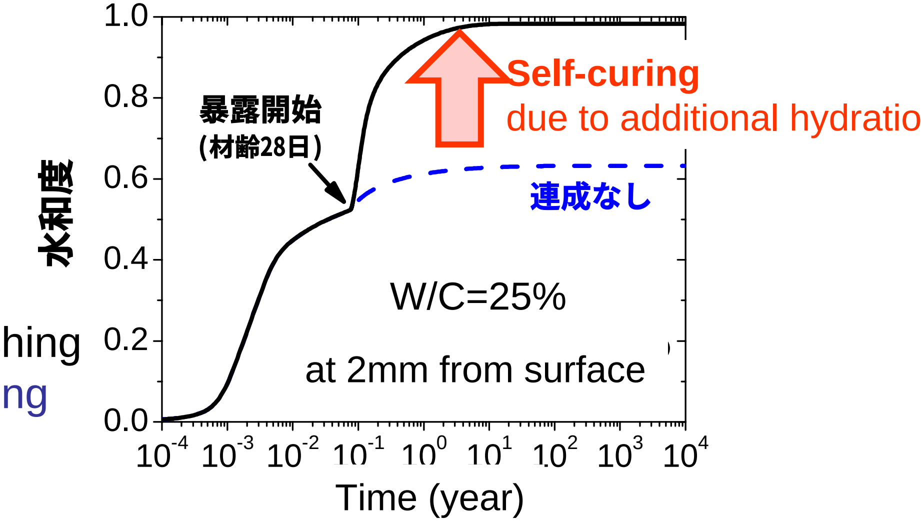
3. Influence of W/C on calcium leaching

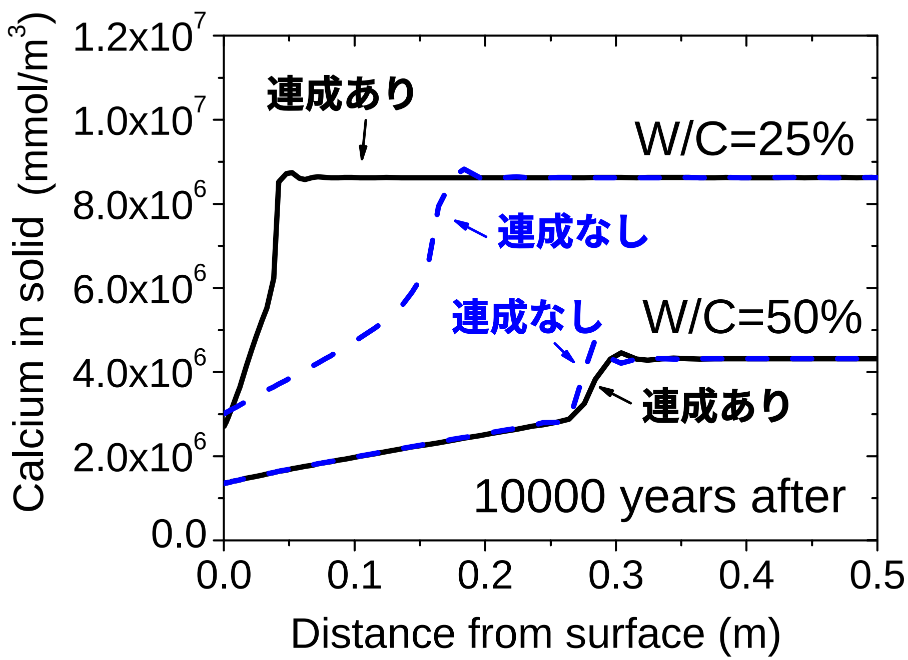
簡易解析（空隙モデルとの簡易連成）

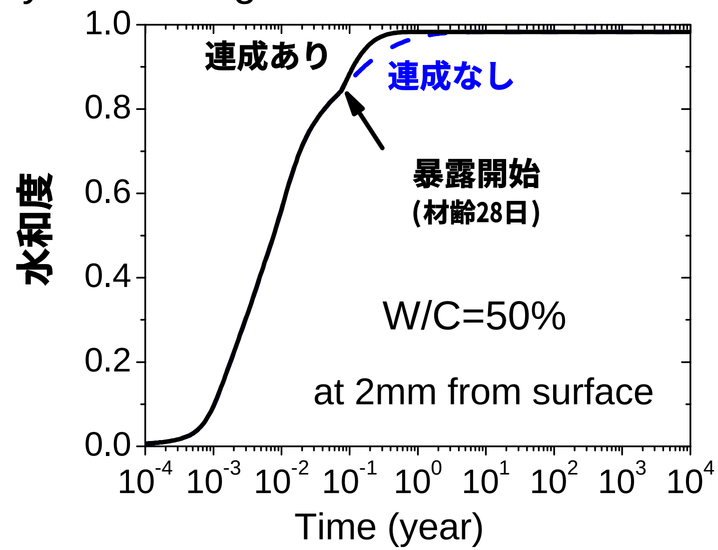
Boundary condition
Ca^{2+} : 2mmol/l



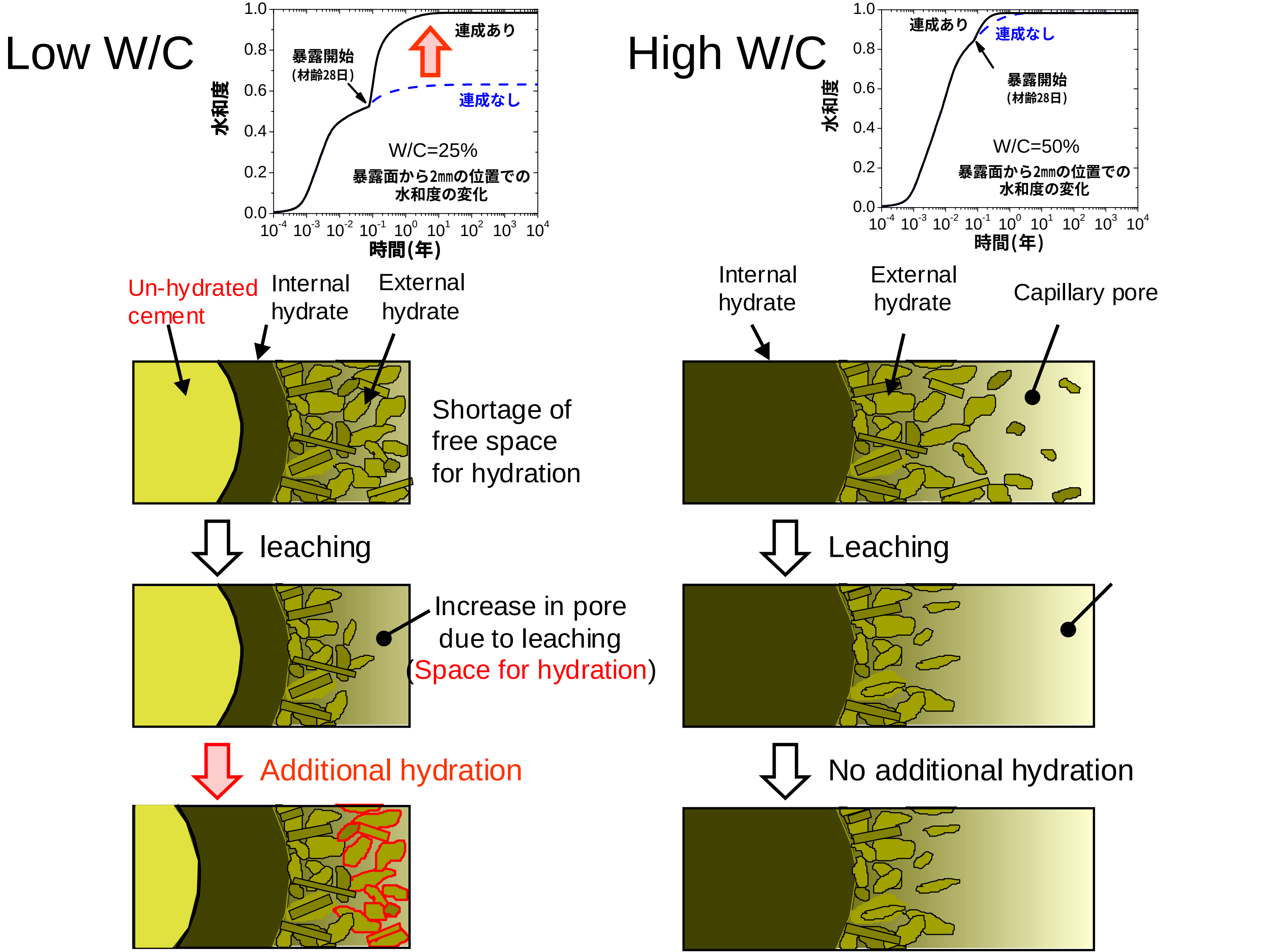
Black line: Consider additional hydration due to leaching
Blue line : Neglect additional hydration due to leaching







4. Self-curing function of low W/C concrete for leaching



Concluding Remarks

- A numerical simulation system that can assess structural behaviors under coupled environmental actions was proposed in this paper.

- In the system, generation and transfer of heat, moisture, gas and ions in micro-pore structures were formulated based on thermodynamics and electrochemistry.

- Coupling these materials modeling, an early age development process and deterioration phenomenon during the service period can be evaluated for arbitrary materials, curing and environmental conditions in a unified manner.

- Numerical verifications show that this method can roughly predict ingress of ion, carbonation and corrosion phenomena for different materials, curing and environmental conditions.