SSCS 2012
Numerical Modeling
Strategies for Sustainable Concrete Structures

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AFGC

A multiphase concrete model with application to high temperature, structural repair, leaching and Alkali-Silica reaction

F. Pesavento, B.A. Schrefler, G. Sciumè

Dept. of Civil, Environmental and Architectural Engineering
University of Padova – ITALY

D. Gawin

Department of Building Physics and Building Materials
Technical University of Lodz – POLAND

Layout

- ☐ Introduction
- ☐ Mathematical model of concrete as multiphase porous material
- ☐ (Numerical model)
- ☐ Applications of the model and numerical examples
  - Modelling of concrete at early ages and beyond
  - Modelling of concrete leaching
  - Modelling of ASR in concrete structures
  - Concrete at high temperature
- ☐ (Simplification of the model and its application to concrete structures repair)
- ☐ Conclusions & final remarks

Theoretical Model

Fundamental hypotheses

- ☐ Concrete treated as a deformable, multiphase porous material
- ☐ Phase changes and chemical reactions (hydration, leaching, etc) are taken into account
- ☐ Full coupling:

  hygro-thermo-mechanical (stress – strain) ⇔ chemical reaction

  (cement hydration, leaching, ASR, etc)
- ☐ Transport mechanisms of moisture- and energy- typical for the specific phases of concrete are considered.
- ☐ Evolution in time (aging) of material properties, e.g. porosity, permeability, strength properties according to the hydration degree.
- ☐ Non-linearity of material properties due to temperature, gas pressure, moisture content and material degradation.

Theoretical Model

Transport Mechanisms

Capillary water (free water):

✓ advective flow *(water pressure gradient)*

Physically adsorbed water:

✓ diffusive flow *(water concentration gradient)*

Chemically bound water:

✓ no transport

Water vapour:

✓ advective flow *(gas pressure gradient)*

✓ diffusive flow *(water vapour concentration gradient)*

Dry air:

✓ advective flow *(gas pressure gradient)*

✓ diffusive flow *(dry air concentration gradient)*

Ions (Ca^{++}, Na^{+}):

✓ advective flow *(water pressure gradient)*

✓ diffusive flow *(calcium ions concentration gradient)*

✓ ~~electrical flow *(electrical potential gradient)*~~ ⇦ **E**=0

Theoretical Model

Chemical reactions & Phase Changes

- ✓ ***Dehydration:*** solid matrix + energy ⇒ bound water
- ✓ ***Hydration:*** chemically bound water ⇒ solid matrix + energy
- ✓ ***Evaporation:*** capillary water + energy ⇒ water vapour
- ✓ ***Condensation:*** water vapour ⇒ capillary water + energy
- ✓ ***Desorption:*** phys. adsorbed water + energy ⇒ water vapour
- ✓ ***Adsorption:*** water vapour ⇒ phys. adsorbed water + energy
- ✓ ***Leaching:*** calcium in solid skeleton ⇒ calcium in liquid solution
- ✓ ***ASR:*** silica+alkali+water ⇒ hydrophilic gel+absortpion

Theoretical Model

Micro- $\Rightarrow$ macro- description

Balance equations:

local formulation (micro- scale)

upscaling

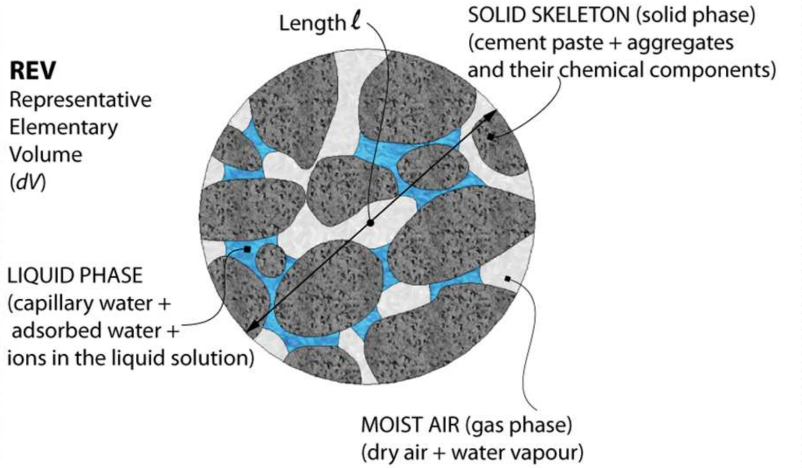
Volume Averaging Theory

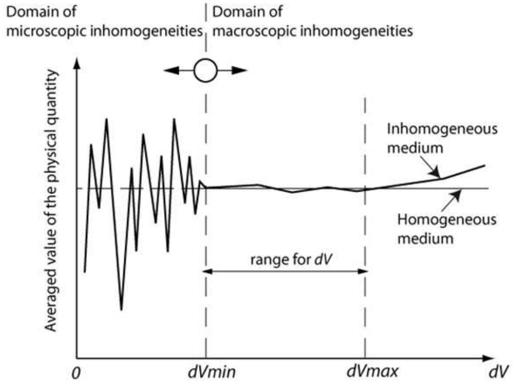
by Hassanizadeh & Gray, 1979,1980

macroscopic formulation

(macro- scale)

Rational Thermodynamics





Model development:

- ***Lewis & Schrefler, 1998;*** ***Schrefler, 2002;***
- ***Gray & Schrefler, 2007;*** ***Gray, Pesavento, Schrefler, 2009;***

Theoretical Model

Macroscopic balance equations & evolution equations

- ✓ The dry air and skeleton mass balance
- ✓ The water species and skeleton mass balance
- ✓ The multiphase medium enthalpy balance
- ✓ The calcium mass conservation equation
- ✓ ~~Electrical charge balance equatio~~ ⇐ Electrical field neglected
- ✓ The multiphase medium momentum balance (mechanical equilibrium)

- ✓ Evolution equation for hydration/dehydration
- ✓ Evolution equation for mechanical damage
- ✓ Evolution equation for thermo-chemical damage (leaching, etc.)
- ✓ Evolution equation for ASR process

Mathematical model

Macroscopic balance equations

Solid skeleton mass balance equation

$$\frac{(1-n)}{\rho^s}\frac{D^s\rho^s}{Dt}-\frac{D^s n}{Dt}+(1-n)\,div\,\mathbf{v}^s=\frac{\dot{m}_{hydr}}{\rho^s}-\frac{\dot{m}_{diss}}{\rho^s}$$

Dry air (and skeleton) mass balance equation

$$-n\frac{D^s S_w}{Dt}-\beta_s(1-n)S_g\frac{D^s T}{Dt}+S_g\,div\,\mathbf{v}^s+\frac{S_g n}{\rho^{ga}}\frac{D^s\rho^{ga}}{Dt}+\frac{1}{\rho^{ga}}div\,\mathbf{J}_g^{ga}+$$

$$\frac{1}{\rho^{ga}}div\left(nS_g\rho^{ga}\mathbf{v}^{gs}\right)=-\frac{\dot{m}_{dis}}{\rho^s}S_g$$

Mathematical model

Macroscopic balance equations

Water species (liquid+vapor) (and skeleton) mass balance equation

$$n\left(\rho^{w}-\rho^{gw}\right)\frac{D^{s}S_{w}}{Dt}+\left(\rho^{w}S_{w}+\rho^{gw}S_{g}\right)\alpha\,div\,\mathbf{v}^{s}-\beta_{swg}^{*}\frac{D^{s}T}{Dt}+S_{g}n\frac{D^{s}\rho^{gw}}{Dt}+div\,\mathbf{J}_{g}^{gw}+$$

$$div\left(nS_{w}\rho^{w}\mathbf{v}^{ls}\right)+div\left(nS_{g}\rho^{gw}\mathbf{v}^{gs}\right)-\left(\rho^{w}S_{w}+\rho^{gw}S_{g}\right)\frac{\left(1-n\right)}{\rho^{s}}\left[\frac{D^{s}\rho^{s}}{D\Gamma_{leach}}\frac{D^{s}\Gamma_{leach}}{Dt}\right]=$$

$$-\frac{\dot{m}_{diss}}{\rho^{s}}\left(\rho^{gw}S_{g}+\rho^{w}S_{w}\right)$$

Energy balance equation (for the whole system)

$$\left(\rho C_{p}\right)_{eff}\frac{\partial T}{\partial t}+\left(\rho_{w}C_{p}^{w}\mathbf{v}^{w}+\rho_{g}C_{p}^{g}\mathbf{v}^{g}\right)\cdot grad\,T-div\left(\chi_{eff}\,grad\,T\right)=-\dot{m}_{vap}\Delta H_{vap}+\dot{m}_{dis}\Delta H_{dis}$$

Mathematical model

Macroscopic balance equations

Calcium mass balance equation

$$(1-n)C_{Ca}S_w\frac{1}{\rho^s}\frac{D^s\rho^s}{D\Gamma_{leach}}\frac{D^s\Gamma_{leach}}{Dt}+nC_{Ca}\frac{D^sS_w}{Dt}+nS_w\frac{D^sC_{Ca}}{Dt}+\alpha C_{Ca}S_w\,div\,\mathbf{v}^s+\frac{1}{\rho^w}div\,\mathbf{J}_d^{Ca}+$$

$$\frac{1}{\rho^w}div\left(C_{Ca}nS_w\rho^w\mathbf{v}^{ls}\right)=\frac{\dot{m}_{dis}}{\rho^w}-\frac{\dot{m}_{dis}}{\rho^s}C_{Ca}S_w$$

Linear momentum balance equation (for the multiphase system)

$$div\left(\dot{\mathbf{t}}^{total}\right)+\dot{\rho}\mathbf{g}=0$$

Theoretical Model

State variables & **internal variables**

- ✓ Gas pressure – p^g
- ✓ Capillary pressure – p^c
- ✓ Temperature – T;
- ✓ Calcium concentration – c_{Ca}
- ✓ Displacement vector – $[u_x, u_y, u_z]$

- ✓ Hydration/Dehydration degree – Γ_{hydr}
- ✓ Mechanical damage degree – d
- ✓ Themo-chemical damage degree – V
- ✓ ASR reaction extent – Γ_{ASR}
- ✓ Leaching degree – Γ_{leach}

Theoretical fundamentals and model development:

- ➢ ***Gawin, Pesavento, Schrefler**, CMAME 2003, Mat.&Struct. 2004, Comp.&Conc. 2005*
- ➢***Gawin, Pesavento, Schrefler**, IJNME 2006 (part 1, part2)*
- ➢***Gawin, Pesavento, Schrefler**, IJSS 2008 (part 1, part2), CMAME 2009*
- ➢***Pesavento et al.** CMAME 2012*

Modelling of concrete at early ages and beyond

Creep in concrete

- ✓ Bazant, Wittmann (eds)- 1982
- ✓ Bazant et al. - 1972-2002
- ✓ Harmathy - 1969
- ✓ Bazant, Chern – 1978 - 1987
- ✓ Hansen - 1987
- ✓ Bazant, Prasannan - 1989
- ✓ De Schutter, Taerwe - 1997
- ✓ Sercombe, Hellmich, Ulm, Mang - 2000

Hydration of cement

- ✓ Jensen - 1995
- ✓ van Breugel - 1995
- ✓ De Schutter, Taerwe - 1995
- ✓ Singh et al. – 1995
- ✓ Ulm, Coussy -1996
- ✓ Bentz et al. – 1998, 1999
- ✓ Sha et al. - 1999

Chemo - hygrothermal interactions

Evolution of the hydration process

Evolution of the hydration degree Γ_{hydr}

[Gawin, Pesavento, Schrefler, IJNME 2006 part 1 and part 2]

$$\frac{d\Gamma_{hydr}}{dt} = \tilde{A}_{\Gamma}(\Gamma_{hydr})\boxed{\beta_{\varphi}(\Gamma_{hydr},\varphi)}\exp\left(-\frac{E_a}{RT}\right)$$

Effect of relative humidity

where

$$\Gamma_{hydr} = \frac{\chi}{\chi_{\infty}} = \frac{m_{hydr}}{m_{hydr\infty}}$$

$\tilde{A}_{\Gamma}(\Gamma_{hydr})$ - hydration degree-related, normalized affinity, χ - hydration extent,

E_a – hydration activation energy, R – universal gas constant, t – time.

$$\tilde{A}_{\Gamma}(\Gamma_{hydr}) = A_1\left(\frac{A_2}{\kappa_{\infty}} + \kappa_{\infty}\Gamma_{hydr}\right)(1-\Gamma_{hydr})\exp(-\bar{\eta}\Gamma_{hydr})$$

- from: *[Cervera, Olivier, Prato, 1999]*

Chemo- mechanical interactions

Strain components

In general, a total strain of maturing concrete, $\boldsymbol{\varepsilon}_{tot}$, can be split into the following components:

1. *free thermal strain*
2. *thermo-chemical strain*
3. *creep strain*
4. *mechanical strain (caused by mechanical load and shrinkage)*

Strain decomposition

$$\boxed{d\boldsymbol{\varepsilon}_{mech} = d\boldsymbol{\varepsilon}_{tot} - d\boldsymbol{\varepsilon}_{c} - d\boldsymbol{\varepsilon}_{th} - d\boldsymbol{\varepsilon}_{ch}}$$

Free thermal strain strain

$$d\boldsymbol{\varepsilon}_t = \beta_s \, dT \, \mathbf{I}$$

Shrinkage strain

$$d\boldsymbol{\varepsilon}_{sh} = -\frac{\alpha}{3K_T}\left(d\chi^{ws} p^c + \chi^{ws} dp^c \right)\mathbf{I}$$

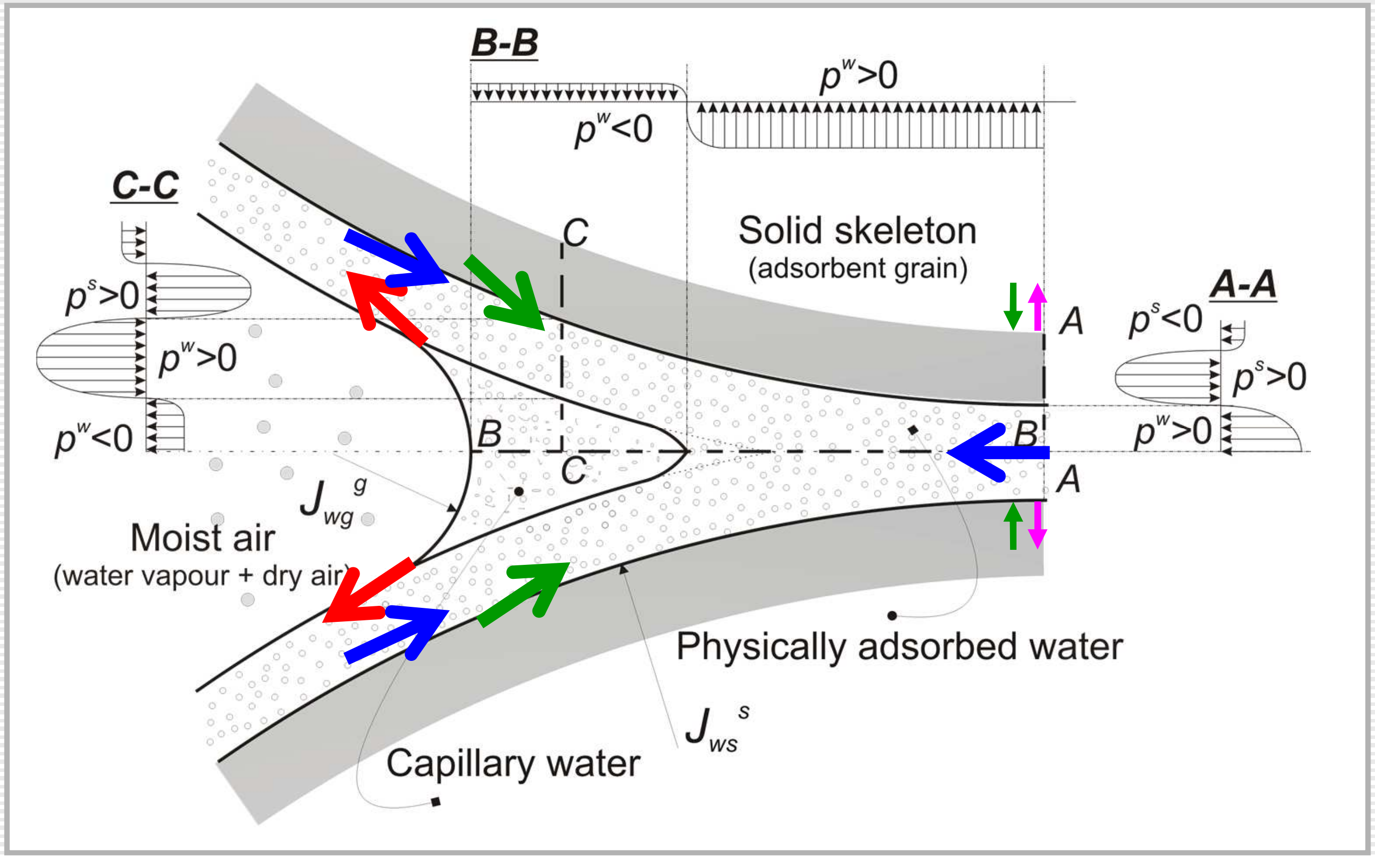
Thermo-chemical strain

$$d\boldsymbol{\varepsilon}_{ch} = \beta_{ch} \, d\Gamma_{hydr} \, \mathbf{I}$$

Hygro-mechanical interactions

Shrinkage of concrete

Capillary pressure & disjoining pressure



Forces:

in water

Capillary pressure

←

Disjoining pressure

←

in skeleton

Capillary pressure

←

Disjoining pressure

←

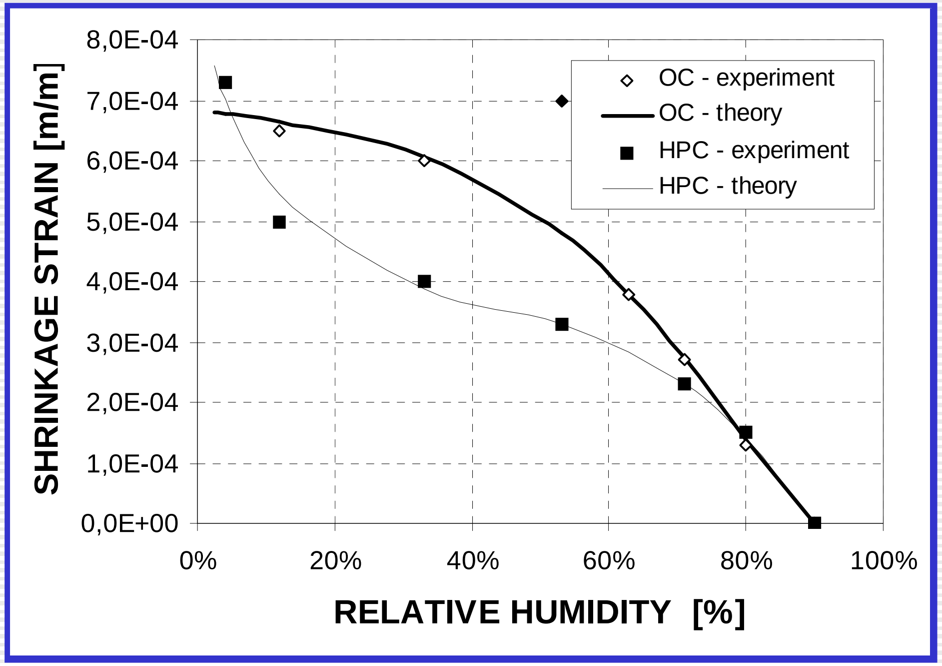
Hygro-mechanical interactions

Shrinkage of concrete

Effective stress principle:

$$\mathbf{t}^{ef} = \mathbf{t}^{tot} + \alpha P^s \mathbf{1}$$

$$p^s = \alpha P^s = p^g - \chi_s^{ws} p^c$$



- *[Gray & Schrefler, 2001]*
- *[Gray & Schrefler 2006]*
- *[Gray, Pesavento, Schrefler 2009]*

where x_s^{ws} is the solid surface fraction in contact with the wetting film,

$\mathbf{I}$ - unit, second order tensor, α - Biot's coefficient,

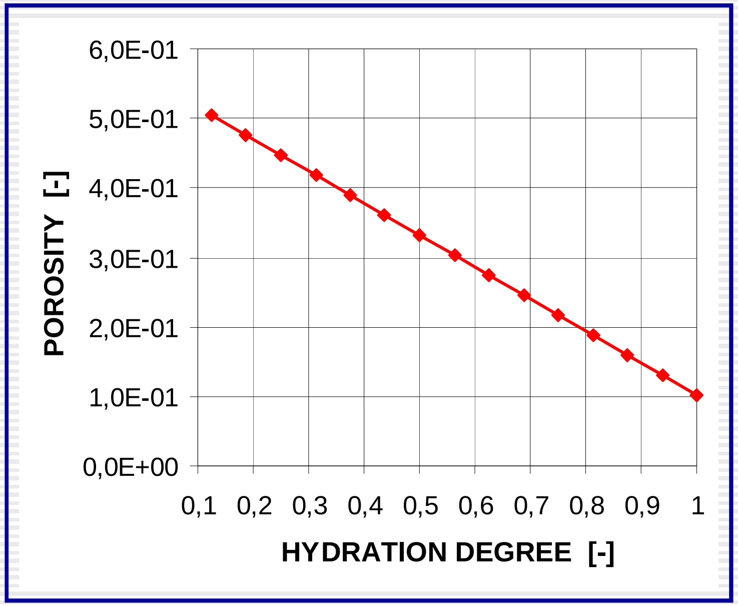
p^s - pressure in the solid phase and p^c is given by $p^c = \Pi^f - s^{wg} J_{wg}^w$

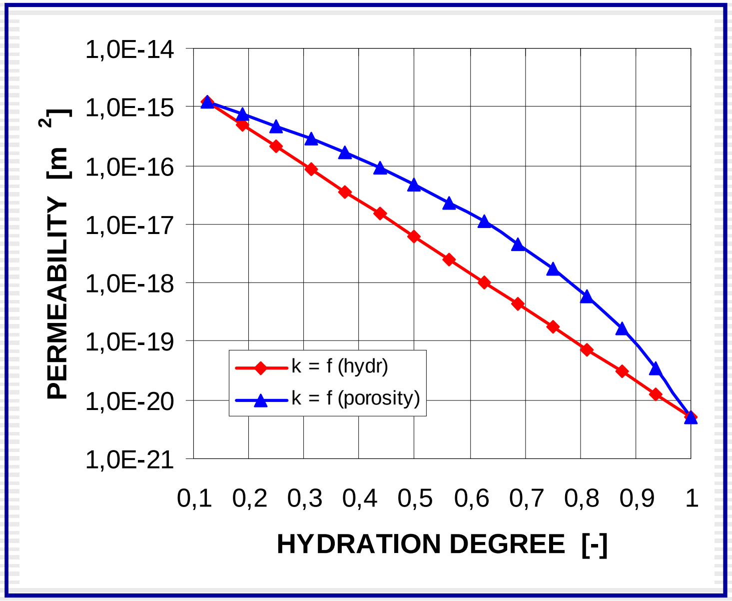
with Π^f - disjoining pressure

Hygro-structural - chemical interactions

Evolution of the material properties

Evolution of concrete porosity & permeability:





$$n\boxed{\left(\Gamma_{hydr}\right)} = n_\infty + A_n\left(\Gamma_{hydr} - 1\right)$$

$$k\boxed{\left(n\right)} = k_\infty \cdot 10^{A_{kn}\left(n - n_\infty\right)}$$

$$k\boxed{\left(\Gamma_{hydr}\right)} = k_\infty \cdot 10^{A_{k\Gamma}\Gamma_{hydr}}$$

[Halamickova, Detwiler, Bentz, Garboczi, 1995]

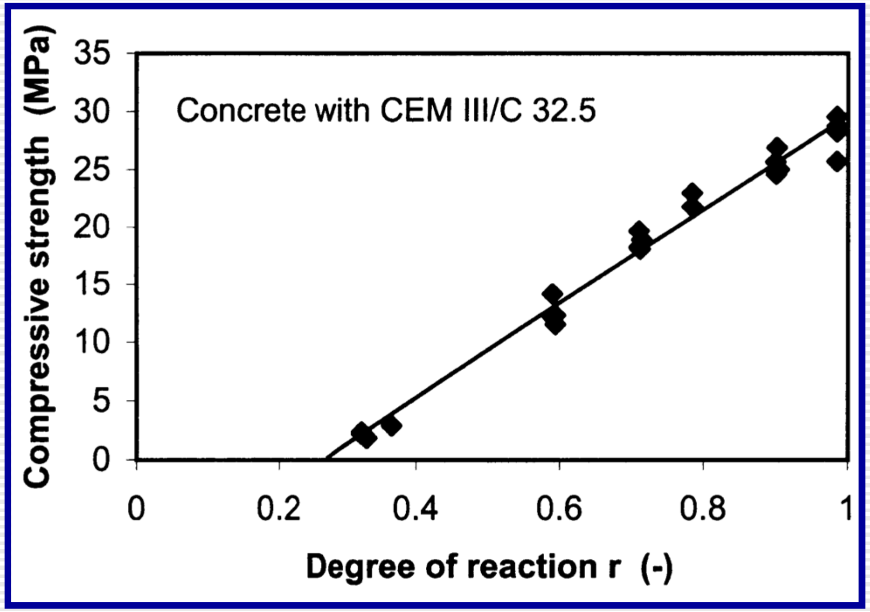
[Halamickova et al., 1995, Kaviany, 1999]

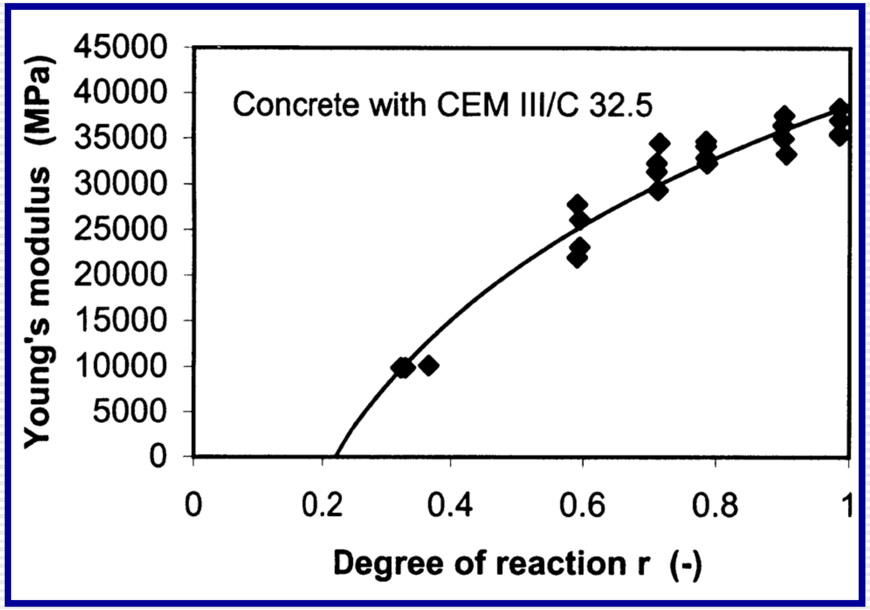
Hygro-structural - chemical interactions

Evolution of the material properties

Evolution of concrete strength properties:

[De Schutter, 2002]





Mathematical model

Constitutive law for creep strain

Solidification theory for basic creep

$$\boxed{\begin{aligned} d\boldsymbol{\sigma}_e^s &= \mathbf{D}\left(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}_c - d\boldsymbol{\varepsilon}_{th} - d\boldsymbol{\varepsilon}_{ch}\right) \\ &+ d\mathbf{D}\left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_{th} - \boldsymbol{\varepsilon}_{ch}\right) \end{aligned}}$$

$$\boxed{d\boldsymbol{\varepsilon}_c = d\boldsymbol{\varepsilon}_v + d\boldsymbol{\varepsilon}_f}$$

where

Hydration degree

$$\boxed{\dot{\varepsilon}_v(t) = \frac{\dot{\gamma}(t)}{\boxed{\Gamma_{hydr}(t)}}}$$

$$\boxed{\dot{\varepsilon}_f(t) = \frac{\boxed{\sigma_e^s(t)}}{\eta(t)}}$$

Effective stress

$\dot{\varepsilon}_c$ - creep strains (as sum of viscoelastic and viscous (flow) term);

$\dot{\varepsilon}_v$ - viscoelastic term;

$\dot{\varepsilon}_f$ - flow term;

γ - viscoelastic microstrain;

η - apparent macroscopic viscosity

Details:

➢ *[Bazant Z.P. Prasannan S.,Solidification theory for concrete creep I: formulation, J. Eng. Mech., **115**(8), 1989]*

Numerical example

Autogenous shrinkage in High Performance Cement Paste (Lura, Jensen, van Breugel test)

- ✓ Cubic specimen – 50x50x200 mm;

- ✓ Initial conditions:

  T_o= 293.15 K, φ_o= 99.0% RH, Γ_{hydr}=0.1;

- ✓ Boundary conditions:

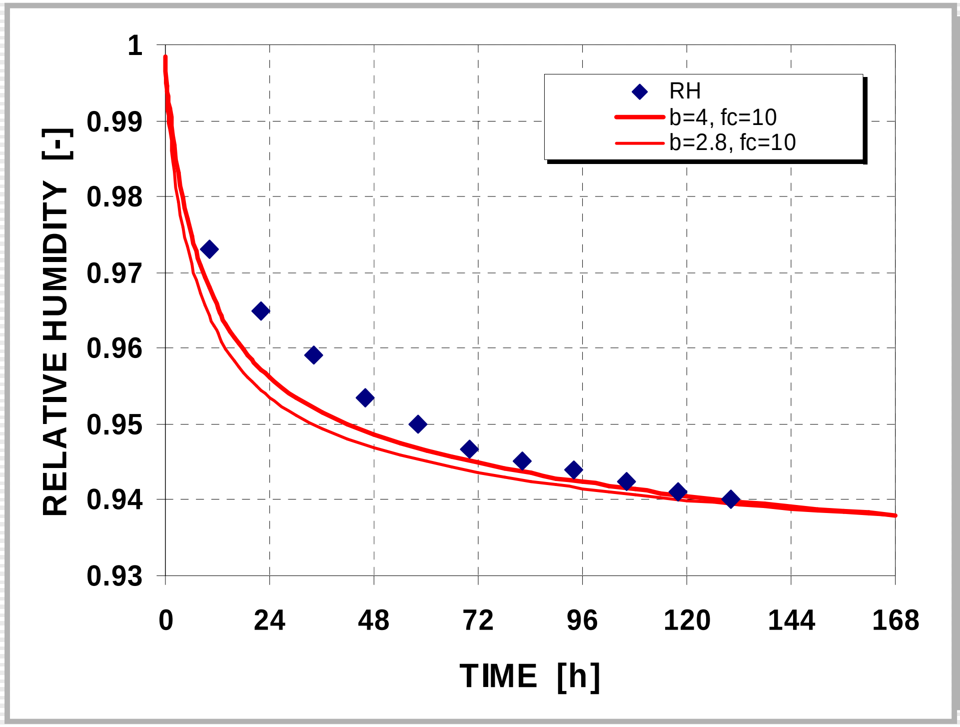
  - convective heat and mass exchange: sealed (adiabatic)
  - surface mechanical load: unloaded

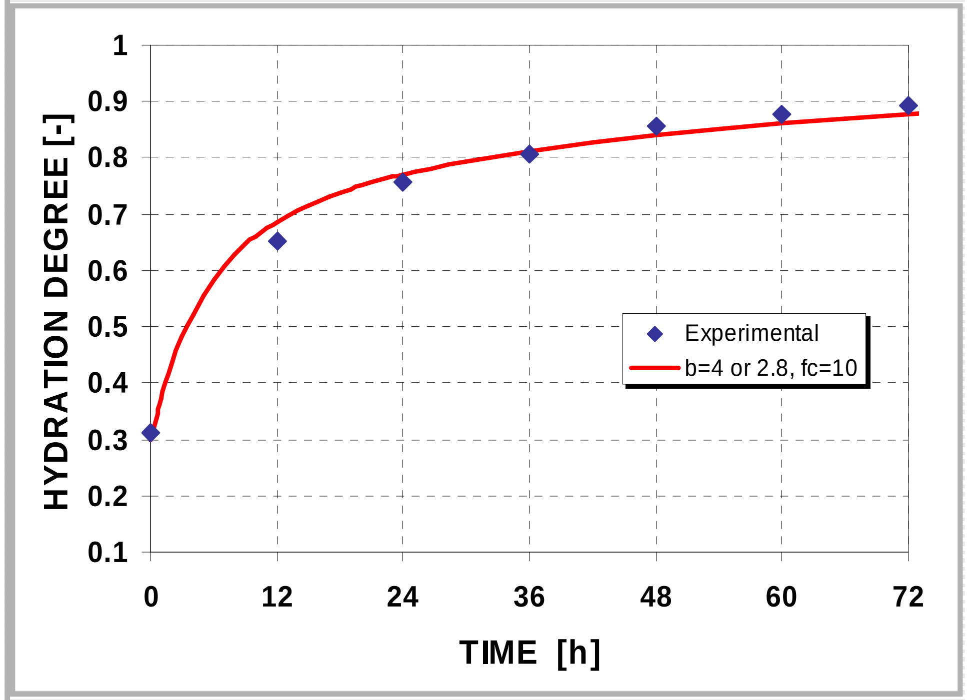
- ✓ Properties of the cement paste:

  - Elastic modulus measured prior the test (1, 3 and 7 days), curing temperature 20°C

Numerical example

Autogenous shrinkage in High Performance Cement Paste (Lura, Jensen, van Breugel test)



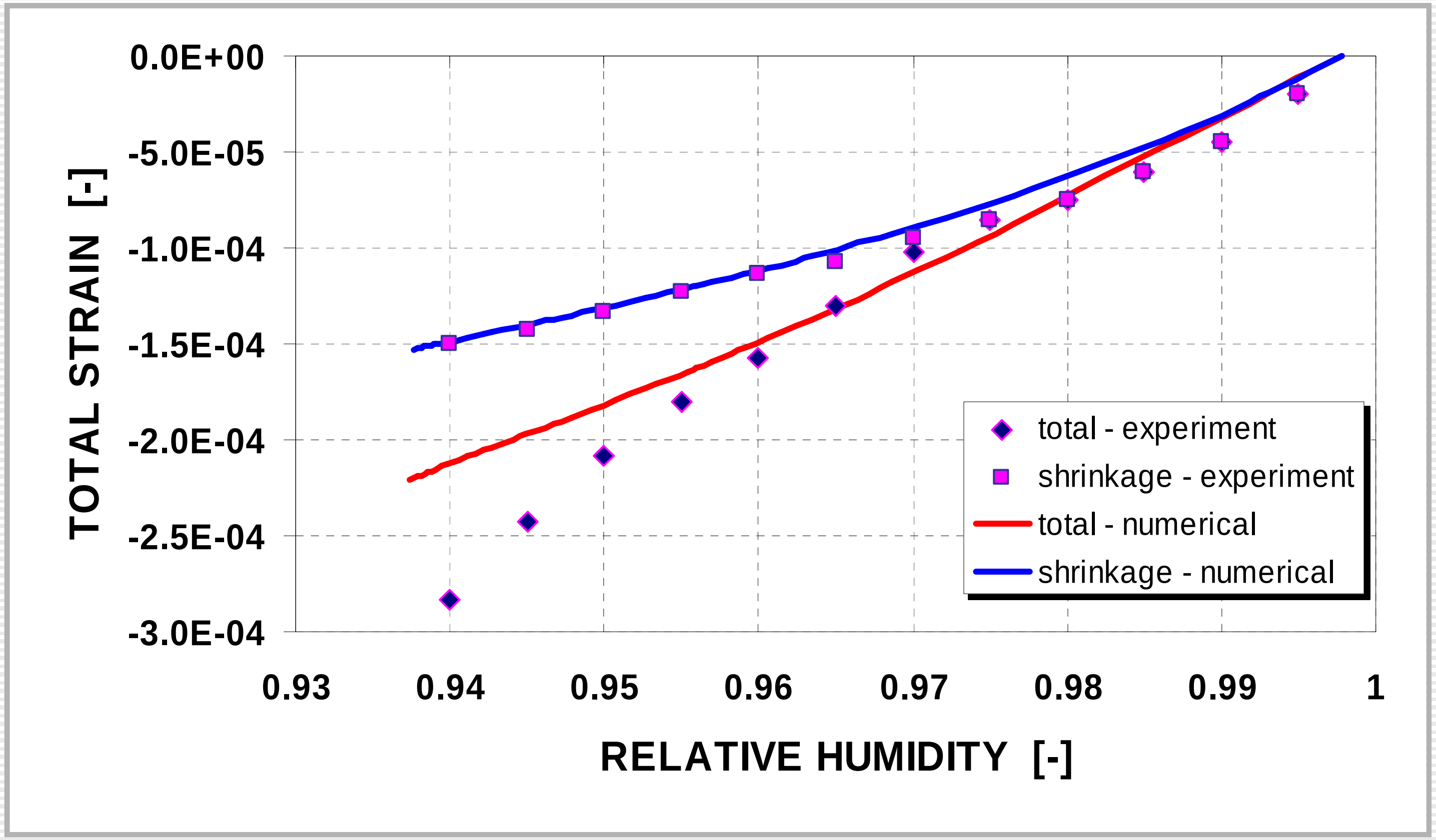


R.H. development in time

Hydr. Degree development in time

Numerical example

Autogenous shrinkage in High Performance Cement Paste (Lura, Jensen, van Breugel test)



Effect of shrinkage – creep coupling

Numerical example

Tests of Bryant and Vadhanavikkit (1987)

- ✓ **Slab** – thickness=30 cm; concrete: C50
- ✓ Material: concrete C50
    - ☐ - final porosity: 0.122, density: $\rho = 1900\ kg/m^3$,
    - ☐ - intrinsic permeability: $ko = 5 \cdot 10^{-19}\ m^2$,
    - ☐ - Young modulus: E= 49.2 GPa,
    - ☐ - water/cement ratio w/c=0.45.
- ✓ Initial conditions:

$T_o = 293.15\ K$, $\varphi_o = 99.8\%$ RH, $\Gamma_{hydr} = 0.3$;

- ✓ Boundary conditions:

Shrinkage *(from day 7)*

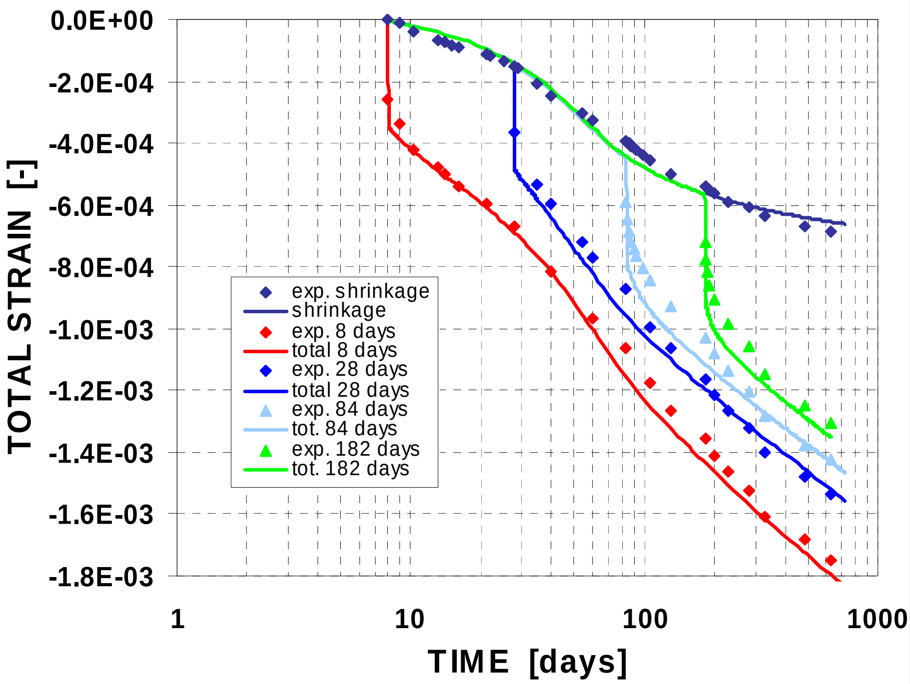
- convective heat and mass exchange: $\alpha_c = 5 W/m^2K$; $T_{amb} = 293.15K$; $\beta_c = 0.002 m/s$; $RH_{amb} = 60\%$
- surface mechanical load: unloaded or load=7 MPa at 8,28,84,182 days

Sealed *(for the first 7 days and basic creep)*

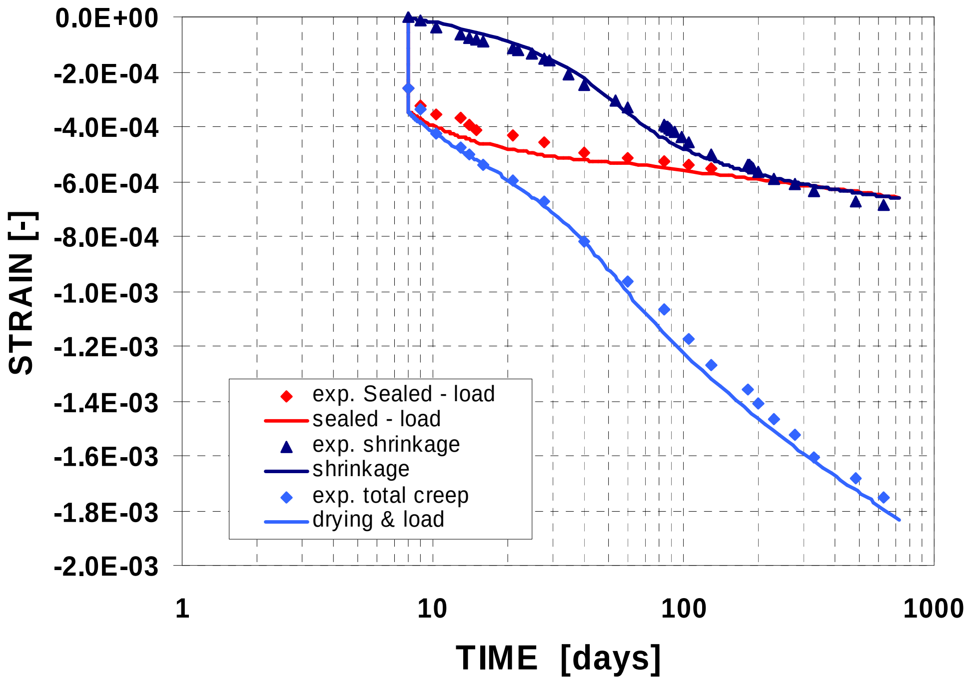
- convective heat and mass exchange: $\alpha_c = 5 W/m^2K$; sealed
- surface mechanical load: unloaded or load=7 MPa at 8,28,84,182 days

Numerical example

Tests of Bryant and Vadhanavikkit (1987)

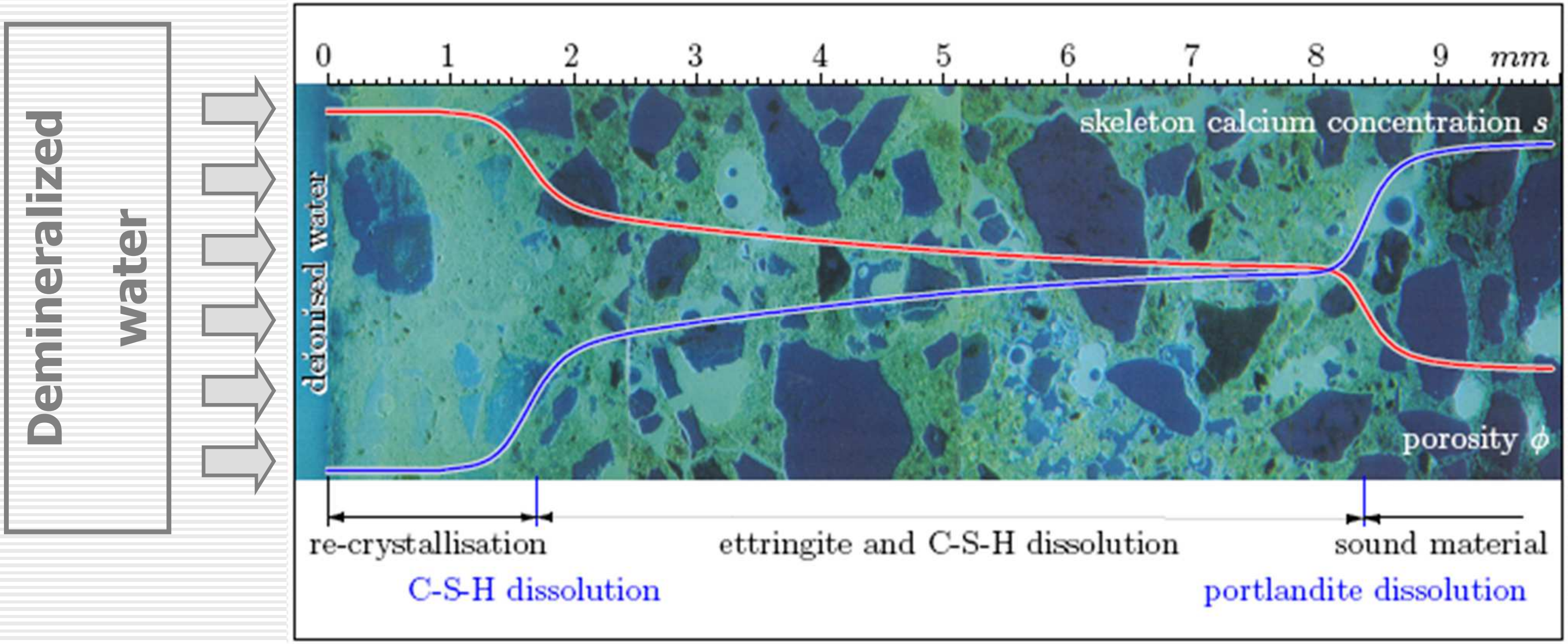


Drying & Load



Pickett's effect (8 days)

Modelling of concrete leaching



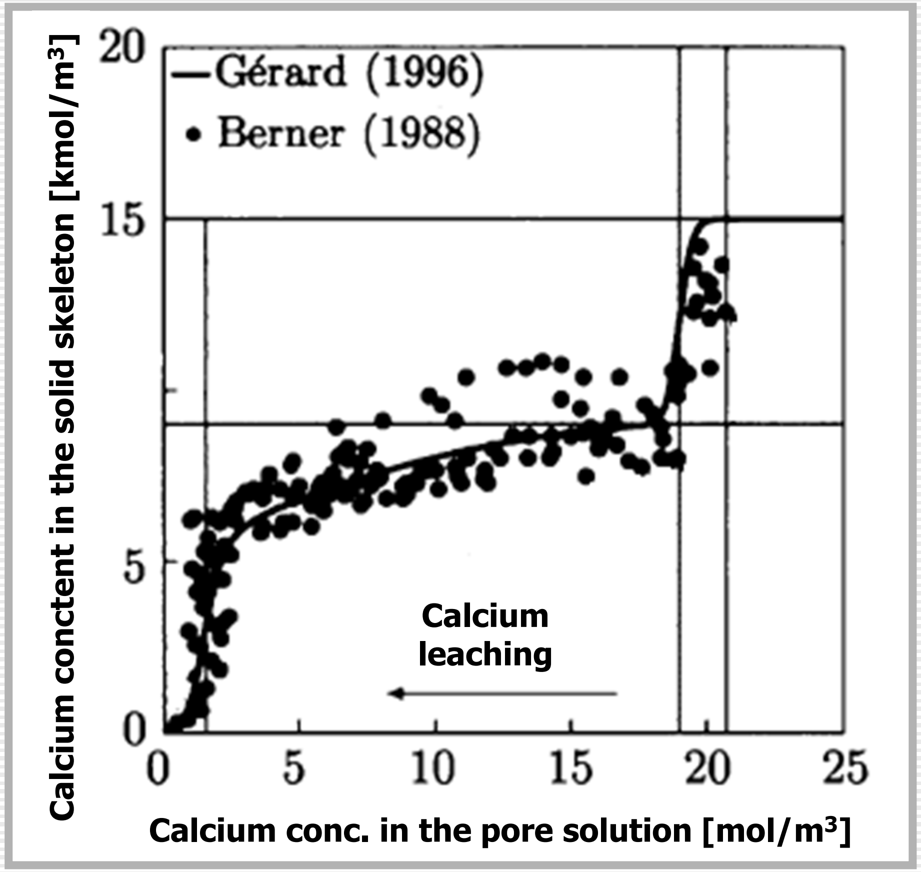
Picture of a leached cement paste sample, obtained by means of microscopic analysis in a fluorescent light.

Equilibrium based models: Gérard (1996), Kuhl et al. (2004), Kuhl and Meschke (2007)

Process kinetics based models:
Ulm, Torrenti, Adenot – *J. Engineering. Mechanics,* 1999
Gawin, Pesavento, Schrefler - Part 1 & Part 2 , *Solids and Structures,* 2008
Gawin, Pesavento, Schrefler, CMAME 2009.

Concrete leaching process kinetics

Curve describing equilibrium between solid and liquid calcium



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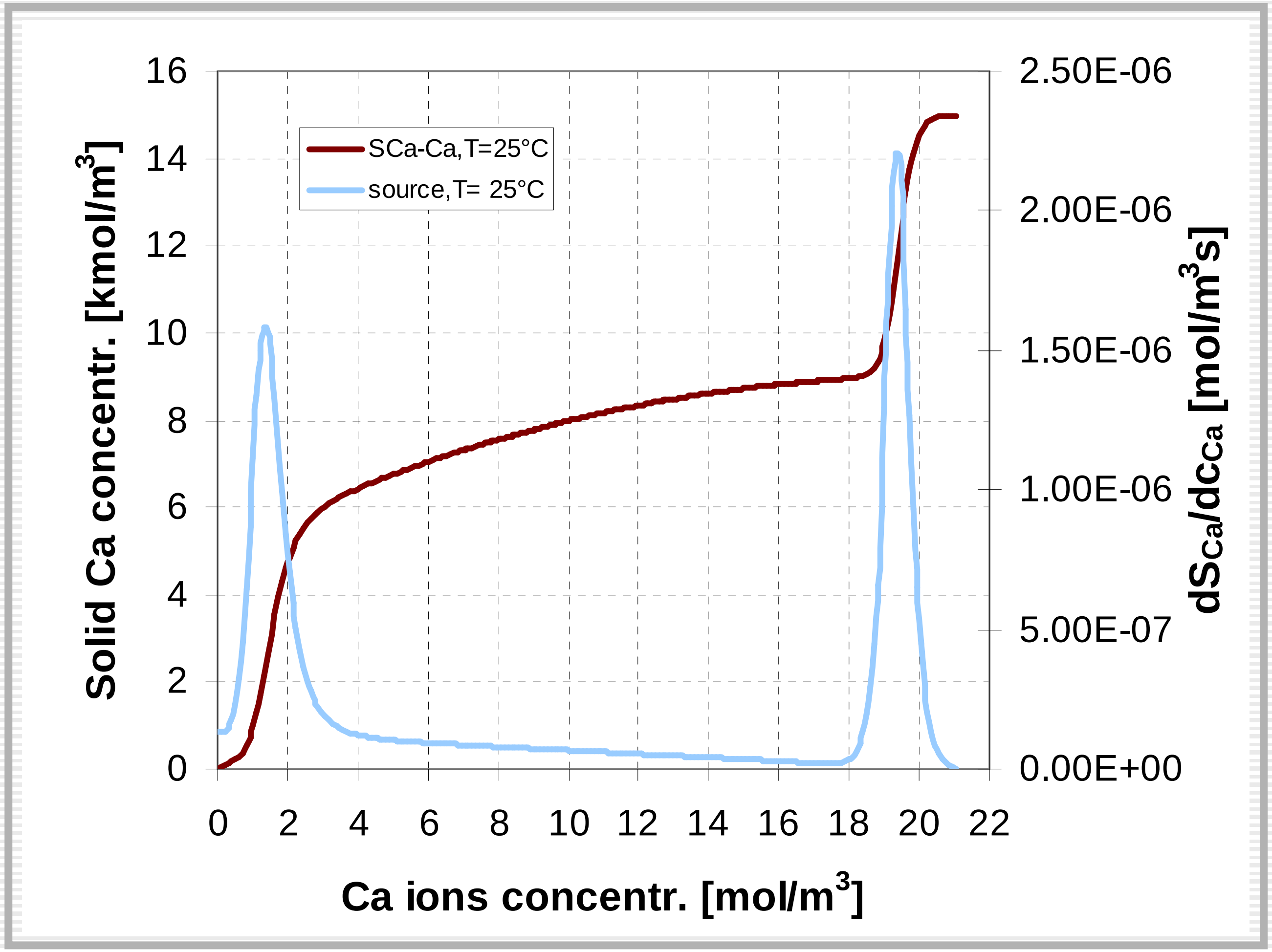

Kinetics of leaching process

Thermodynamic description of the process

[Ulm, Torrenti, Adenot – J. Engng. Mech. 1999]

$$A_s = \mu^s - \Gamma = \eta \frac{ds_{Ca}}{dt}$$

η- parameter dependent on micro-diffusion of Ca^{2+},

μ^s – chemical potential of liquid calcium,

Γ – chemical potential of solid calcium.

$$dA_s = RT\frac{dc_{Ca}}{c_{Ca}} - \mathbf{B} : \left(d\boldsymbol{\varepsilon} - d\boldsymbol{\varepsilon}^p \right) + kd\chi - \kappa ds_{Ca}$$

Effect of *Ca* concentration

Effect of the material elastic properties

Effect of micro-cracking

Effect of *Ca* content in skeleton

Kinetics of leaching process

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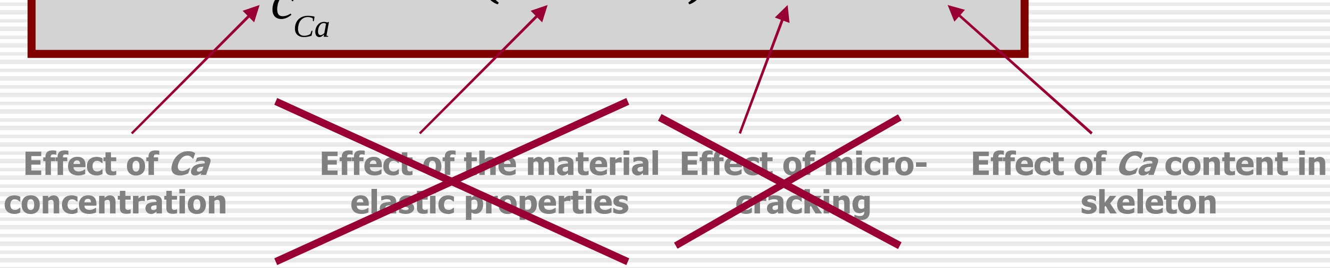

Effect of *Ca* concentration

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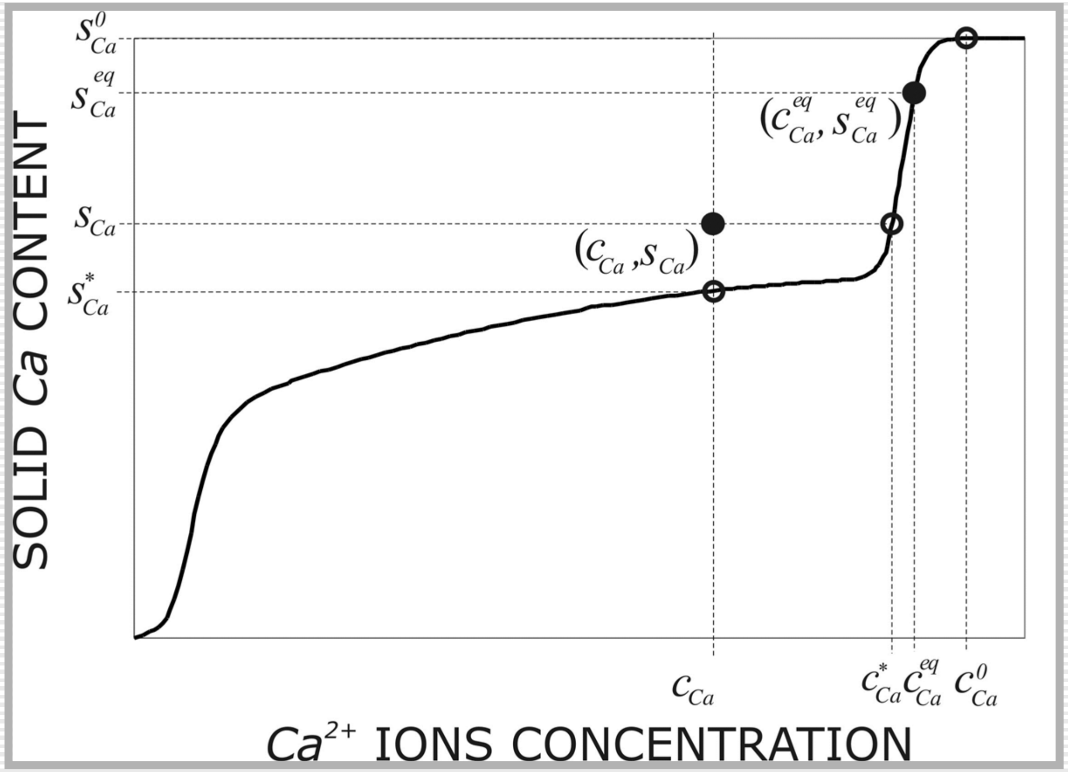
Effect of *Ca* content in skeleton

Kinetics of leaching process

Thermodynamic description of the process



$$\boxed{\frac{\partial s_{Ca}}{\partial t} = \frac{1}{\eta}\left[\int_{s^0_{Ca}}^{s^*_{Ca}} \kappa\left(\bar{s}, T\right) d\bar{s} - \int_{s^0_{Ca}}^{s_{Ca}} \kappa\left(\bar{s}, T\right) d\bar{s}\right]}$$

R – universal constant of gas,

κ – process equilibrium constant,

η - parameter dependent on micro-diffusion of Ca^{2+}

$$\boxed{\tau_s = \frac{\eta}{RT}}$$

Characteristic time of the process

Kinetics of leaching process

Extension to the non-isothermal conditions

The values of the *equilibrium constant*

$$\boxed{\kappa\left(s_{Ca},T\right)}$$

can be found from the thermodynamic equilibrium condition at temperature *T*, which can be written in the incremental form as

$$dA_s = RT\frac{dc_{Ca}}{c_{Ca}} - \kappa ds_{Ca} = 0$$

in this way we get

$$\kappa\left(s_{Ca},T\right) = \frac{RT}{c_{Ca}}\left(\left.\frac{ds_{Ca}}{dc_{Ca}}\right|_T\right)^{-1}$$

and taking into account the expression

$$c_{Ca}^{ef}\left(T\right) = c_{Ca} \times \exp\left[-\frac{E_{leach}}{R}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right]$$

one can write

$$\boxed{\kappa\left(s_{Ca},T\right) = \kappa\left(s_{Ca},T_{ref}\right)\frac{T}{T_{ref}}}$$

This allows writing the general relationship describing the thermodynamic of the process as:

$$\boxed{\frac{\partial s_{Ca}}{\partial t} = \frac{1}{\tau_{leach}\left(T\right)}\frac{1}{RT_{ref}}\left[\int_{s_{Ca}^0}^{s_{Ca}^*}\kappa\left(\bar{s},T_{ref}\right)d\bar{s} - \int_{s_{Ca}^0}^{s_{Ca}}\kappa\left(\bar{s},T_{ref}\right)d\bar{s}\right]}$$

i.e. the dependence on the temperature is concentrated in the function $\boxed{\tau_{leach}\left(T\right)}$

Chemo - hygral interactions

Evolution of the material properties

Evolution of a material porosity & permeability:

[Kuhl et al. - 2004]

$$n = n_0 + \Delta n_{ch}\left(\Gamma_{leach}\right),$$

$$\Delta n_{ch} = \frac{M_{diss}}{\rho^{diss}} s^0_{Ca} \cdot \Gamma_{leach}$$

[Saito and Deguchi - 2000]

$$k^* = B \cdot 10^{A_n n^*}$$

$$k = k\left(n_0\right) \cdot 10^{A_\Gamma \Gamma_{leach}}$$

Effect of mechanical and chemical damage

[Gawin et al. - 2009, CMAME accepted]

$$k = k\left(n_0\right) \cdot 10^{A_n \Delta n^*_{ch}}$$

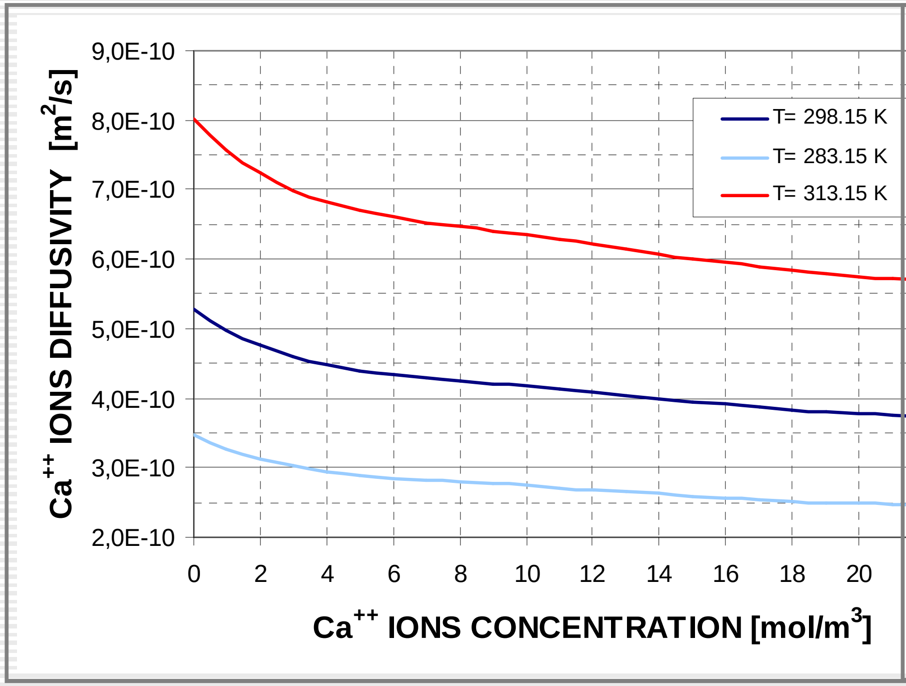
with

$$A_\Gamma = A_n \frac{\Delta n_{ch}}{\bar{V}_{paste}} = \frac{A_n}{\bar{V}_{paste}} \frac{M_{diss}}{\rho^{diss}} s^0_{Ca}$$

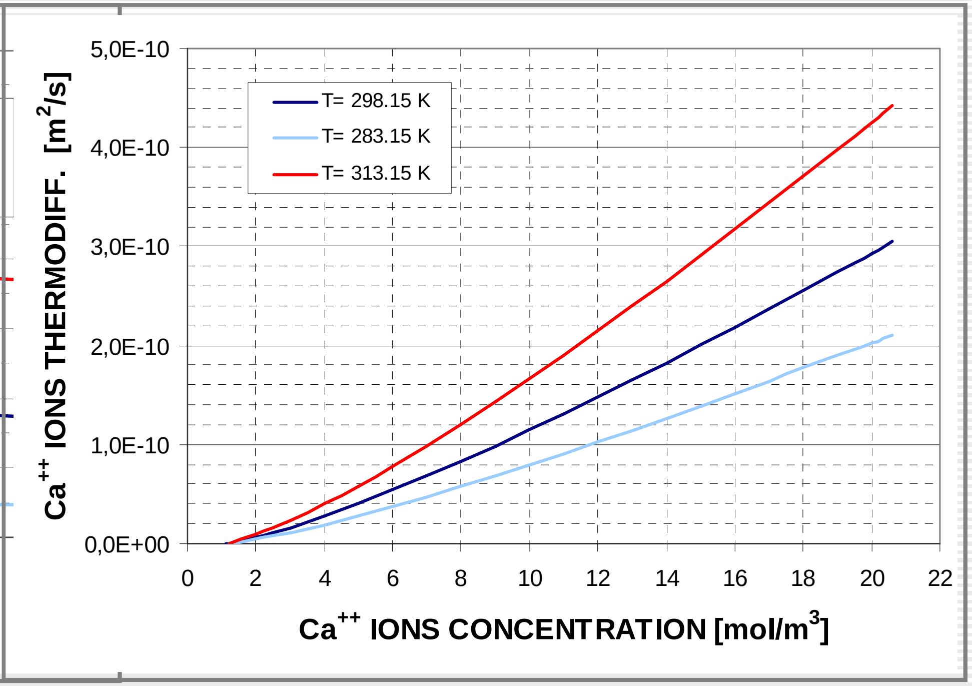
Hygral - chemical interactions

Calcium transport

Ions diffusion



Ions thermo-diffusion



$$\mathbf{D}_d^{Ca} = D_d^{Ca}\mathbf{I} = n S_w \tau D_{d0}^{Ca}\cdot\exp\left[A_4\left(T-T_{ref}\right)\right]\mathbf{I}$$

$$\mathbf{D}_T^{Ca} = D_T^{Ca}\mathbf{I} = n S_w \tau D_{T0}^{Ca}\frac{c_{Ca}}{T}\cdot\exp\left[\alpha_T\left(T-T_{ref}\right)\right]\mathbf{I}$$

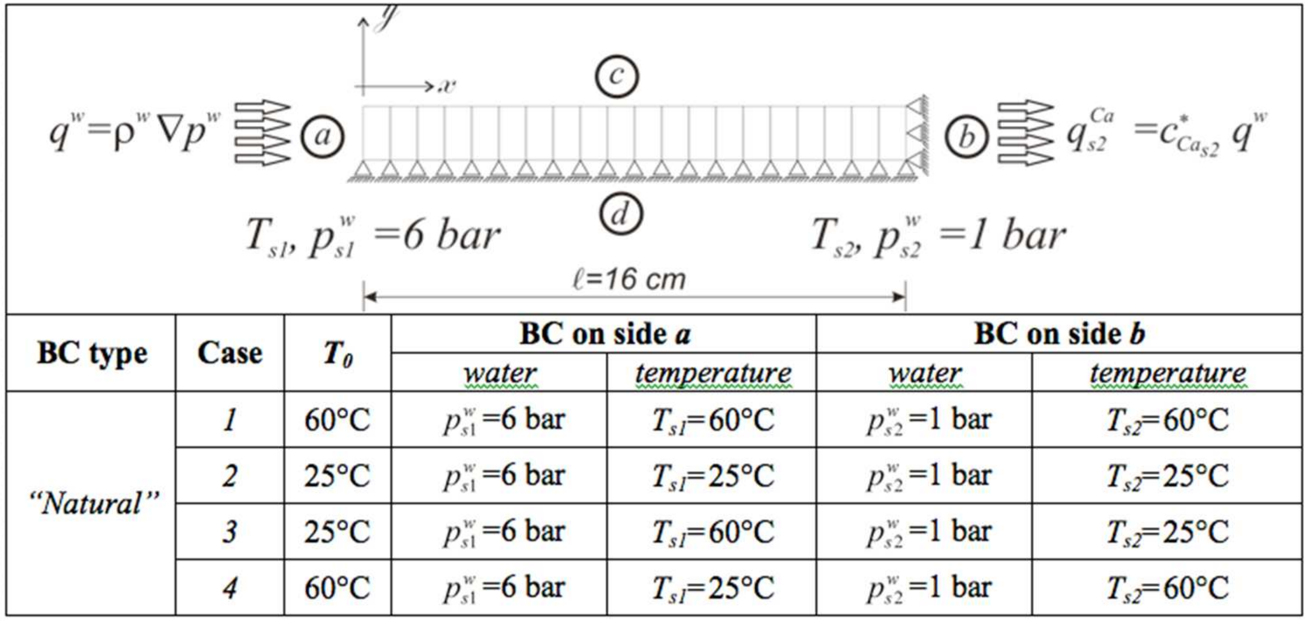
[Samson et al. - 2007, Kuhl and Meschke - 2003]

[Samson et al. - 2007]

Numerical simulation results

Modeling of a wall subject to reaction-diffusion-advection process

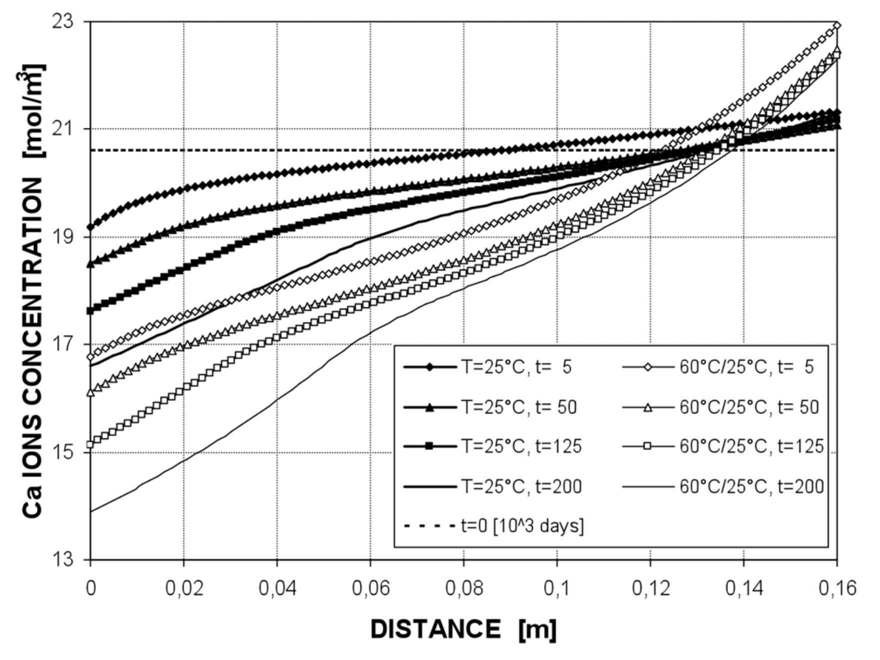
Boundary Conditions



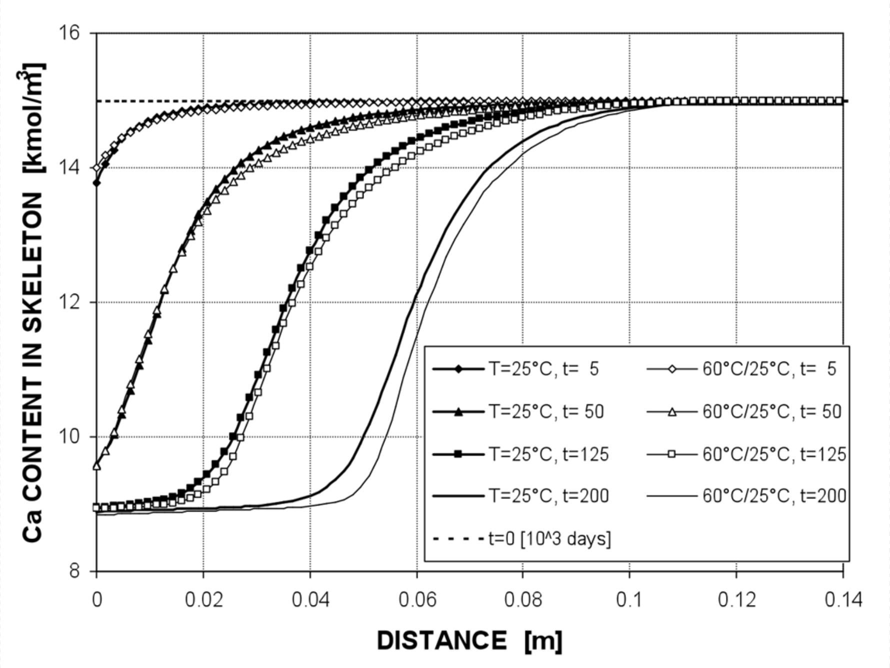
BC type	Case	T_0	BC on side ***a***		BC on side ***b***	
			water	temperature	water	temperature
"Natural"	*1*	60°C	p_{s1}^w =6 bar	T_{s1}=60°C	p_{s2}^w =1 bar	T_{s2}=60°C
	2	25°C	p_{s1}^w =6 bar	T_{s1}=25°C	p_{s2}^w =1 bar	T_{s2}=25°C
	3	25°C	p_{s1}^w =6 bar	T_{s1}=60°C	p_{s2}^w =1 bar	T_{s2}=25°C
	4	60°C	p_{s1}^w =6 bar	T_{s1}=25°C	p_{s2}^w =1 bar	T_{s2}=60°C

Numerical simulation results

Reaction-diffusion-advection process: 25°C and 60°C-25°C cases (2 and 3)



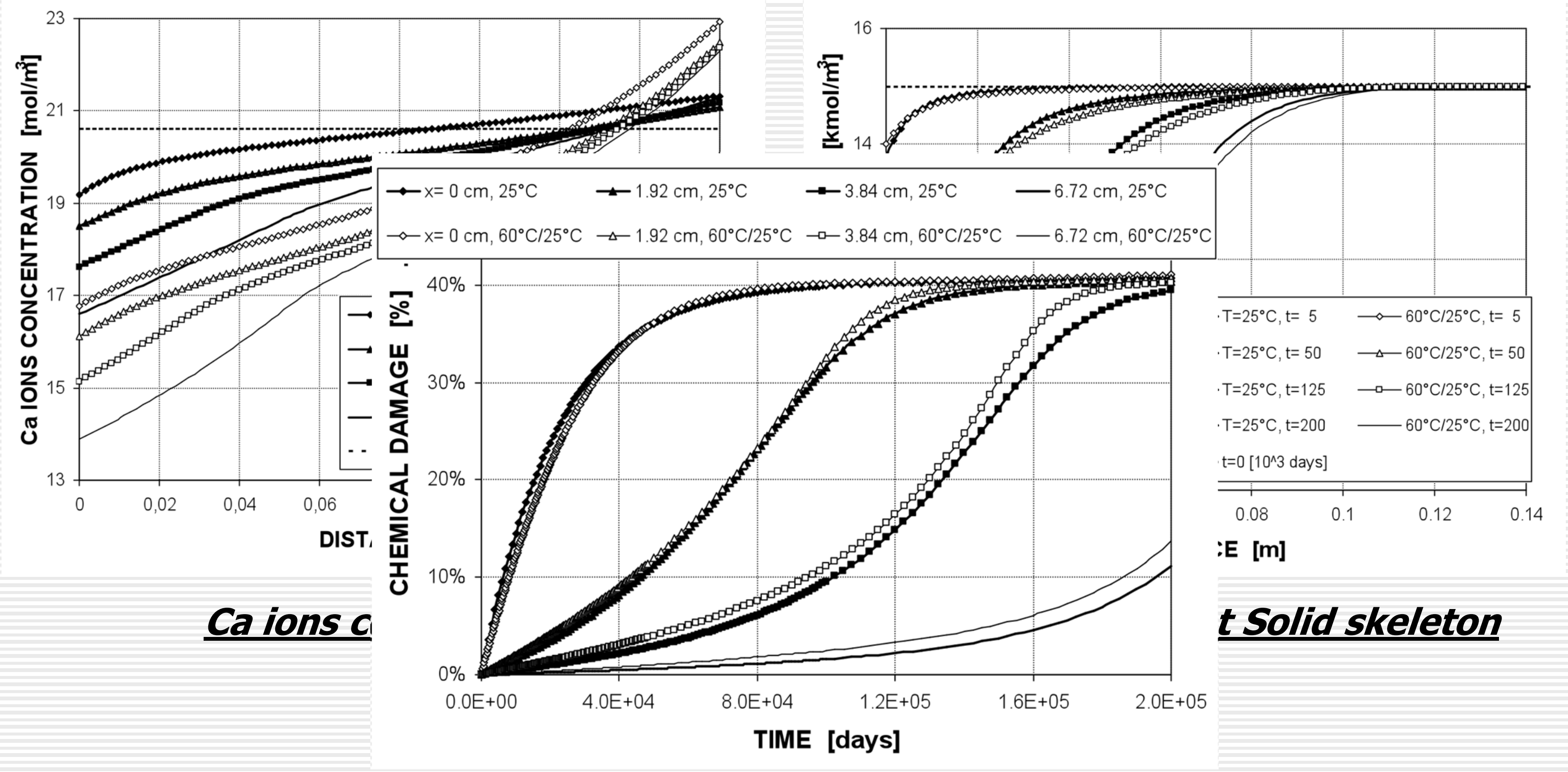
<u>Ca ions concentration</u>



<u>Calcium content Solid skeleton</u>

Numerical simulation results

Reaction-diffusion-advection process: 25°C and 60°C-25°C cases (2 and 3)



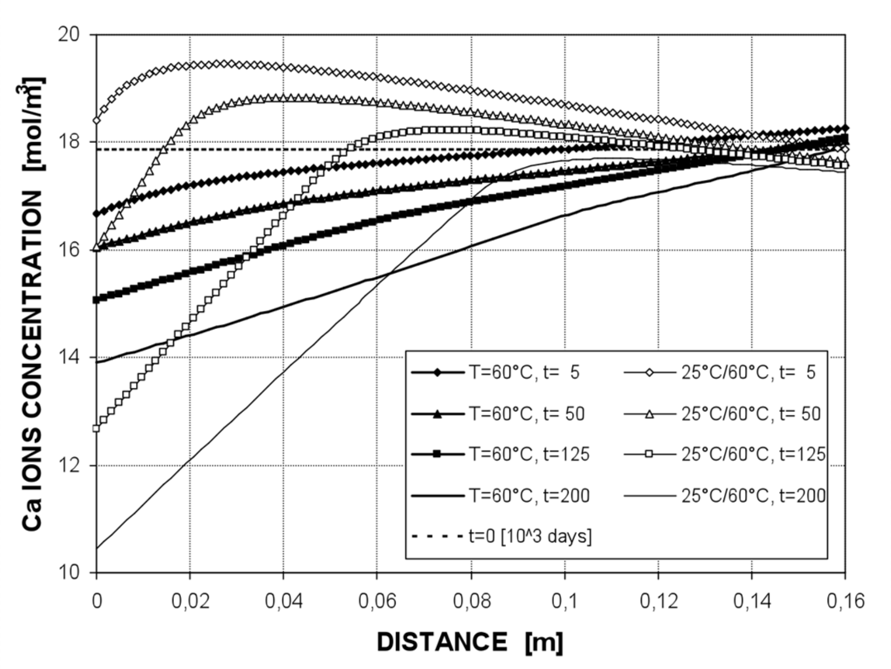
Ca ions c

t Solid skeleton

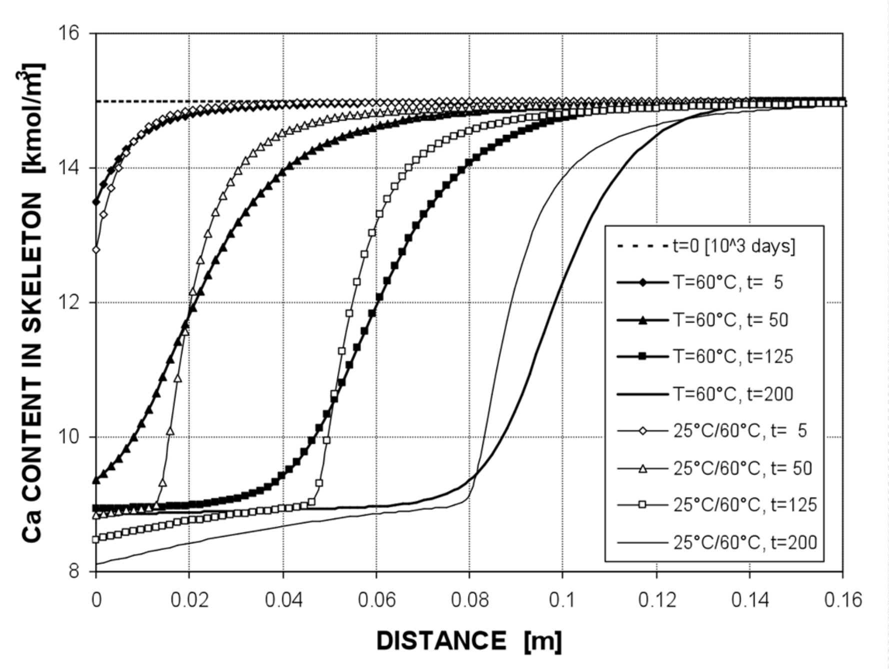
Chemical Damage

Numerical simulation results

Reaction-diffusion-advection process: 60°C and 25°C-60°C cases (1 and 4)



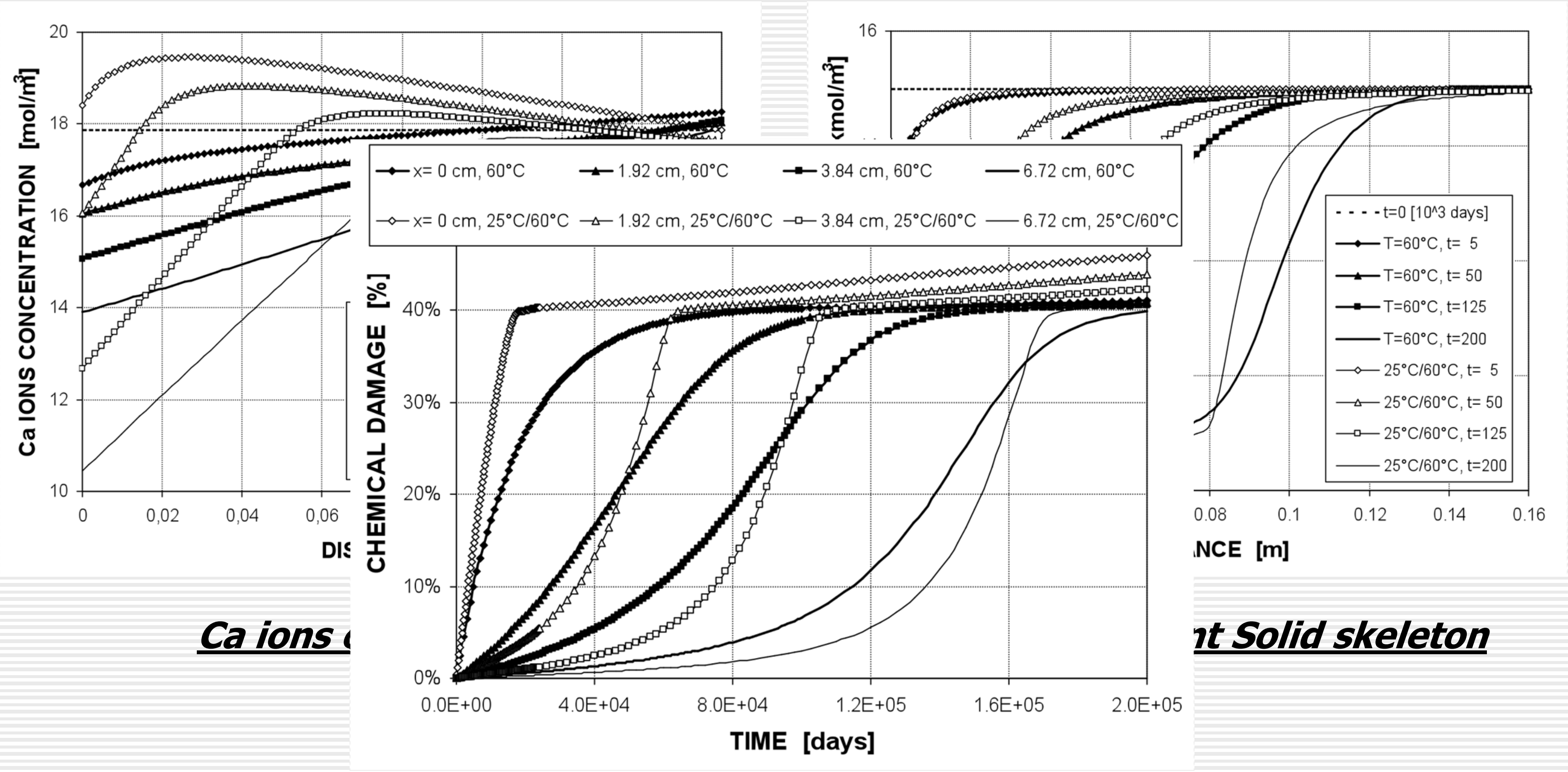
Ca ions concentration



Calcium content Solid skeleton

Numerical simulation results

Reaction-diffusion-advection process: 60°C and 25°C-60°C cases (1 and 4)



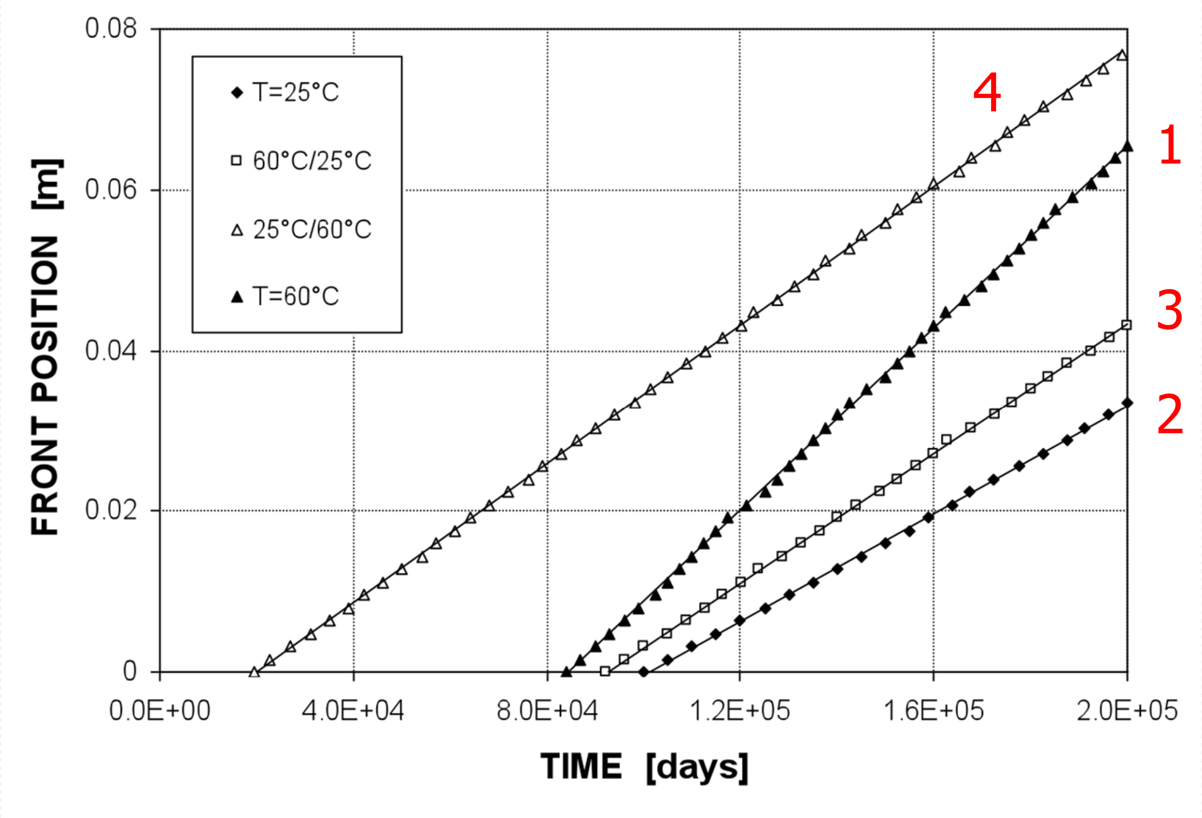
Ca ions

nt Solid skeleton

Chemical Damage

Numerical simulation results

Modeling of a wall subject to reaction-diffusion-advection process



Leaching front evolution

Modelling of Silica Alkali Reaction

Introduction

Difficulties related to ASR process simulation

☐ *The reaction between alkali and the aggregates takes place at microscopic level and consists in the formation of a hydrophilic gel from the chemical combination of the silica contained in the aggregates, the alkali in the cement klinker (ions K^+ and Na^+ mainly) and the saline water solution, which fills partly or fully the pores of the material.*

☐ *While the first stage of the ASR (i.e. the dissolution of the silica) is known and can be simulated by means of a first order kinetic law, the second part of the process is less clear. In particular the mechanism of the formation of the amorphous gel, its combination with water and the related swelling, which leads to the macroscopically observable expansion and deterioration of the concrete structures, is under discussion.*

Modelling of Silica Alkali Reaction

Introduction

Existing models and model proposed

☐ *The **existing models** can be classified essentially into two classes: models which attribute the process progression to the water imbibitions (temperature independent) [1, 2] and models which consider temperature as the main parameter, i.e. ASR is considered as a pure thermally activated process [3, 4].*

☐ *In the **present model** the ASR is modelled as a two-stage process, involving chemical reactions causing first silica dissolution and then gel formation, [1]. The effect of moisture content on the kinetics of the first process is considered similarly as in [1, 2] and effect of temperature following approach proposed in [3, 4]. It is assumed that the gel formation process causes expansion of the material skeleton and the maximal chemical strain is dependent on the moisture content and to a much lesser extent on the temperature value. The gel is assumed to be in equilibrium with moisture in its pores, hence any variation of relative humidity causes an immediate change of chemical strains, also during decrease of water content.*

① *A. Steffens et al., Aging Approach to Water Effect on Alkali–Silica Reaction Degradation of Structures, Journal of Engineering Mechanics, 129, 50-59, (2003).*

② *F. Bangert et al., Chemo-hygro-mechanical modelling and numerical simulation of concrete deterioration caused by alkali-silica reaction, Int. J. Numer. Anal. Meth. Geomech., 28(78), 689-714, (2004).*

③ *Larive, C. Apports combinés de l'expérimentation et la modélisation à la compréhension de l'alcali-réaction et de ses effets mécaniques, Monograph LPC, 0A28, Laboratoire Central des Ponts et Chaussées, Paris (1998).*

④ *F-J Ulm et al., Thermo-chemo-mechanics of ASR expansion in concrete structures, Journal of Engineering Mechanics, 126(3), 233-242, (2000).*

Mathematical model

Model of Silica Alkali Reaction

First stage of the process: evolution of the reaction extent Γ_{ASR}

$$\dot{\Gamma}_{ASR} = \frac{1-\Gamma_{ASR}}{t_r}$$

where (at constant T and S_w):

$$\Gamma_{ASR}(t) = \frac{\varepsilon_{ASR}(t)}{\varepsilon_{ASR,\infty}}$$

$t_r = k_r/A_0$ is the reaction time (A_0 is the initial chemical affinity and k_r is the kinetic coefficient)

The chemical affinity is: $A_r(\Gamma_{ASR}) = A_{r0}(1-\Gamma_{ASR})$

❑ ***Ref.: Larive et al**, Journal of Engineering Mechanics 2000*

The reaction time is: $t_r = \tau_r(T,\boxed{S_w})\cdot\lambda(T,\boxed{S_w},\Gamma_{ASR})$ where $\lambda(T,S_w,\Gamma_{ASR}) = \dfrac{1+\exp(-\tau_L/\tau_r)}{\Gamma_{ASR}+\exp(-\tau_L/\tau_r)}$

with

Latency time

$$\tau_L(T,S_w) = \tau_{L0}\left[U_L\left(\frac{1}{T}-\frac{1}{T_0}\right)\right]\boxed{(A_L\cdot S_w + B_L)}$$

Influence of saturation level

Characteristic time

$$\tau_r(T,S_w) = \tau_{r0}\left[U_r\left(\frac{1}{T}-\frac{1}{T_0}\right)\right]\boxed{(A_L\cdot S_w + B_L)}$$

$\tau_{L0}, \tau_{r0}, A_L, B_L$ are material parameters

Mathematical model

Strain components

In general, a total strain of concrete, ε_{tot}, can be split into the following components:

1. *free thermal strain*
2. *ASR strain*
3. *thermo-chemical strain*
4. *creep strain*
5. *mechanical strain (caused by mechanical load and shrinkage)*

Strain decomposition

$$d\boldsymbol{\varepsilon}_{mech} = d\boldsymbol{\varepsilon}_{tot} - d\boldsymbol{\varepsilon}_{ASR} - d\boldsymbol{\varepsilon}_{c} - d\boldsymbol{\varepsilon}_{th} - d\boldsymbol{\varepsilon}_{ch}$$

Free thermal strain strain

$$d\boldsymbol{\varepsilon}_t = \beta_s \, dT \, \mathbf{I}$$

Shrinkage strain

$$d\boldsymbol{\varepsilon}_{sh} = -\frac{\alpha}{3K_T}\left(d\chi^{ws} p^c + \chi^{ws} dp^c\right)\mathbf{I}$$

Thermo-chemical strain

$$d\boldsymbol{\varepsilon}_{ch} = \beta_{ch} \, d\Gamma_{hydr} \, \mathbf{I}$$

Mathematical model

Model of Silica Alkali Reaction

Second stage of the process: evolution of ASR strain ε_{ASR}

$$\boxed{\dot{\boldsymbol{\varepsilon}}_{ASR}(t) = \frac{\alpha}{\rho^{ASR}} \cdot \dot{m}_{ASR}(t)\mathbf{I}}$$

where $\dot{m}_{ASR}$ is the rate of water mass combination with the gel $\dot{m}_{ASR} \propto \dot{\Gamma}_{ASR}$;

α is the chemo-elastic dilatation coefficient;

ρ^{ASR} the density of the formed gel.

❑ ***Ref.: Pesavento et al**, Comp. Methods in Appl. Mech. and Eng. 2012*

Water Aging

Due to peculiar physico-chemical processes a loss of swelling potential is experimentally observed; this loss can be considered as a sort of "material aging":

$$\boxed{\dot{\Gamma}_a = \frac{1-\Gamma_a}{t_a}}$$

with Γ_a is the aging process extent;

t_a is the characteristic time of aging.

❑ ***Ref.: Steffens et al**, Journal of Engineering Mechanics 2003*

The water-gel combination rate is now:

$$\boxed{m_{ASR} = M_{ASR}(S_w)\cdot(1-\Gamma_a)\cdot\dot{\Gamma}_{ASR}}$$

in which $M_{ASR}(S_w)$ is the water combination coefficient at saturation level S_w

Mathematical model

Model of Silica Alkali Reaction

Second stage of the process: evolution of ASR strain ε_{ASR}

$$M_{ASR}\left(S_w\right)=M_{ASR0}\left(\tilde{A}_{ASR}\cdot S_w+\tilde{B}_{ARS}\right) \qquad \text{linear formulation}$$

$$M_{ASR}\left(S_w\right)=M_{ASR0}\cdot\exp\left(\tilde{C}_{ASR}\cdot S_w+\tilde{D}_{ASR}\right) \qquad \text{power formulation}$$

- ❑ **Ref.: Steffens et al**, *Journal of Engineering Mechanics 2003*
- ❑**Ref.: Bangert et al**, *IJNME 2004*

in which $M_{ASR0}=M_{ASR}\left(S_w=1\right)$ and $\tilde{A}_{ASR},\tilde{B}_{ARS},\tilde{C}_{ASR}$ and $\tilde{D}_{ASR}$ are material parameters

After some mathematical transformations Steffens showed that:

$$1-\Gamma_a=\left(1-\Gamma_{ASR}\right)^{\tau_{r0}/\tau_{a0}}$$

Hence, the ASR strain evolution law is now:

- ❑ **Ref.: Pesavento et al**, *Comp. Methods in Appl. Mech. and Eng. 2012*

$$\dot{\boldsymbol{\varepsilon}}_{ASR}=\frac{\alpha}{\rho^{ASR}}M_{ASR}\left(S_w\right)\cdot\left(1-\Gamma_{ASR}\right)^{\tau_{r0}/\tau_{a0}}\cdot\dot{\Gamma}_{ASR}\,\mathbf{I}$$

Mathematical model

Model of Silica Alkali Reaction: constitutive relationships

Const. relationships for the solid density

- *Density of the solid phase:*

$$\rho^s = \frac{\rho^{s0} + m_{ASR}(t)\left(1-n\right)^{-1}}{1+\varepsilon_{ASR}^{vol}(t)}$$

✧ In general the constitutive relationship for the solid skeleton has the form :

$$\rho^s = \rho^s\left(T, P^s, tr\,\mathbf{t}^{ef}, \varepsilon_{ASR}^{vol}, m_{ASR}\right)$$

✧ *Rate of the first invariant of the effective stress tensor:*

$$\frac{\overset{s}{D}\left(tr\,\mathbf{t}^{ef}\right)}{Dt} = 3\tilde{K}_T\left(div\,\boldsymbol{\nabla}^s + \frac{1}{\tilde{K}_s}\frac{\overset{s}{D}P^s}{Dt} - \beta_s\frac{\overset{s}{D}T}{Dt}\right)$$

Variation of the pore volume

$$V_p\left(T, P^s, tr\,\mathbf{t}^{ef}, \varepsilon_{ASR}^{vol}\right) = V_p\left(T, P^s, tr\,\mathbf{t}^{ef}, \varepsilon_{ASR}^{vol} = 0\right)\left[1 + \varepsilon_{ASR}^{vol}(t)\right]$$

Mathematical model

Model of Silica Alkali Reaction: constitutive relationships

Const. relationships for the porosity

$$\boxed{n = constant}$$

Const. relationships for the intrinsic permeability

$$\boxed{k = k\left(m_{ASR}, d\right) = k_o \cdot 10^{A_k\left(m_{ASR}/m_{ASR\infty}\right)} 10^{A_d d}}$$

Sorption isotherms

✧ Suction curve for "***unreacted***" and for "***fully reacted***" material (Van Genuchten type):

$$\boxed{S_w = \left[\left(\frac{p^c}{a}\right)^{\frac{b}{b-1}} + 1\right]^{-1/b}}$$

✧ Evolution of the sorption isotherm during ASR process:

$$\boxed{S_w\left(p^c, m_{ASR}\right) = S_w\left(p^c, 0\right) + \frac{m_{ASR}}{m_{ASR,\infty}}\left[S_w\left(p^c, m_{ASR,\infty}\right) - S_w\left(p^c, 0\right)\right]}$$

Mathematical model

Model of Silica Alkali Reaction: additional shrinkage

Evolution of the solid surface fraction due to ASR

New microstructure due to the gel formation ⇒ modification of the solid pressure formulation by means a new form of the solid surface fraction

$$\chi^{ws}_{ASR}\left(S_w,\Gamma_{ASR}\right)=\chi^{ws}_{s}\left[1+\frac{m_{ASR}}{m_{ASR\infty}}\delta_{ASR}\right]$$

with

δ_{ASR} constant (material parameter)

This allows of taking into account an additional shrinkage due to water loss from the ASR gel during the drying phases (the gel occupies less volume)

Solid pressure

$$p^s=p^g-\chi^{ws}_{ASR}p^c$$

Modelling Silica Alkali Reaction

Experimental-Numerical results comparison

Poyet's experimental tests at constant relative humidity

✓ Material properties as in:

S. Poyet, Etude de la dégradation des ouvrages en béton atteints de la réaction alcali–silice: approche expérimentale et modélisation numérique multi-échelle des dégradations dans un environnement hydrochemo–mécanique variable, PhD thesis, Université de Marne la Vallée, France (2003).

✓ Size of the specimens:

Cylindrical specimens – radius=1cm, height=16cm

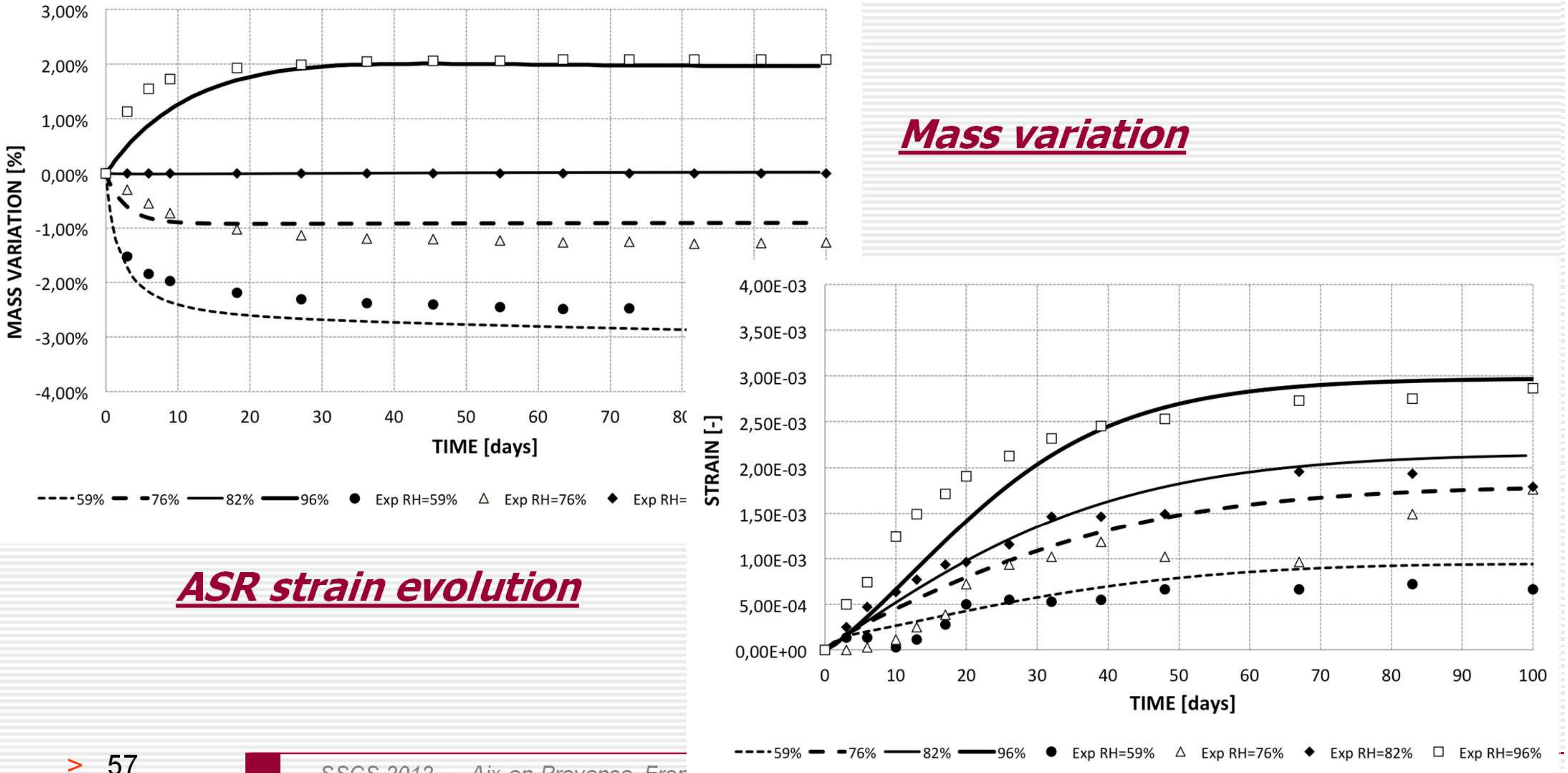
✓ Boundary conditions:

- convective heat and mass exchange:
  - RH_∞=82%, and then 59%, 76%, 82%, 96% or 100% kept constant in time with β_c=0.002 m/s (drying cases) and β_c=0.002 m/s (swelling cases)
  - T=60°C with α_c=5 W/Km^2
- surface mechanical load: unloaded

Modelling Silica Alkali Reaction

Experimental-Numerical results comparison

Poyet’s experimental tests at constant relative humidity



Mass variation

ASR strain evolution

Modelling Silica Alkali Reaction

Experimental-Numerical results comparison

Poyet's experimental tests at variable relative humidity

✓ Material properties as in:

S. Poyet, Etude de la dégradation des ouvrages en béton atteints de la réaction alcali–silice: approche expérimentale et modélisation numérique multi-échelle des dégradations dans un environnement hydrochemo–mécanique variable, PhD thesis, Université de Marne la Vallée, France (2003).

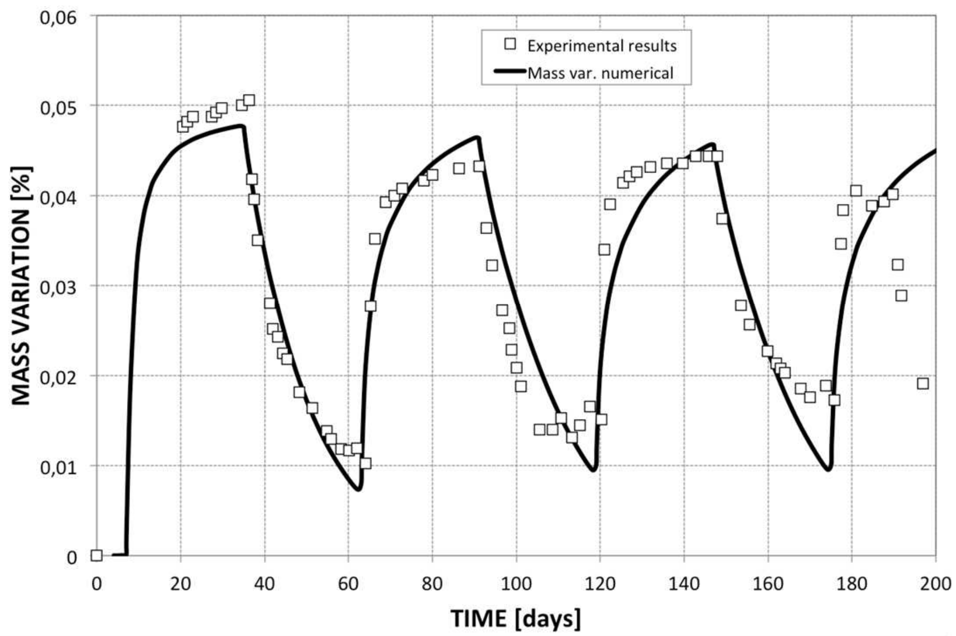
✓ Size of the specimens:
Cylindrical specimens – radius=1cm, height=16cm

✓ Boundary conditions:
- convective heat and mass exchange:
  - RH_∞=59-96% variable in time with two different cycles: short (14 days) and long (28 days) β_c=0.002 m/s (drying phases) and β_c=0.002 m/s (swelling phases)
  - T=60°C with α_c=5 W/Km^2

Modelling Silica Alkali Reaction

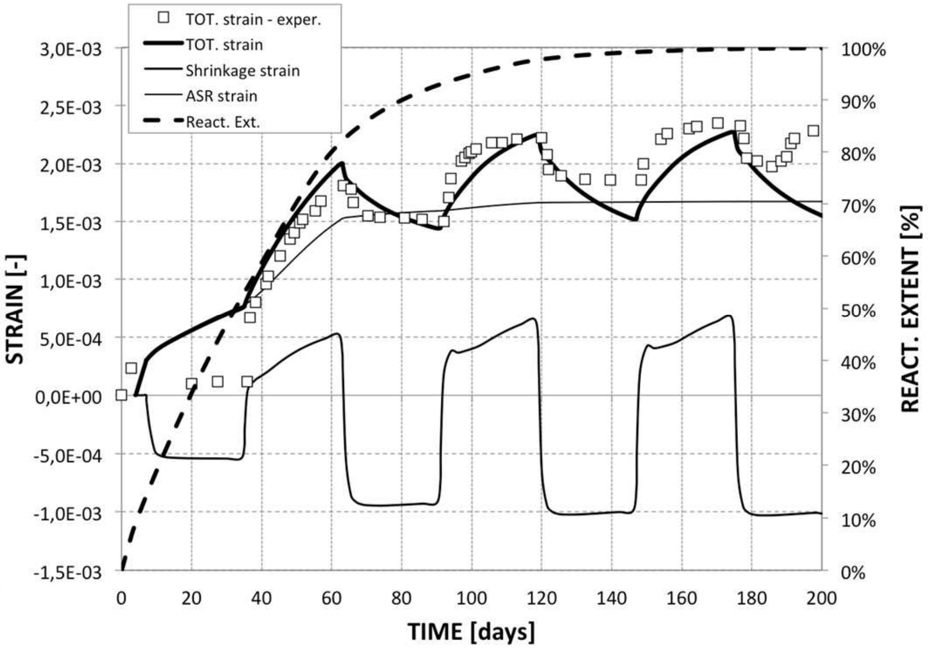
Experimental-Numerical results comparison

<u>Poyet's experimental tests at variable relative humidity (long cycle)</u>



Mass variation

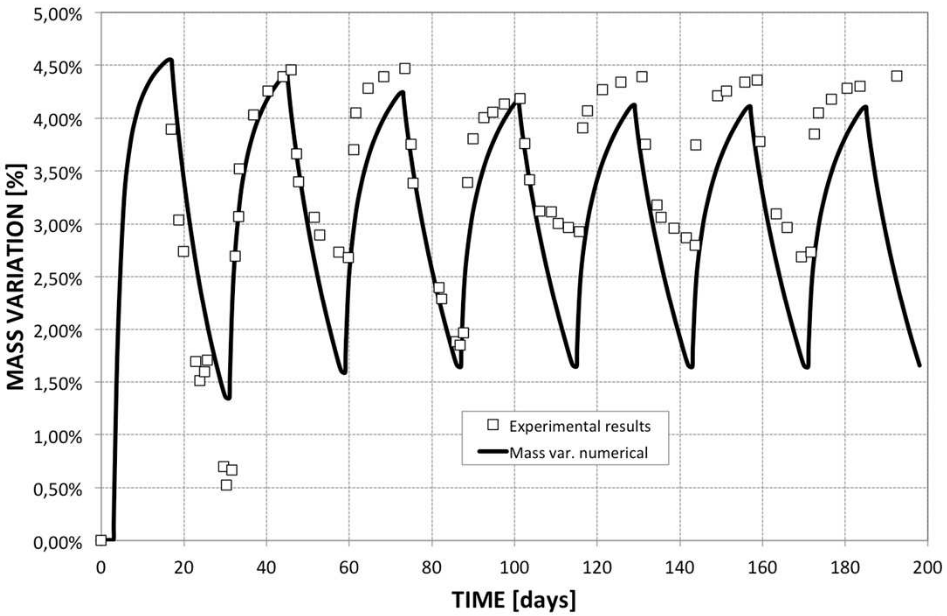
ASR strain and react. extent evolution



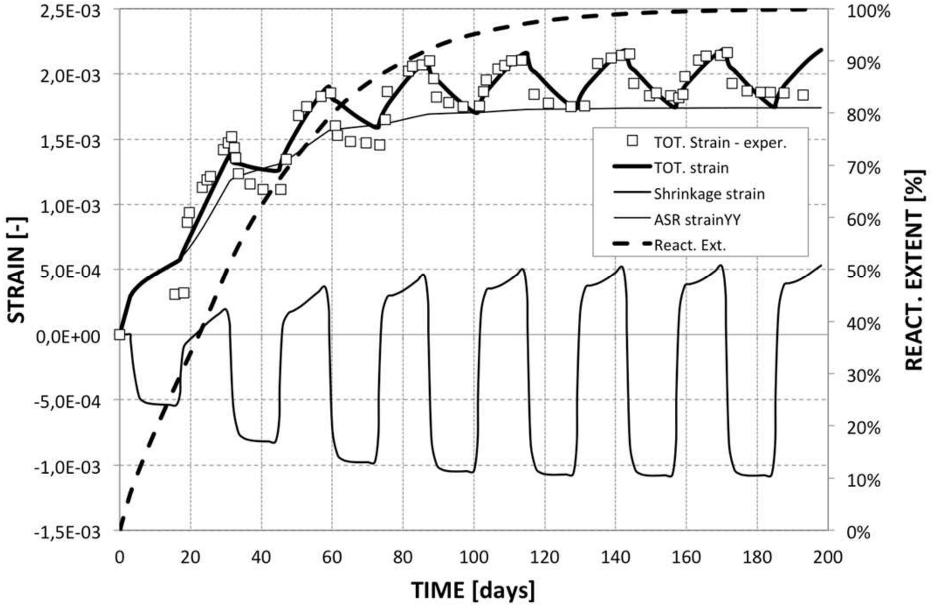
Modelling Silica Alkali Reaction

Experimental-Numerical results comparison

Poyet’s experimental tests at variable relative humidity (short cycle)



Mass variation



ASR strain and react. extent evolution

Modelling of concrete at high temperature

Concrete at high temperature

- ✓ Bazant, Thonguthai – 1978
- ✓ Thelandersson – 1987
- ✓ England, Khoylou - 1995
- ✓ Bazant, Kaplan – 1996
- ✓ Gerard, Pijaudier-Cabot, Laborderie - 1998
- ✓ Gawin, Majorana, Schrefler - 1999
- ✓ Bentz – 2000
- ✓ Nechnech, Reynouard, Meftah - 2001

Thermal spalling

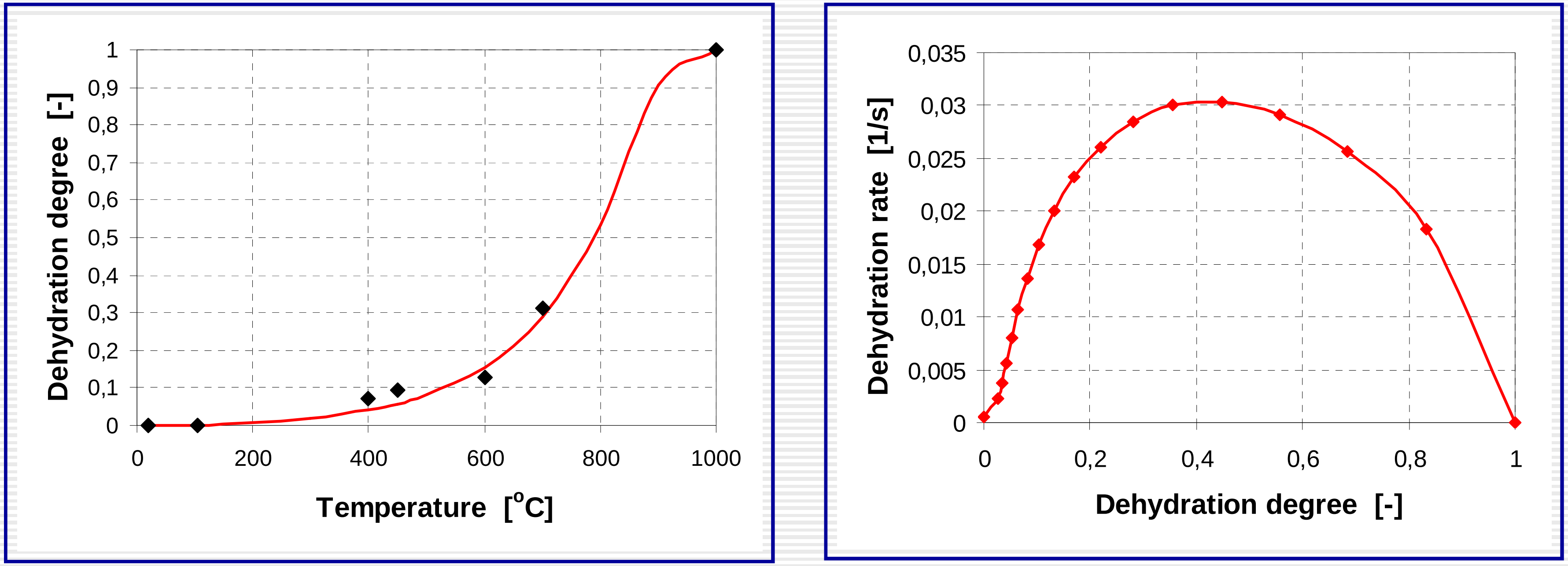
- ✓ Phan – 1996
- ✓ Ulm, Coussy, Bazant – 1999
- ✓ Sullivan – 2001
- ✓ Phan, Lawson, Davis - 2001

- ✓ HITECO project – 1995-2000
- ✓ NIST workshop – 1997
- ✓ UPTUN project – 2002-2006

Thermo-chemical interactions

Concrete at high temperature

Dehydration of concrete



$$\Gamma_{dehydr}(t) = \Gamma_{dehydr}\left[T_{\max}(t)\right]$$

$$\frac{\partial\Gamma}{\partial t} = A_{\Gamma}(\Gamma)\cdot exp\left(-\frac{E_a}{RT}\right)$$

T –temperature of concrete

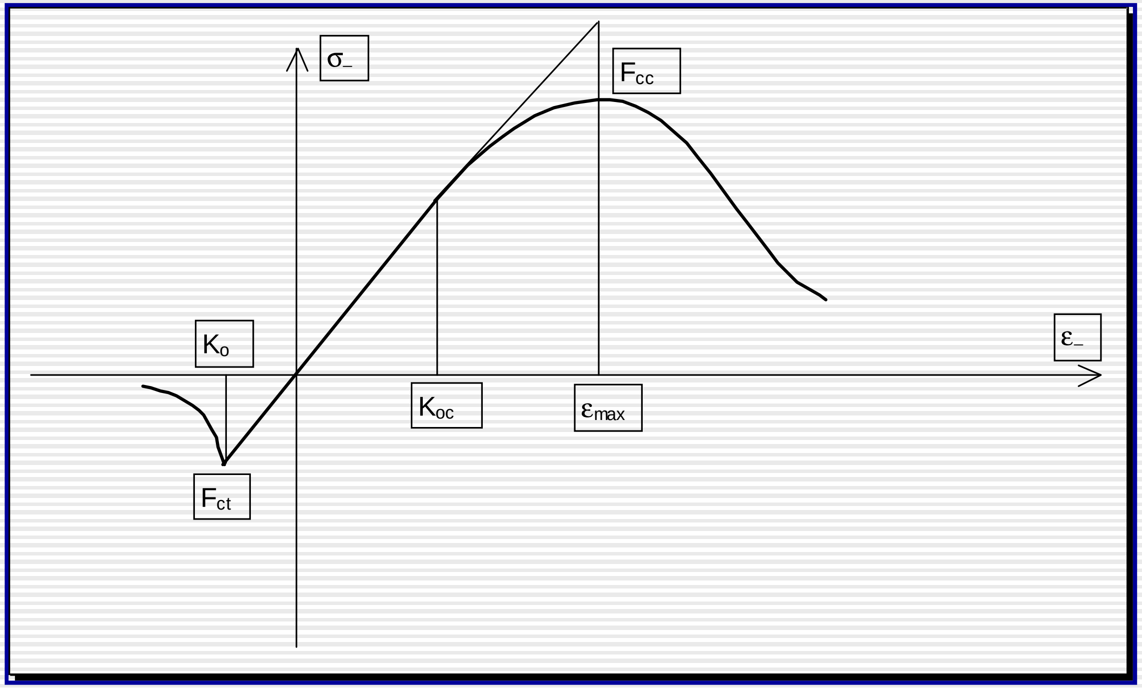
A_{Γ} – chemical affinity

Mechanical – mat. degradation interactions

Mechanical material degradation description

Non-local isotropic damage theory

[Mazars & Pijaudier-Cabot, 1989]



$$d = \alpha_t d_t + \alpha_c d_c$$

$$\tilde{\varepsilon} = \sqrt{\sum_{i=1}^{3} \left(\langle \varepsilon_i \rangle_+ \right)^2}$$

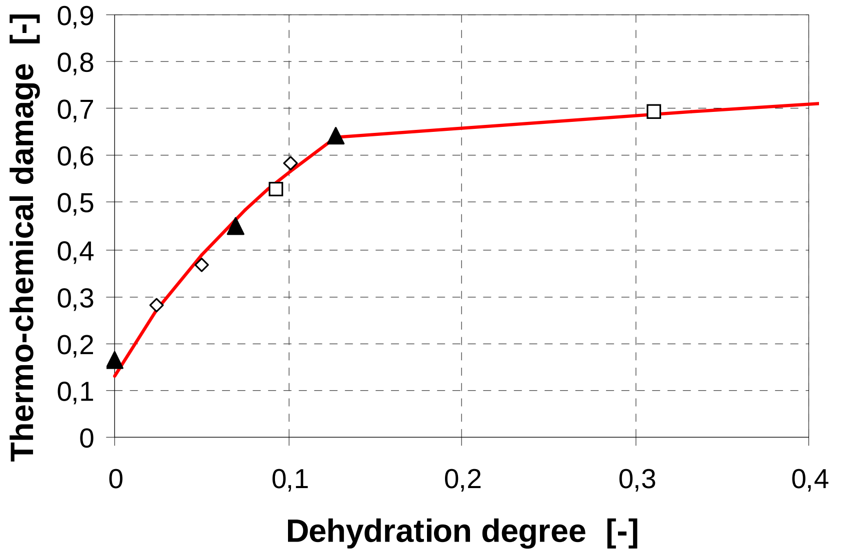
$$\overline{\varepsilon}(x) = \frac{1}{V_r(x)} \int_V \Psi(x-s)\tilde{\varepsilon}(s)\, dv$$

$$\Psi(x-s) = \Psi_o \exp\left(-\frac{\|x-s\|^2}{2 l_c^2} \right)$$

Chemo - mechanical interactions

Concrete at high temperature

Correlation of dehydration degree & thermo-chemical damage



$$V = 1 - \frac{E_o(T)}{E_o(T_a)}$$

$$\tilde{\sigma} = \sigma \frac{S}{\tilde{S}} = \frac{\sigma}{(1-d)(1-V)}$$

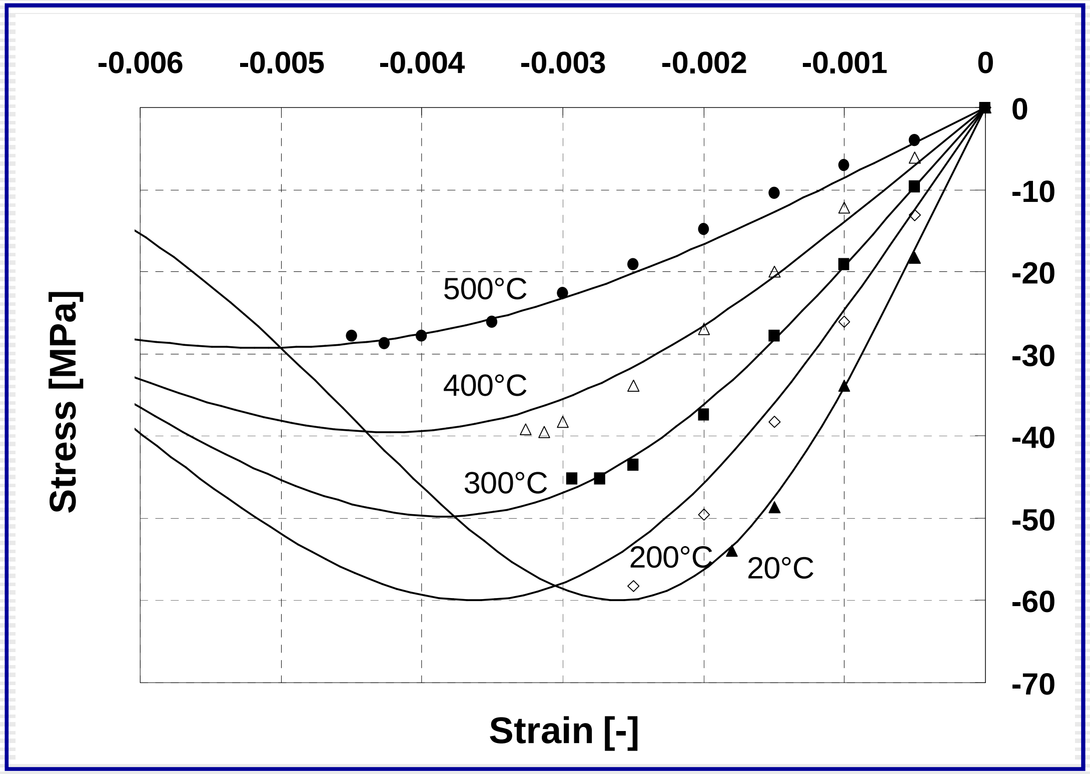
$$\boldsymbol{\sigma} = (1-d)(1-V)\boldsymbol{\Lambda}_0 : \boldsymbol{\varepsilon}^e = (1-D)\boldsymbol{\Lambda}_0 : \boldsymbol{\varepsilon}^e$$

$$D = 1 - \frac{E(T)}{E_o(T_a)} = 1 - \frac{E(T)}{E_o(T)}\frac{E_o(T)}{E_o(T_a)} = 1 - (1-d)\cdot(1-V)$$

Thermochemical - mechanical interactions

Concrete at high temperature

Effect of thermo-chemical material degradation on the stress – strain curves for C-60 concrete

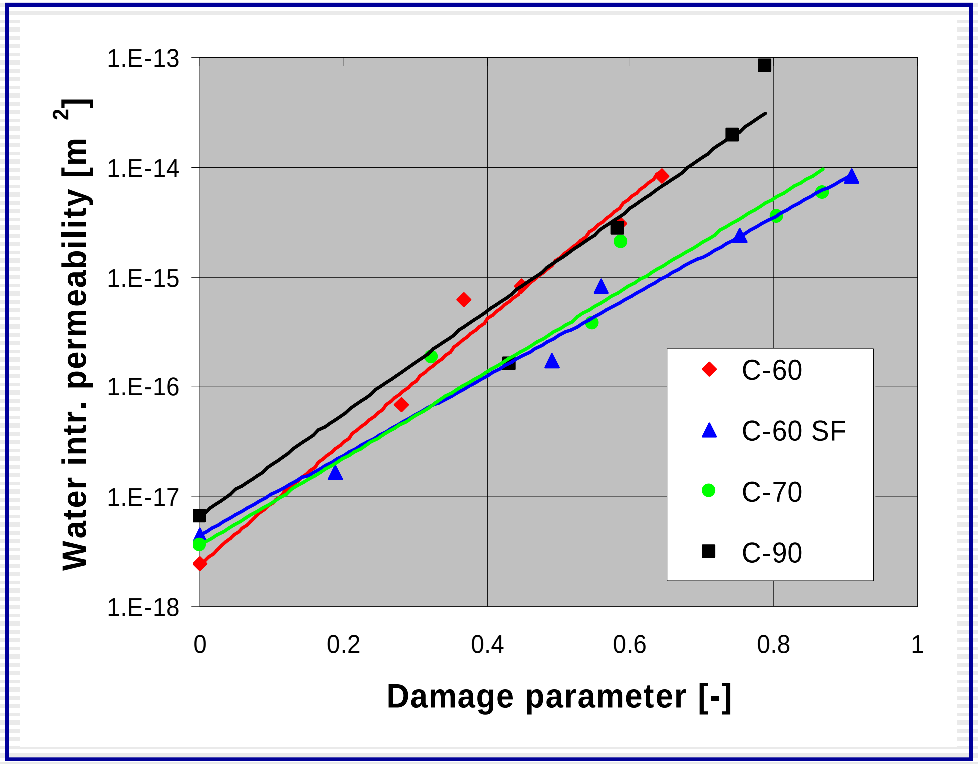


Experimental results from the EURAM-BRITE "HITECO" project

Mechanical - hygral interactions

Concrete at high temperature

Intrinsic permeability – damage relationship



$$k = k_o \cdot 10^{f(T)} \cdot \left(\frac{p^g}{p_o^g} \right)^{A_p} \cdot 10^{A_D D}$$

Details:
[Gawin, Pesavento & Schrefler, CMAME 2003]

Experimental results from the EURAM-BRITE “HITECO” project

Stress and strains of concrete

Strain decomposition

Mechanical strain

$$\boxed{d\varepsilon_{mech} = d\varepsilon_{tot} - d\varepsilon_{th} - d\varepsilon_{tchem} - d\varepsilon_{tr}}$$

Where:

ε_{mech}	mechanical strain (contains also shrinkage strain)
ε_{tot}	total strain
ε_{th}	thermal strain
ε_{tchem}	thermo-chemical strain
ε_{tr}	thermal transient strain

Stress and strains of concrete

Load Free Thermal Strain (LFTS) model

By using Load Free Thermal Strain (LFTS, i.e. irreversible part of thermal strain) model we get:

1. *free thermal strain*
2. *shrinkage strain*
3. *thermo-chemical strain*

Free thermal strain strain

$$d\boldsymbol{\varepsilon}_{th} = \beta_s(T)\, dT$$

Shrinkage strain

$$d\boldsymbol{\varepsilon}_{sh} = \frac{\alpha}{K_T}\left(d\chi^{ws} p^c + \chi^{ws} dp^c \right)\mathbf{I}$$

Thermo-chemical strain assessment

$$d\boldsymbol{\varepsilon}_{tchem} = d\boldsymbol{\varepsilon}_{tot} - d\boldsymbol{\varepsilon}_{th} - d\boldsymbol{\varepsilon}_{sh}$$

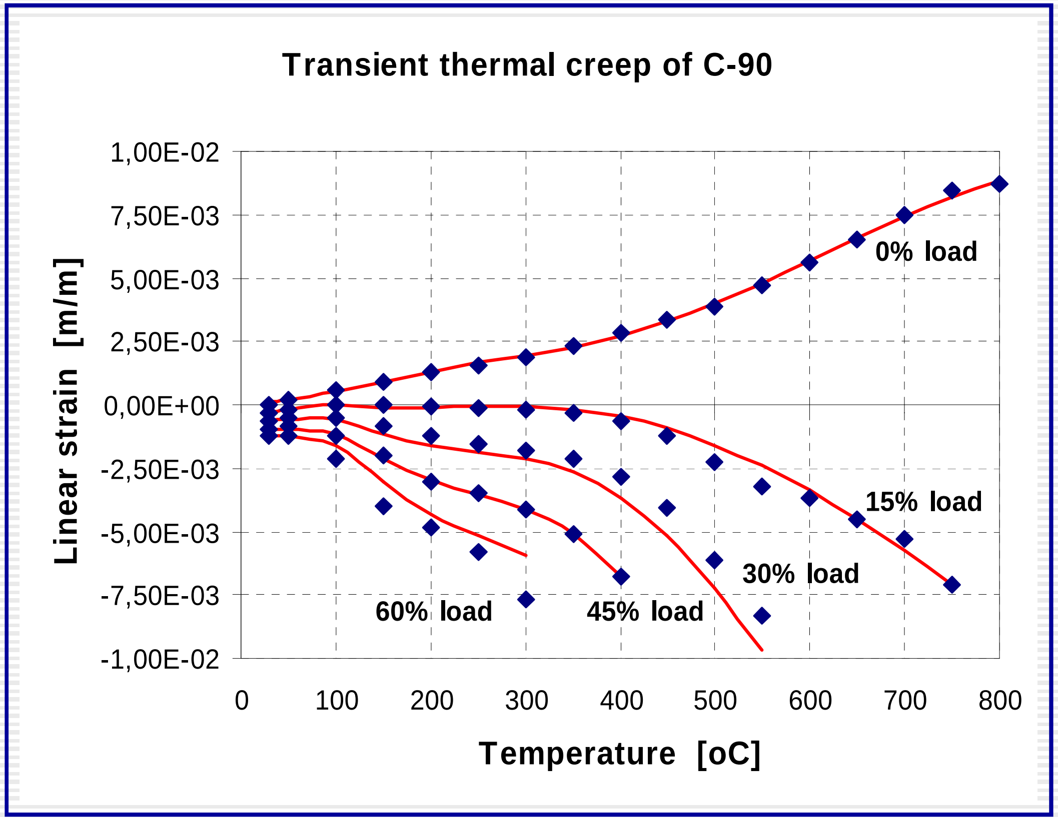
Constitutive relationship for ε_{tchem}

$$\boxed{d\boldsymbol{\varepsilon}_{tchem} = \beta_{tchem}(V)\, dV}$$

LFTS model according to: *[Gawin, Pesavento, Schrefler, Materials and Structures, 2004]*

Stress and strains of concrete

Load Induced Thermal Strain (LITS) model



$$d\boldsymbol{\varepsilon}_{tr} = \frac{\bar{\beta}_{tr}(V)}{\mathrm{f_c}(T_a)}\mathbf{Q} : \boldsymbol{\sigma}_e^s \, dT$$

$$Q_{ijkl} = -\gamma\delta_{ij}\delta_{kl} + \frac{1}{2}(1+\gamma)\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)$$

3-D modelling of LITS:

[Thelandersson, 1987]

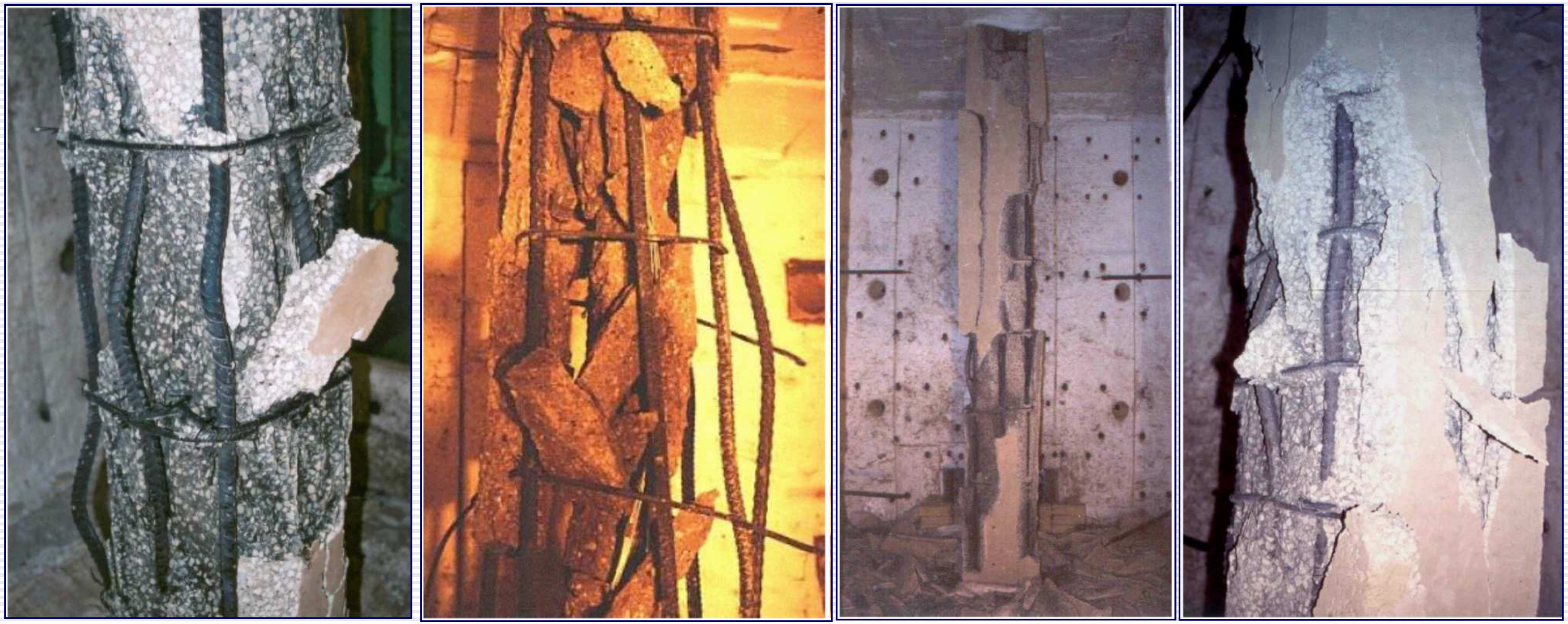
$\beta_{tr}(V)$ relation according to:

[Gawin, Pesavento & Schrefler, Mat&Struct 2004]

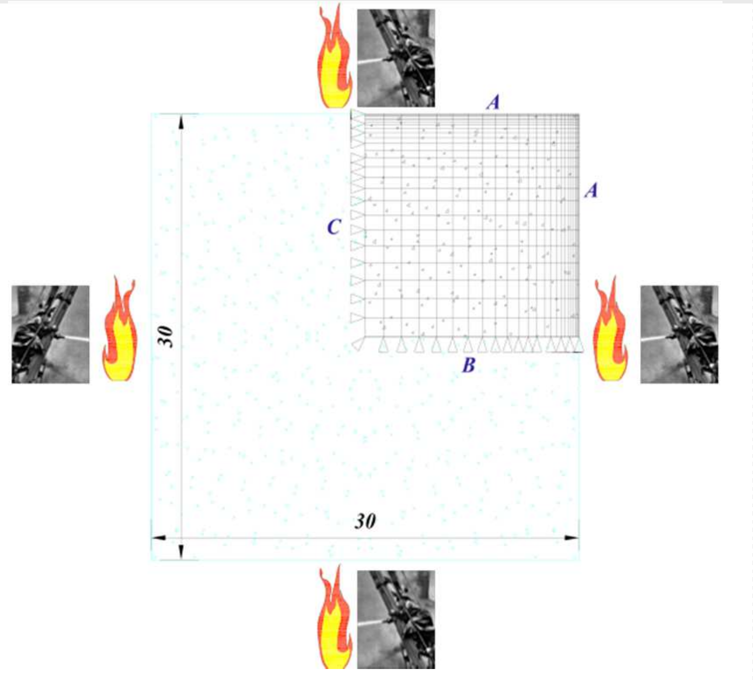
Numerical simulations

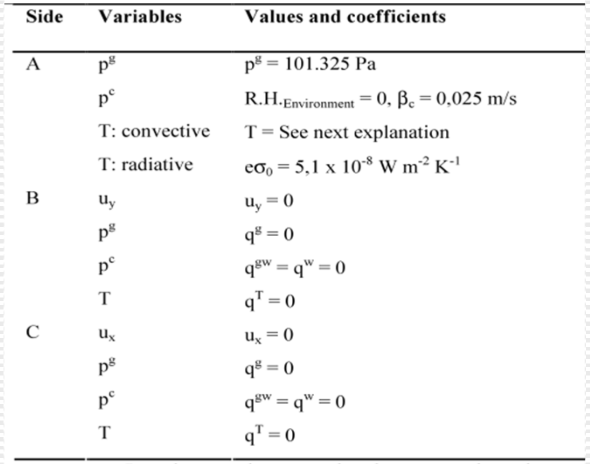
Analysis of cooling processes in HSC square columns

AIM: **qualitative analysis of the effect of cooling processes on the hygro-thermo-chemo-mechanical state of a square column, manufactured with HSC, during the development of a natural fire in a high-rise building.**



C60 (HSC)





Side	Variables	Values and coefficients
A	p^g	$p^g = 101.325$ Pa
	p^c	$R.H._{Environment} = 0$, $\beta_c = 0{,}025$ m/s
	T: convective	T = See next explanation
	T: radiative	$e\sigma_0 = 5{,}1 \times 10^{-8}$ W m^{-2} K^{-1}
B	u_y	$u_y = 0$
	p^g	$q^g = 0$
	p^c	$q^{gw} = q^w = 0$
	T	$q^T = 0$
C	u_x	$u_x = 0$
	p^g	$q^g = 0$
	p^c	$q^{gw} = q^w = 0$
	T	$q^T = 0$

Boundary conditions used in the numerical simulation

HEATING PARAMETRIC CURVE:

- Slow fire curve

-Eurocode 1, Part 1-2 is used (O = 0,013 m$^{1/2}$)

$$\Theta_g = 20 + 1.325 \cdot (1 - 0{,}324 \cdot e^{-0{,}0077 \cdot t} - 0{,}204 \cdot e^{-0{,}06545 \cdot t} - 0{,}472 \cdot e^{-0{,}7315 \cdot t})$$

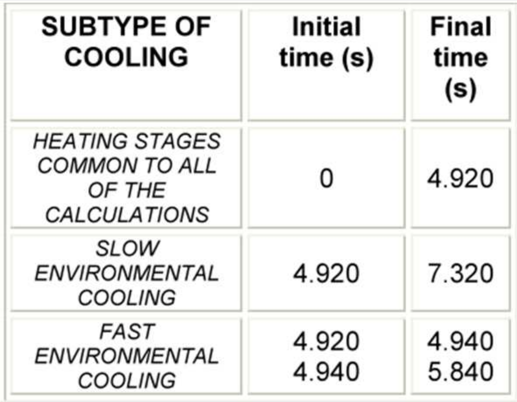
(Θ_g [ºC] , t [h])

+

2 TYPES OF ENVIRONMENTAL COOLING:

Cooling Rates of the Air:

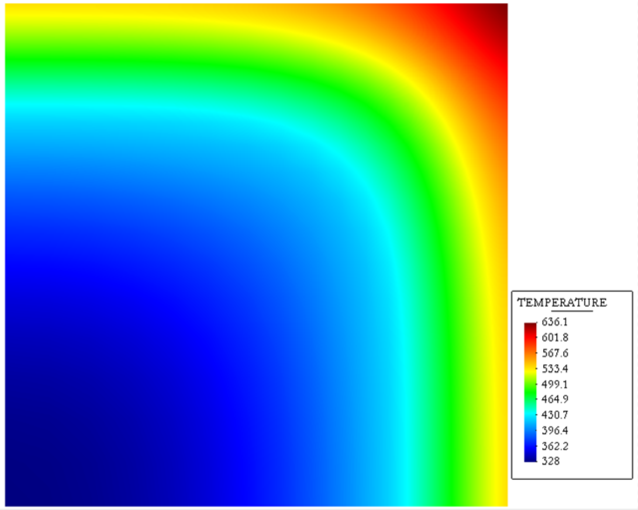
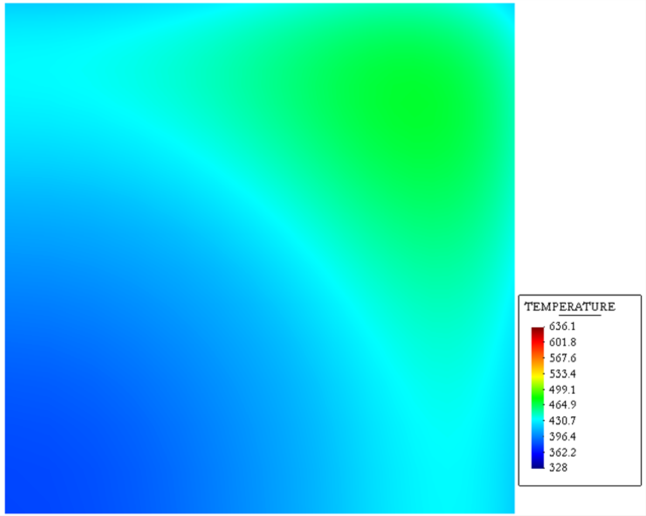
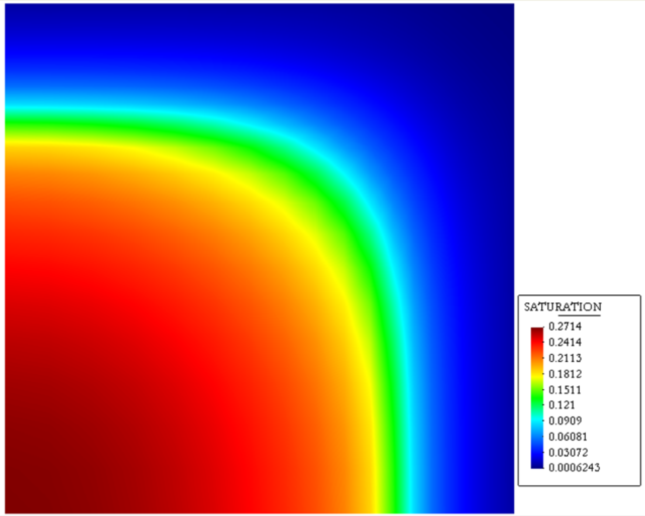
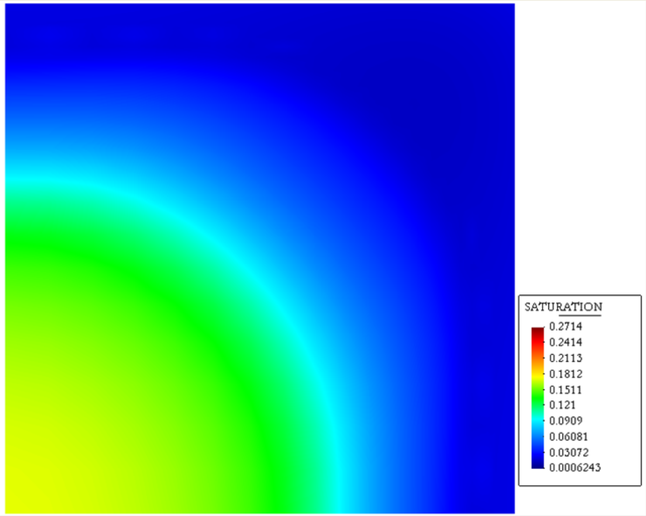
- **"Slow cooling": – 0.20 ºC/s**
- **"Fast cooling": – 20.0 ºC/s**



SUBTYPE OF COOLING	Initial time (s)	Final time (s)
HEATING STAGES COMMON TO ALL OF THE CALCULATIONS	0	4.920
SLOW ENVIRONMENTAL COOLING	4.920	7.320
FAST ENVIRONMENTAL COOLING	4.920 4.940	4.940 5.840

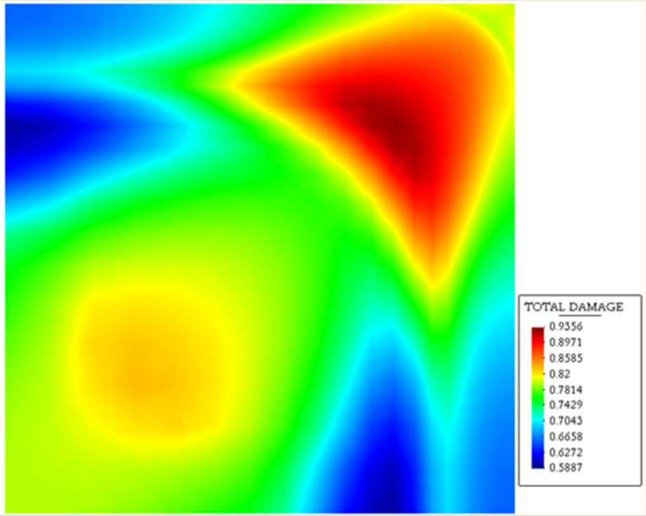
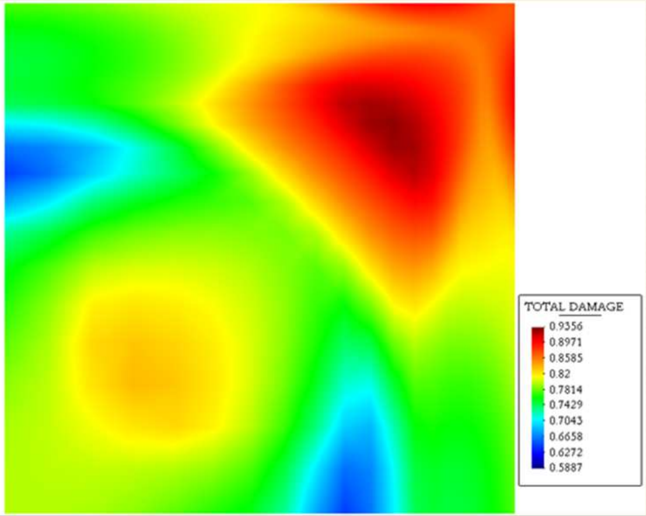
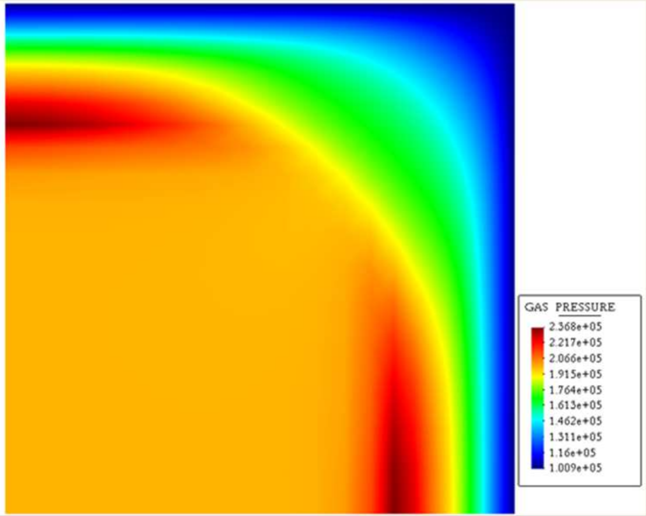
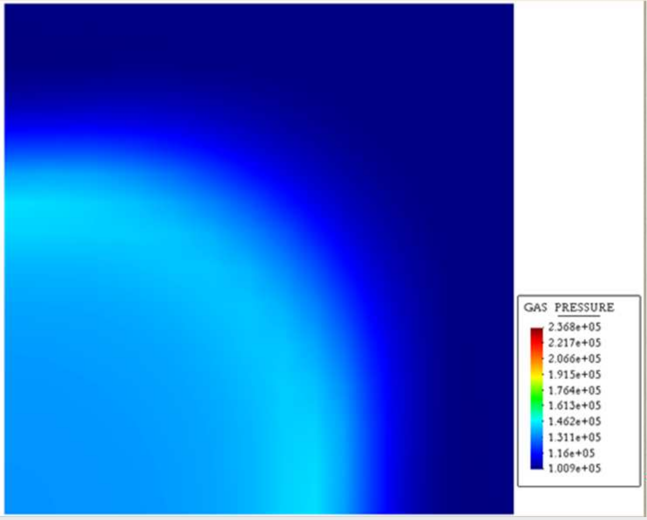
Analysis of cooling processes

SLOW (40 min) ENVIRONMENTAL COOLING

Par.	82 min. from fire start – at the beginning of cooling	122 minutes from fire start – at the end of slow cooling
TEMPERATURE T [K]		
SATURATION S [-]		

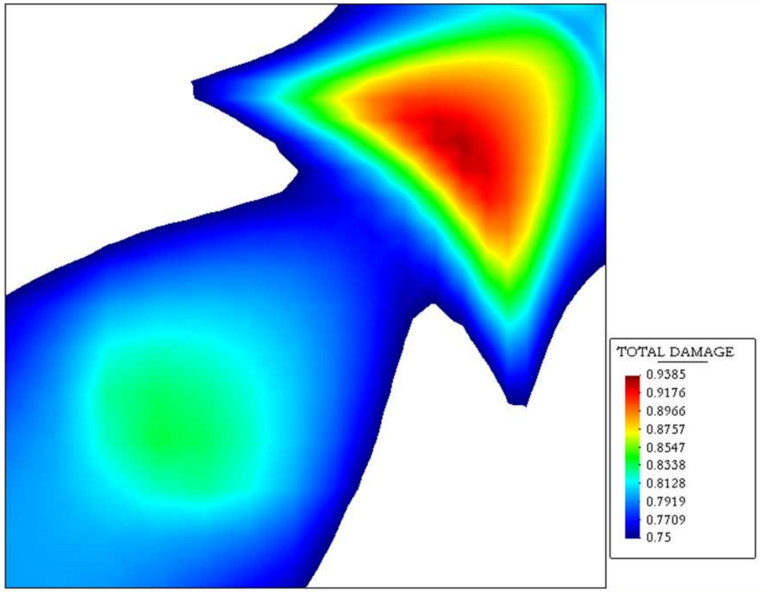
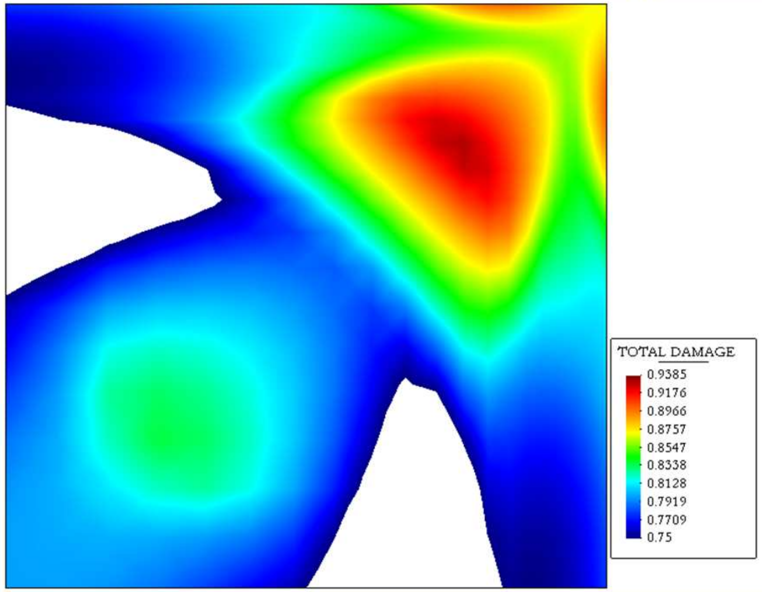
Analysis of cooling processes

SLOW (40 min) ENVIRONMENTAL COOLING

Par.	82 min. from fire start – at the beginning of cooling	122 minutes from fire start – at the end of slow cooling
TOTAL DAMAGE D [-]		
GAS PRESSURE Pg [Pa]		

Analysis of cooling processes

SLOW (40 min) ENVIRONMENTAL COOLING

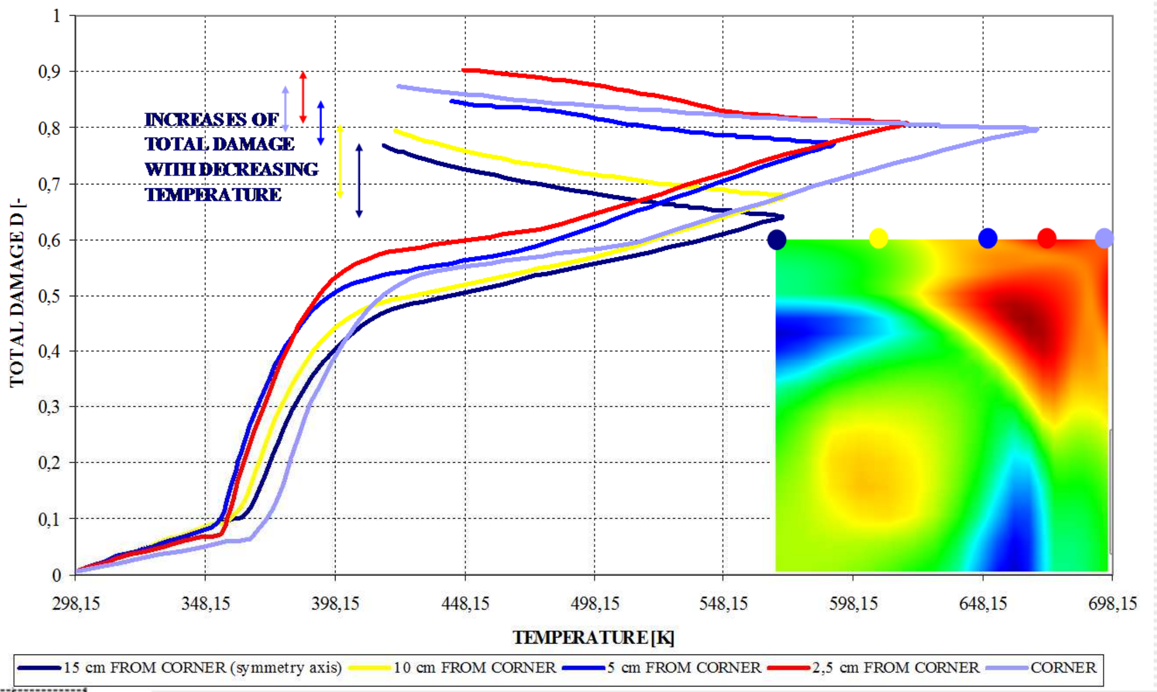
Param.	**82 min. fromfire start – at the beginningof slow cooling**	**122 minutesfromfire start – at the end of slow cooling**
TOTAL DAMAGE D [-]		

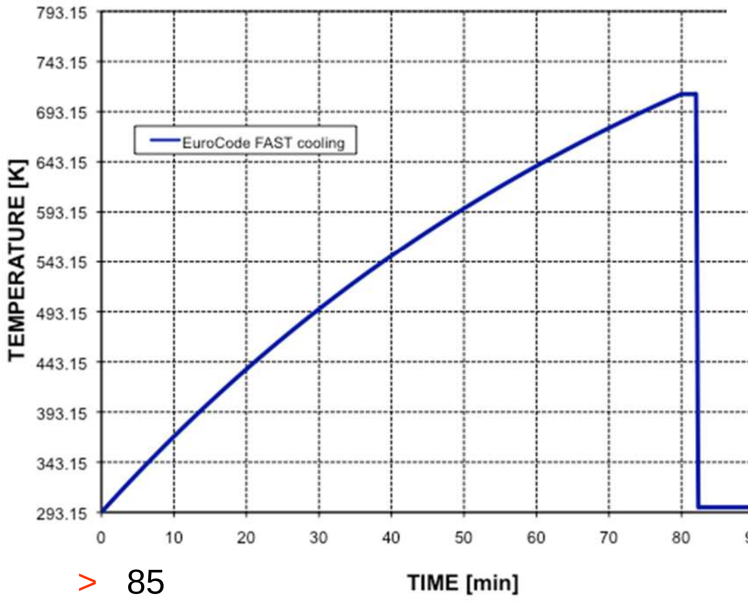
ZONES WITH AN INCREASE OF DAMAGE DUE TO COOLING (ESPECIALLY CLOSE TO THE SURFACE)

Analysis of cooling processes

FAST (20 sec) ENVIRONMENTAL COOLING

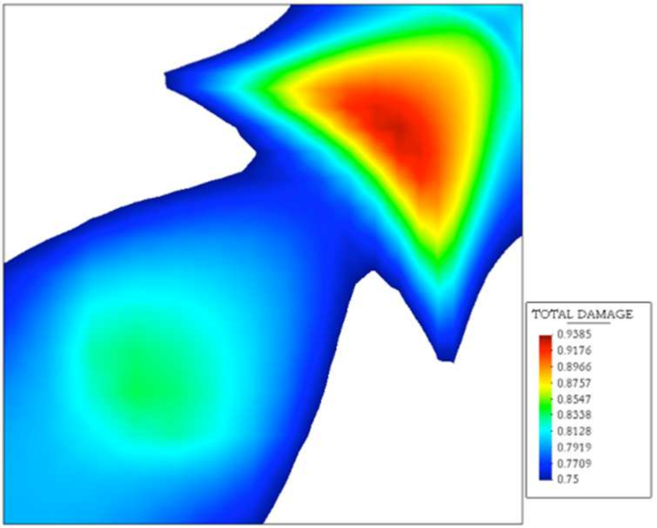
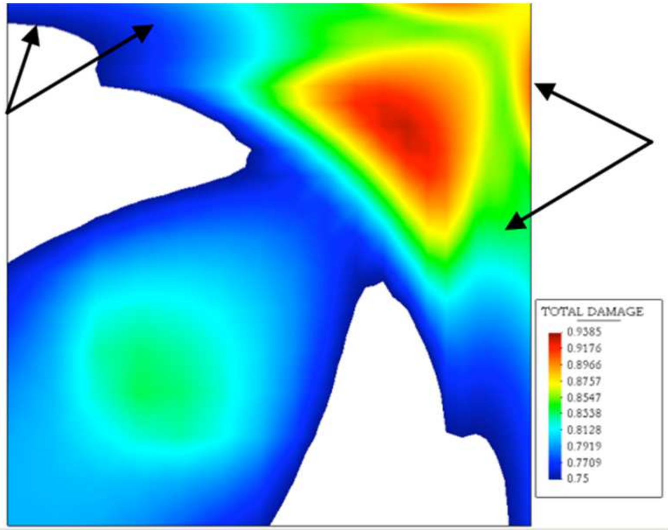
DURING COOLING PHASE IN THE ZONES CLOSE TO THE EXTERNAL SURFACES WE OBSERVE AN INCREASE OF DAMAGE D





Analysis of cooling processes

FAST (20 sec) ENVIRONMENTAL COOLING

Param.	**82 min. fromfire start – at the beginningof fast cooling**	**≈100 mins from fire start – at the end of the phase at constant ambient temperature**
TOTAL DAMAGE [-]		

Zones of the squares column with Total Damage higher than 0.75, at the beginning of the fast environmental cooling and at the end of the phase at constant ambient temperature

Conclusions

- A general model based on the mechanics of multiphase porous media for the analysis of thermo-hygral-chemical and mechanical behaviour of concrete has been presented.
- Some relevant applications of this model have been shown:
  - ✓ Concrete **maturing/hardening** process (i.e. hydration) and **long term behaviour** of concrete structures (i.e. creep development);
  - ✓ Concrete structures under **extreme conditions** in terms of pressure and temperature (high temperature);
  - ✓ Concrete exposed to chemical degradation by pure water (i.e. leaching) in both **isothermal** and **non-isothermal conditions**;
  - ✓ Concrete subject to **Alkali-Silica Reaction**;
- The **leaching model** considers not only the diffusive calcium transport, as other existing models, but additionally also the **advective calcium flow**.
- Calcium leaching process is modeled by considering **thermodynamic imbalance** of the calcium in solid and liquid phases, what allows for the description of **process kinetics**;
- The ASR model accounts for both **water content (i.e. saturation) and temperature** influence on the reaction evolution and the strain development;
- A **simplified version** of the model suitable for practical engineering application (e.g. concrete structures repair) has been formulated.