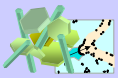
Lifespan simulation for materials and structures

Environmental Actions
Drying-wetting. Wind. Sunlight. ions/salts etc.

Scale 10^{-6}-10^{-9}[m]

Thermo-hygro system
State laws
Mass/energy balance

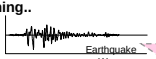


Output: Hydration degree, Microstructure, Distributions of Moisture /Salt /Oxygen /CO2, pH in pore water, corrosion rate etc.

10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} Time (Days)

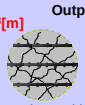
Unified evaluation

Hydration starts — **Heat. Initial defects** — **Corrosion, Carbonation, Leaching..**



Scale 10^{0}-10^{3}[m]

Output: Stress, Strain, Accelerations, Degree of damage, Plasticity, Crack density etc.



Macroscopic cracking

Mechanical Actions
Ground acceleration
Gravity
Temperature and shrinkage effects

Continuum Mechanics
Deformational compatibility
Momentum conservation

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

Hydration computation
Temperature, hydration level of each component

Microstructure computation
Bi-modal porosity distribution, interlayer porosity

Pore pressure computation
Pore pressure, RH and moisture distribution

Chloride transport and equilibrium
Concentrations of free & bound chlorides

CO_2 transport and equilibrium
Gas and dissolved CO2 concentration

Ion equilibrium model
Concentration of each ionic species pH in pore water

O_2 transport and equilibrium
Gas and dissolved O2 concentrations

Corrosion model
Corrosion rate amount of O2 consumption

Conservation laws satisfied ?
no — Next Iteration
yes — Increment time, continue

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

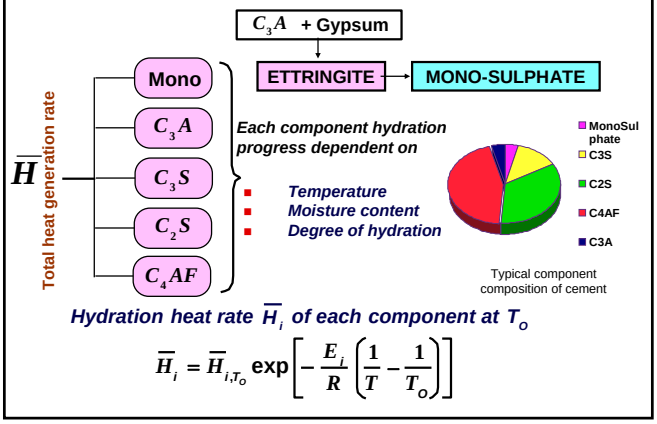
Moisture equilibrium and transport

Micro-pore struc. development

Vapor diffusivity
Liquid permeability
Condensed water
Adsorbed water on pore wall

Governed by mass balance law for moisture

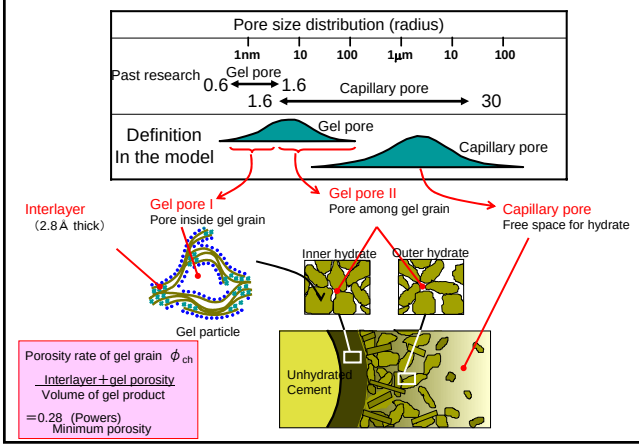
Multi-component cement hydration model



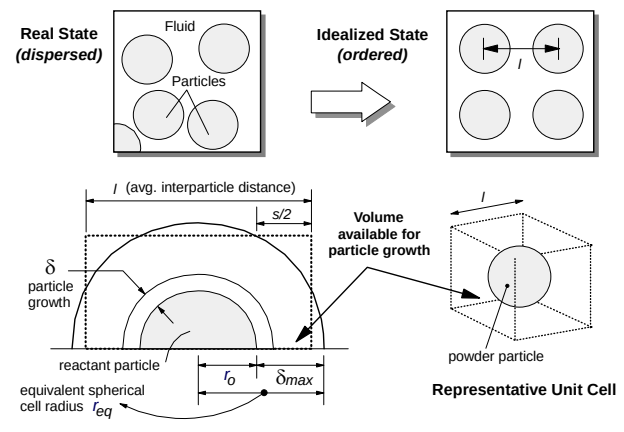
Hydration heat rate $\overline{H}_i$ of each component at T_o

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

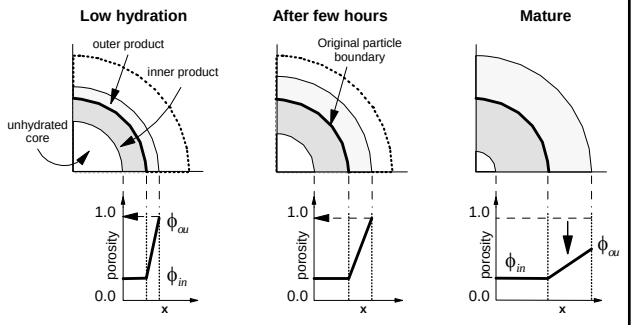
Classification and Definition of Pore Structure



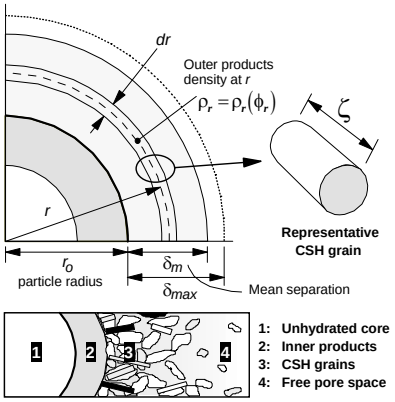
Initial State of Powder Particles



Bulk porosity function of outer product and cluster expansion



A reactant particle at arbitrary stage of hydration



1: Unhydrated core
2: Inner products
3: CSH grains
4: Free pore space

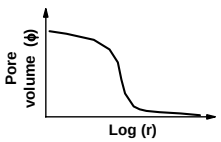
Capillary Surface Area =
Total *external* CSH grains SA

$$S_c = \int_{r_o}^{r_o+\delta_m} dS_c = \int \frac{4\pi r^2}{\zeta}\left(\frac{1-\phi_r}{1-\phi_{in}}\right)dr$$

Gel Surface Area =
Total *internal* CSH grains SA

$$S_g = Weight\ of\ CSH \times sp.\ SA\ of\ CSH$$

Relationship of pore structure parameter B and S/ϕ

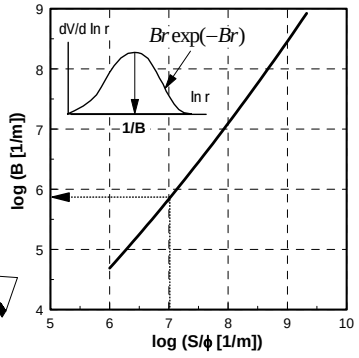


$$\phi(r) = \sum \phi_i \left(1 - \exp(-B_i r)\right)$$

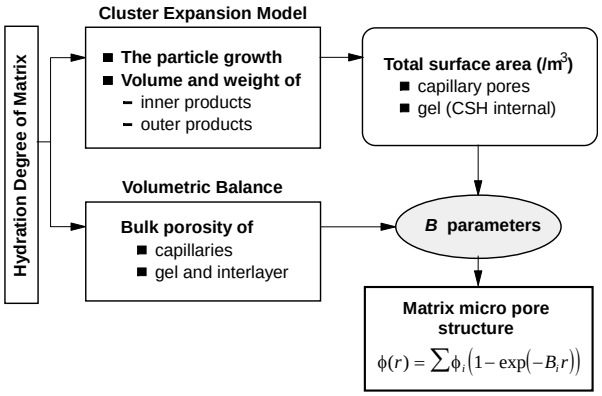
ϕ_i : porosity known
B_i : Pore structure parameter, to be obtained

Fundamental surface area, porosity relationship

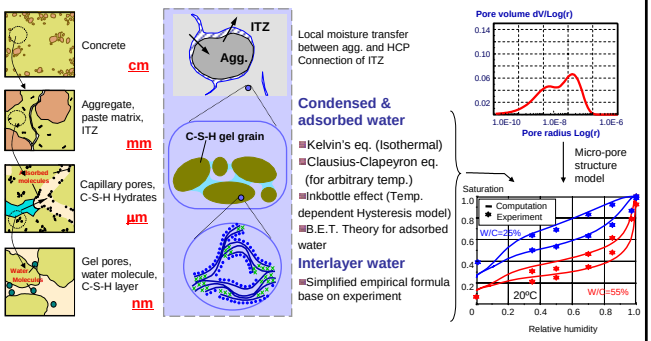
$$S = 2\int d\phi / r$$



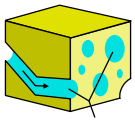
Schematic representation of the pore structure development computation



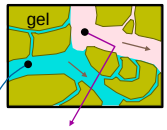
Multi-scale modeling of moisture state in cementitious materials

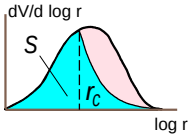


Moisture Conductivity of Concrete



micro-pores





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

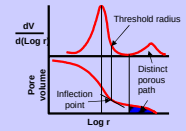
$$K_L = \frac{\phi^2 \rho_l}{50\,\eta}\left[\int_0^r r\,dV\right]^2$$

History dependent liquid viscosity

Total Conductivity K = Liquid Conductivity K_L + Vapor Conductivity K_v

Mass balance equation for vapor and liquid

Flux term



Moisture conductivity

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

Sink term

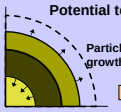
Moisture loss due to hydration

- *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

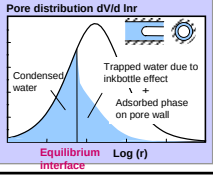


Pore-structure development model

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

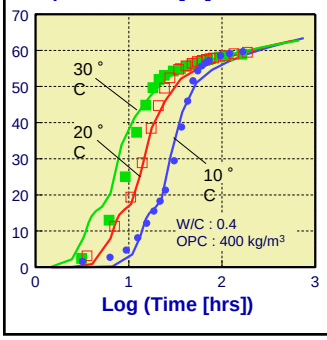
Pore distribution dV/d lnr



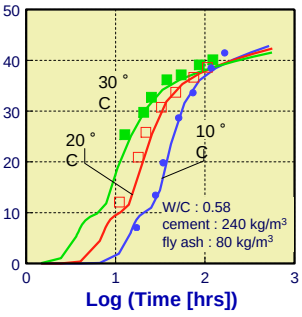
Influence of Casting Temperature

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

Temperature rise [˚C]

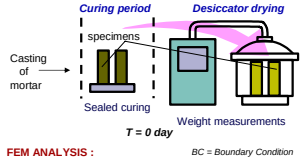


Temperature rise [°C]



Prediction of moisture loss behavior for early age under severe conditions

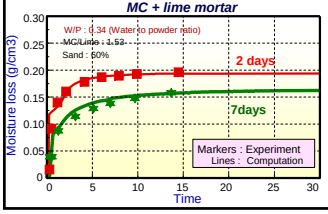
EXPERIMENTAL PROCEDURE :



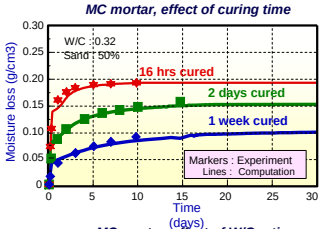
FEM ANALYSIS : *BC = Boundary Condition*

Input ; Mix proportions → Sealed BC, Hydration dominant → BC : 0.001 RH, Moisture transport dominant

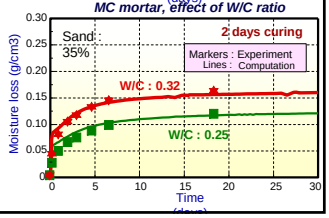
MC + lime mortar



MC mortar, effect of curing time



MC mortar, effect of W/C ratio



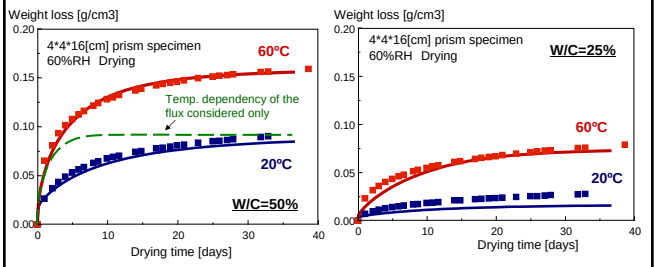
Moisture loss behaviors under different temperature

Time-dependent moisture isotherm model

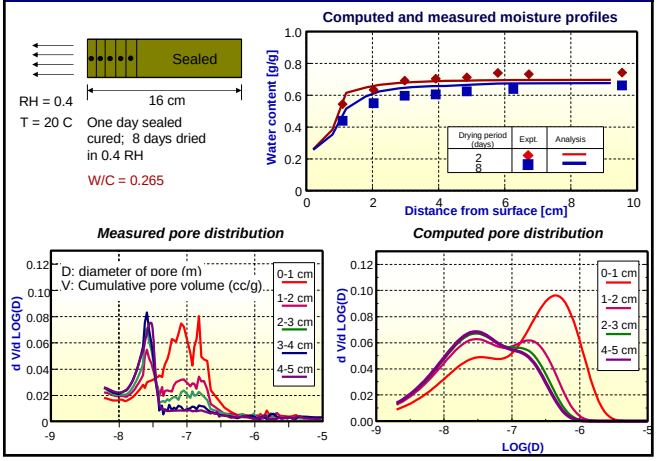
- Two phase equilbrium (Clausius-Clapeyron eq.)
- Temp. dependency of surface tension
- Time-dependency of inkbottle water
- Temp-dependency of interlayer water

Moisture flux under arbitrary pressure & temperature gradient

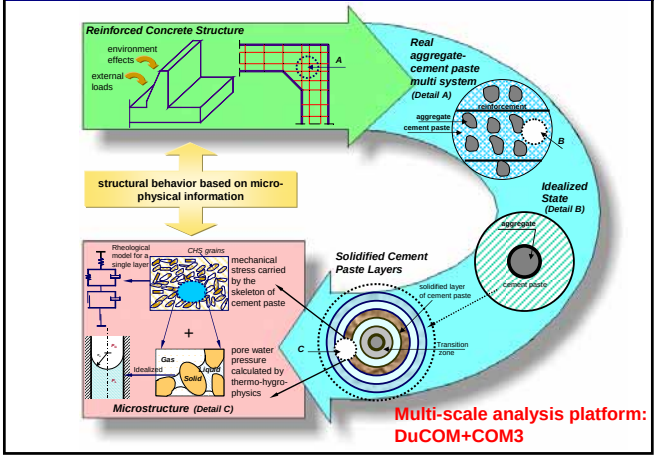
- Mass flux potential based on partial pressure of vapor
- Temp. dependency of vapor diffusivity
- Temp. dependency of liquid viscosity



Verification of the influence of early age drying on microstructure development

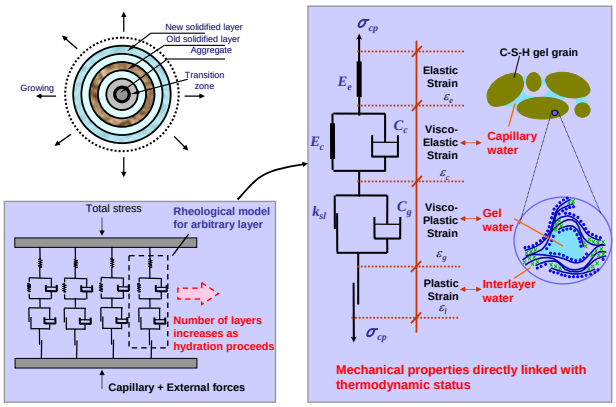


Macrostructure Microstructure Correlation



Solidification Model of Hardening Concrete Composite

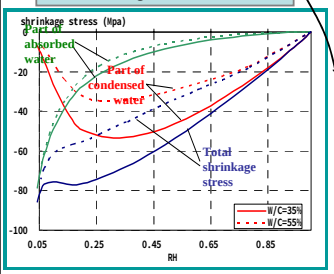
Proposed by Maekawa, Rasha, Zhu, and Ishida



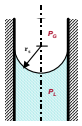
Constitutive Model of Concrete – Modeling of shrinkage stress, 1

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

Inherent driving forces in terms of RH



Theory of capillary tension



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

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

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

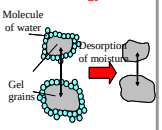
- Kelvin & Laplace equations
- Content of condensed water

Theory of surface energy

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

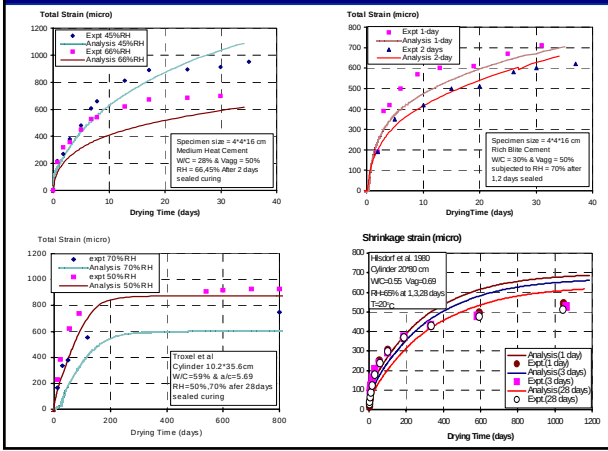
$$S_{sd} = f(h) S_{gel}$$

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



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

Verification (Drying shrinkage)



Verification (Creep)