BUILDING
PHYSICS
IN THE
NORDIC
COUNTRIES

NSB 2011

9th Nordic Symposium on Building Physics

Effect of variable hygro-thermal conditions on chemical degradation of concrete structures due to alkali – silica reaction

Prof. D. Gawin, M.Sc. W. Grymin, Dr. M. Wyrzykowski

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

Dr. F. Pesavento

Department of Structural and Transportation Engineering
University of Padova – ITALY

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

This research was supported in part by the project POIG.01.01.02-10-106/09-00 funded by EU

Motivation

Building materials degradation caused by ASR

Damage due to the Alkali – Silica Reaction

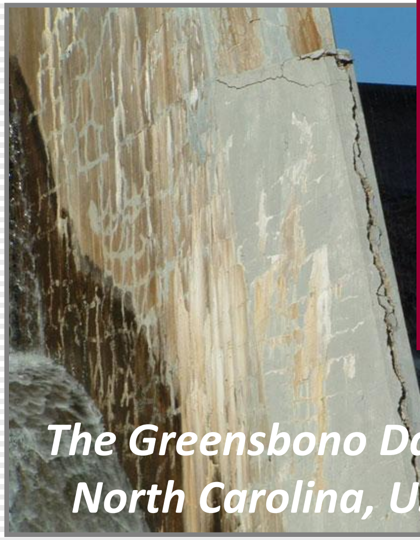
The Greensbono Dam,
North Carolina, USA

Bridge at the 6th Street,
Los Angeles, USA

Motivation

Building materials degradation caused by ASR

Damage due to the Alkali – Silica Reaction



The Greensbono Dam, North Carolina, USA

Expanding amorphous gel

Bridge at the 6th Street, Los Angeles, USA

Introduction

Modeling chemical degradation, leaching and ASR

Modeling chemical degradation

damage theory:
- ✓ Gerard - 1996
- ✓ Pijaudier-Cabot, Gerard, Molez– 1998

chemo-poro-plasticity:
- ✓ Ulm, Torrenti, Adenot - 1999

theory of reactive porous media:
- ✓ Kuhl, Bangert, Meschke - 2004

Modeling calcium leaching

- ✓ Adenot and Buil - 1992
- ✓ Gerard - 1996
- ✓ Ulm, Torrenti, Adenot - 1999
- ✓ Kuhl, Bangert, Meschke – 2004
- ✓ Gawin, Pesavento, Schrefler – 2008, 2009

Modeling salt transport and precipitation (equil. & nonequil.)

- ✓ Samson et al. - 2007
- ✓ Koniorczyk & Gawin –2008, 2011
- ✓ Koniorczyk – 2009, 2010

ASR reaction

- ✓ Larive – 1998
- ✓ Bazant, Steffens - 2000
- ✓ Ulm, Coussy, Kefei, Larive - 2000
- ✓ Poyet – 2003
- ✓ Steffens, Li, Coussy – 2003
- ✓ Bangert, Kuhl, Meschke – 2004
- ✓ Multon et al. – 2006, 2008
- ✓ Comi, Fedele, Perego - 2009

Theoretical Model

Transport Mechanisms

Capillary water (free water):

- ✓ advective flow *(water pressure gradient)*
- ✓ osmotic flow *(salt concentration gradient)*

Physically adsorbed water:

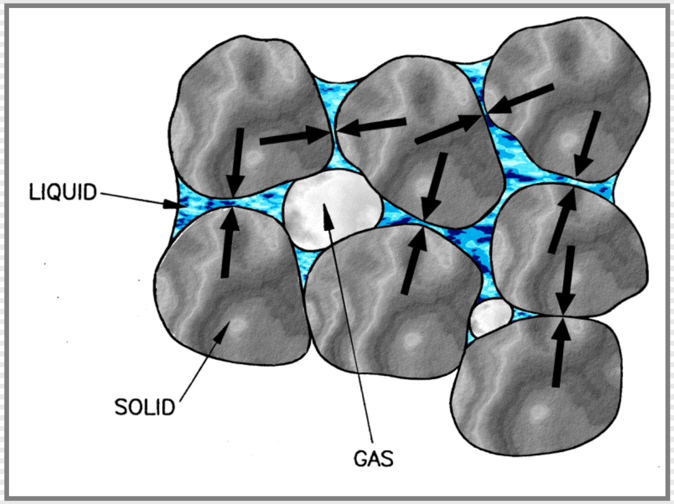
- ✓ diffusive flow *(water concentration gradient)*

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)*



Microscopic view of a three-phase porous material (concrete, rocks)

Theoretical Model

Phase Changes & Chemical Reactions

- ✓ ***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

---

- ✓ ***ASR reaction:*** Alkali (K^+ & Na^+ ions) + silica (aggregate) ⇒ expanding amorphous gel

Theoretical Model

Micro- ⇒ macro- description

Balance equations:

local formulation **(micro- scale)**

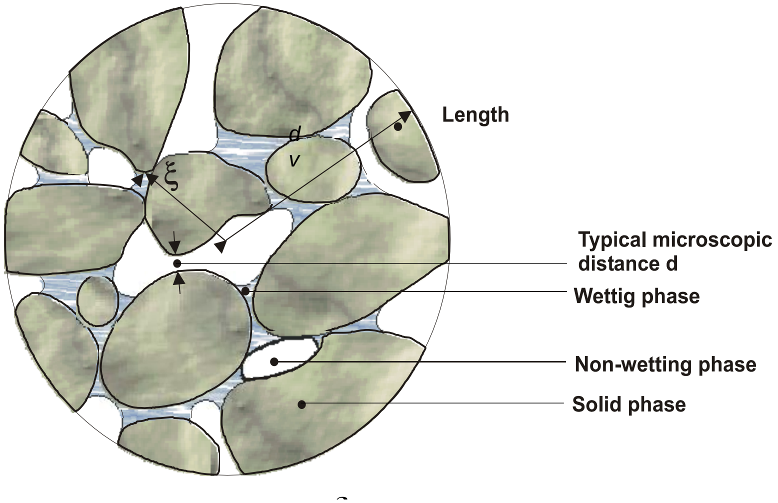
Volume Averaging Theory

by Hassanizadeh & Gray, 1979,1980

macroscopic formulation

(macro- scale)

Rational Thermodynamics



Representative Elementary Volume

Model development:

- ***Lewis & Schrefler:*** *"The FEM in the Static and Dynamic ...", Wiley,* ***1998***
- ***Gawin:*** *" Modelling of coupled hygro-thermal phenomena in building materials …", Hab. Thesis, Łódź,* ***2000***

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 multiphase medium momentum balance (mechanical equilibrium)

- ✓ Evolution equation for mechanical damage
- ✓ Evolution equation for chemical damage (due to ASR)
- ✓ Evolution equation for chemical reaction (ASR)

Theoretical Model

State variables & internal variables

- ✓ Gas pressure – p^g
- ✓ Capillary pressure – p^c
- ✓ Temperature – T;
- ✓ Displacement vector – $[u_x, u_y, u_z]$

- ✓ Mechanical damage degree – *d*
- ✓ Chemical damage degree – *V*
- ✓ Reaction degree (ASR – Γ_{ASR})

Theoretical fundamentals and model development:

- ➢ ***Gawin, Pesavento, Schrefler***, *CMAME 2003, Mat.&Struct. 2004, Comp.& Conc. 2005*
- ➢ ***Gawin, Pesavento, Schrefler***, *IJNME 2006 (part 1, part2)*
- ➢ ***Koniorczyk, Gawin***, *J. Build. Phys. 2008, Transport in Porous Media 2010*

Theoretical Model

Strain decomposition

Total strain of concrete, $\boldsymbol{\varepsilon}_{tot}$, can be split into :

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

Strain decomposition

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

Free thermal strain strain

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

Shrinkage strain

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

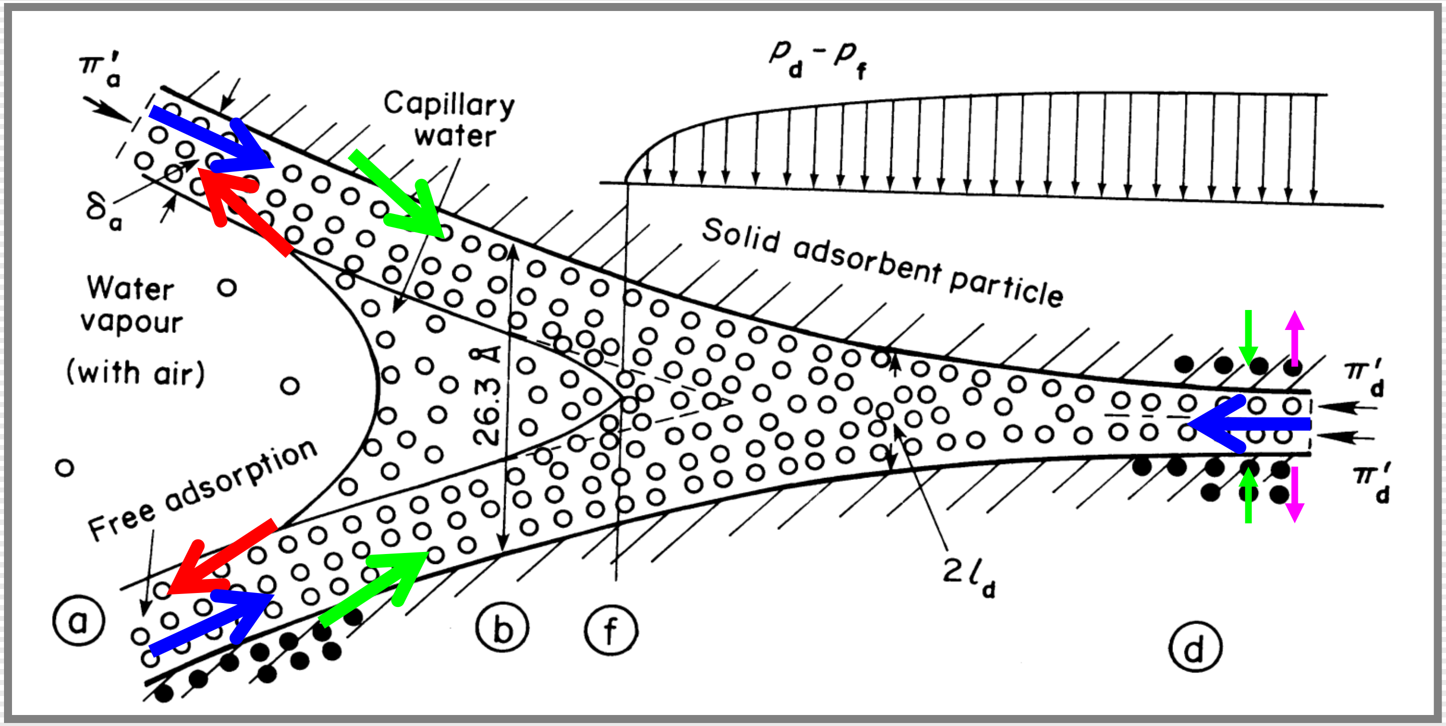
Thermo-chemical strain

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

Theoretical Model

Shrinkage strains of concrete

Capillary pressure & disjoining pressure



Forces:

in water

Capillary pressure

←

Disjoining pressure

←

in skeleton

Capillary pressure

←

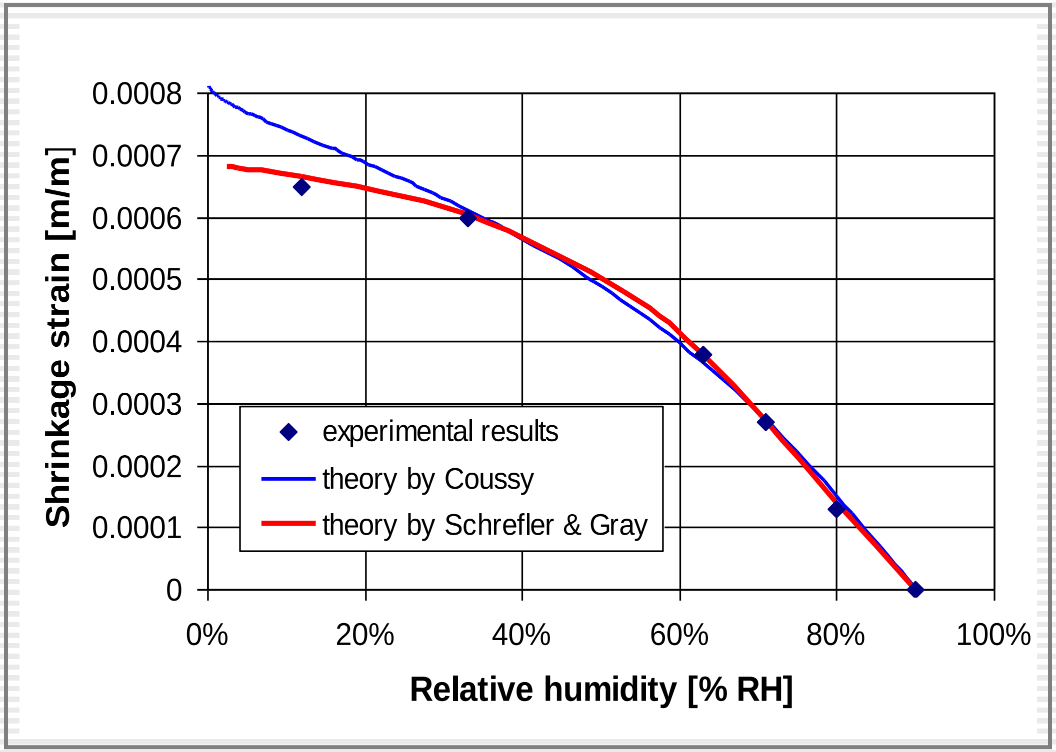
Disjoining pressure

←

Theoretical Model

Shrinkage strains of concrete

Effective stress principle:



- *[Gray & Schrefler, 2001]*

$$\boxed{\boldsymbol{\sigma}_e^s = \boldsymbol{\sigma} + \alpha\,\mathbf{I}\,p^s}$$

$$\boxed{p^s = p^g - \chi_s^{ws}\,p^c}$$

Experimental data from:

- *[Baroghel-Bouny, et al., Cem. Concr. Res. 29, 1999]*

Mathematical model

Model of Alkali – Silica Reaction evolution rate

$$\frac{\partial \Gamma_{ASR}}{\partial t} = \frac{1-\Gamma_{ASR}}{t_r}$$

with

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

☐ ***Ref.: Larive et al,***
J. of Engineering Mechanics 2000

where the reaction time is given by:

$$t_r = \tau_r\left(T,\boxed{S_w}\right)\cdot\lambda\left(T,\boxed{S_w,}\Gamma_{ASR}\right)$$

$$\lambda\left(T,S_w,\Gamma_{ASR}\right) = \frac{1+\exp\left(-\tau_L/\tau_r\right)}{\Gamma_{ASR}+\exp\left(-\tau_L/\tau_r\right)}$$

Latency time

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

Influence of the saturation degree

Characteristic time

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

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

Mathematical model

Model of strains due to Alkali – Silica Reaction

Evolution of ASR strain Γ_{ASR} : final form

$$\frac{\partial \boldsymbol{\varepsilon}_{ASR}}{\partial t} = \tilde{\beta}_{ASR}(S_w)\cdot(1-\Gamma_{ASR})^{\tau_{r0}/\tau_{a0}} \cdot \frac{\partial \Gamma_{ASR}}{\partial t}\,\mathbf{I}$$

Influence of the S_w and T on the strain rate

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

$$\tilde{\beta}_{ASR}(S_w) = \tilde{\beta}_{ASR0}(S_w)^{\tilde{C}_{ASR}} \qquad \text{power formulation}$$

$\tilde{\beta}_{ASR0}, \tilde{A}_{ASR}, \tilde{B}_{ARS}, \left(\text{or } \tilde{C}_{ARS}\right)$

are material parameters

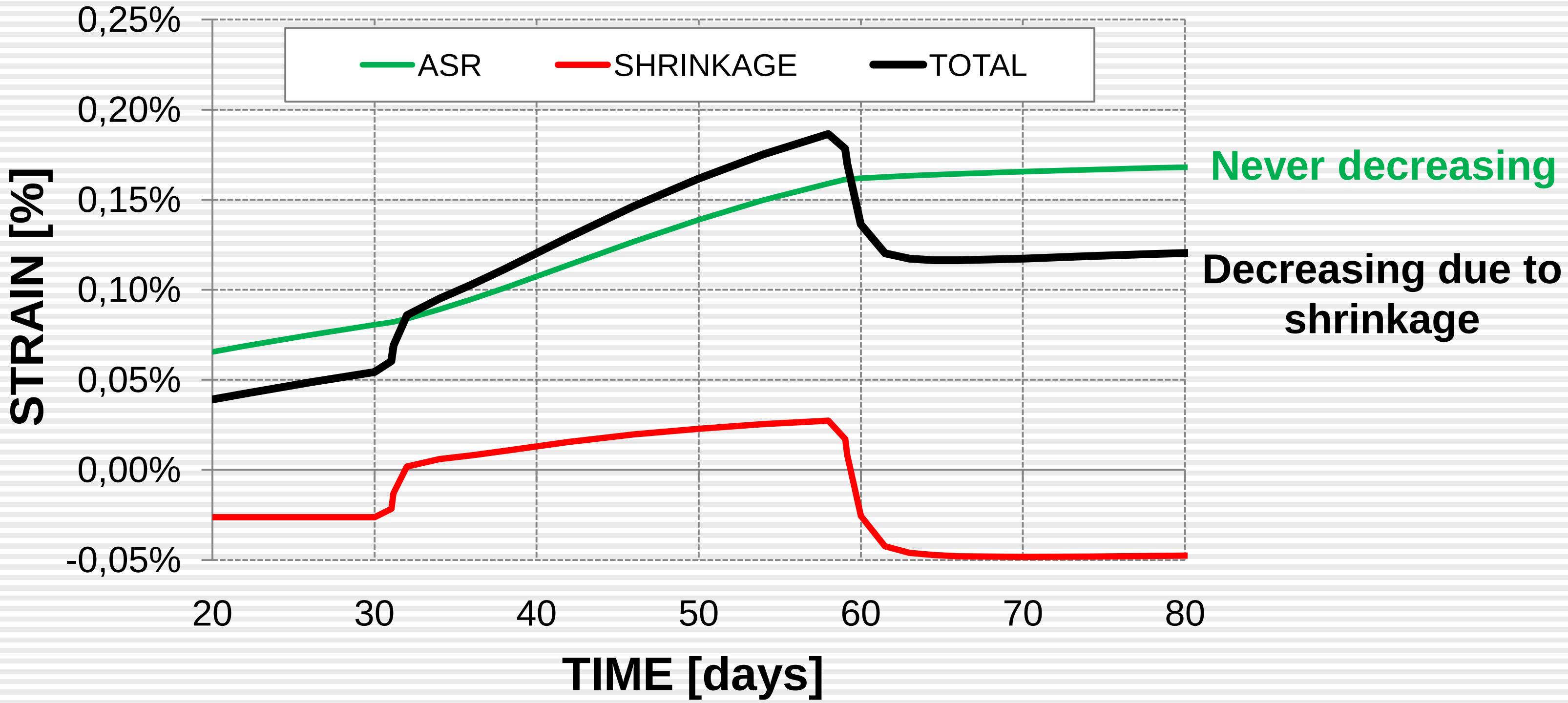
$$\tau_L(T,S_w) = \tau_{L0}\cdot\exp\left[U_L\cdot\left(\frac{1}{T}-\frac{1}{T_0}\right)\right]\cdot(A_L\cdot S_w + B_L)$$

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

- ☐ ***Ref.: Steffens et al****, Eng. Mech. 2003*
- ☐ ***Ref.: Bangert et al****, IJNME 2004*

Theoretical Model

Strains at variable humidity



Strain components:

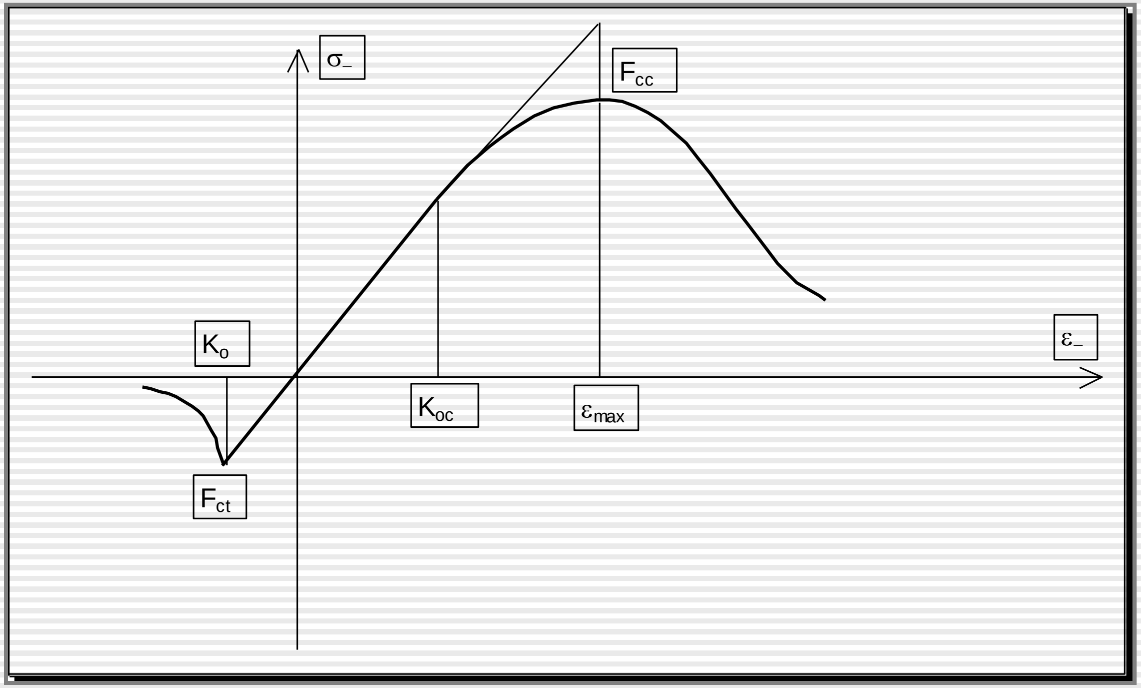
$$\boxed{d\boldsymbol{\varepsilon}_{tot} = d\boldsymbol{\varepsilon}_{shrink} + d\boldsymbol{\varepsilon}_{ASR}}$$

Theoretical Model

Mechanical material degradation

Non-local isotropic damage theory

[Mazars & Pijaudier-Cabot, 1989]



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

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

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

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

Theoretical Model

Constitutive relationships for ASR

Constitutive relationships for the densities

- *Density of the reacted material:*

$$\rho^r = \frac{\rho^u}{1 + \operatorname{tr} \boldsymbol{\varepsilon}^{\infty}_{ASR}}$$

- *Density of the solid phase:*

$$\rho^s = \frac{\rho^u}{1 + \Gamma_{ASR}\left(\rho^u / \rho^r - 1\right)} = \frac{\rho^u}{1 + \Gamma_{ASR} \operatorname{tr} \boldsymbol{\varepsilon}^{\infty}_{ASR}}$$

Constitutive relationships for the sorption isotherms

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

Constitutive relationships for the intrinsic permeability

$$k = k_o \cdot 10^{A_k\left(\varepsilon^{vol}_{ASR} / \varepsilon^{vol}_{ASR,\infty}\right)}$$

Numerical Solution

Discretization and linearization the model equations

Governing equations of the model

Galerkin's (weighted residuum) method

Variational (weak) formulation

FEM (in space)

FDM (in the time domain)

Discretized form (non-linear set of equations)

Numerical Solution

Discretization and linearization the model equations

Discretized form (nonlinear equations)

↓ *the Newton - Raphson method*

Solution of the final, linear equation set

↓ *the frontal, monolithical solver*

Computer code (COMES / HMTRA family)

Numerical Solution

Matrix form of the FEM-discretised governing equations

$$\mathbf{C}_{gg}\frac{\partial\bar{\mathbf{p}}^g}{\partial t}+\mathbf{C}_{gc}\frac{\partial\bar{\mathbf{p}}^c}{\partial t}+\mathbf{C}_{gt}\frac{\partial\bar{\mathbf{T}}}{\partial t}+\mathbf{C}_{gu}\frac{\partial\bar{\mathbf{u}}}{\partial t}+\mathbf{K}_{gg}\bar{\mathbf{p}}^g+\mathbf{K}_{gc}\bar{\mathbf{p}}^c+\mathbf{K}_{gt}\bar{\mathbf{T}}=\mathbf{f}_g$$

$$\mathbf{C}_{cc}\frac{\partial\bar{\mathbf{p}}^c}{\partial t}+\mathbf{C}_{ct}\frac{\partial\bar{\mathbf{T}}}{\partial t}+\mathbf{C}_{cu}\frac{\partial\bar{\mathbf{u}}}{\partial t}+\mathbf{K}_{cg}\bar{\mathbf{p}}^g+\mathbf{K}_{cc}\bar{\mathbf{p}}^c+\mathbf{K}_{ct}\bar{\mathbf{T}}=\mathbf{f}_c$$

$$\mathbf{C}_{sc}\frac{\partial\bar{\mathbf{p}}^c}{\partial t}+\mathbf{C}_{st}\frac{\partial\bar{\mathbf{T}}}{\partial t}+\mathbf{C}_{su}\frac{\partial\bar{\mathbf{u}}}{\partial t}+\mathbf{K}_{sg}\bar{\mathbf{p}}^g+\mathbf{K}_{sc}\bar{\mathbf{p}}^c+\mathbf{K}_{st}\bar{\mathbf{T}}=\mathbf{f}_s$$

$$\mathbf{C}_{ug}\frac{\partial\bar{\mathbf{p}}^g}{\partial t}+\mathbf{C}_{uc}\frac{\partial\bar{\mathbf{p}}^c}{\partial t}+\mathbf{C}_{ut}\frac{\partial\bar{\mathbf{T}}}{\partial t}+\mathbf{C}_{uu}\frac{\partial\bar{\mathbf{u}}}{\partial t}+\mathbf{K}_{uu}\bar{\mathbf{u}}=\mathbf{f}_u$$

where $\mathbf{K}_{ij}$ - related to the primary variables

$\mathbf{C}_{ij}$ - related to the time derivative of the primary variables

$\mathbf{f}_{i}$ - related to the other terms, eg. BCs (*i,j=g,c,t,s,**u***)

Modelling Silica Alkali Reaction

Validation of the model

- ✓ Material properties and size of the specimens as in:

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

- ✓ Boundary conditions:

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

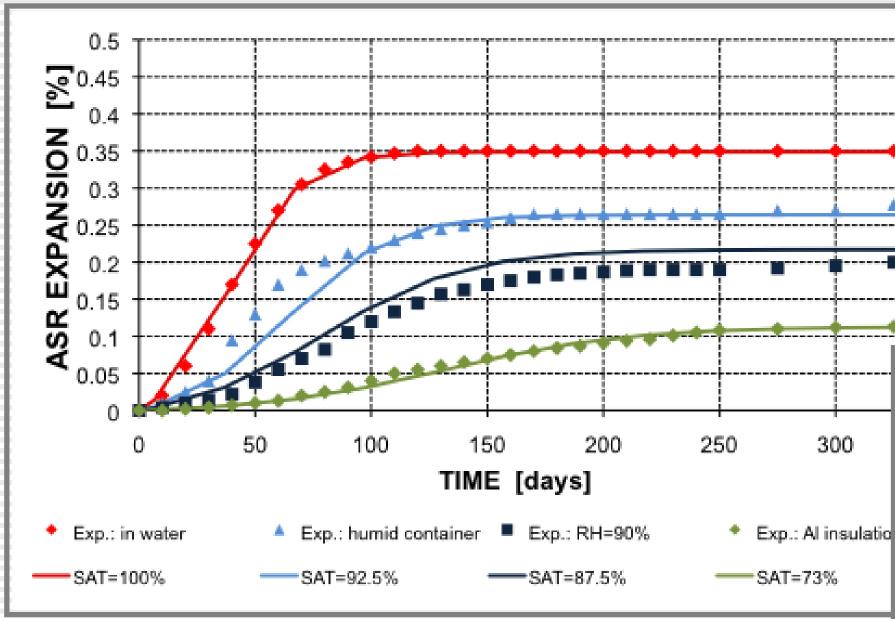
- ✓ Thermo-hygral conditions during the experimental tests (constant):

  T_o= 23 °C, 38°C, 60°C at S_w = 87.5% ;

  S_w= 100%, 92.5%, 87.5%, 73% at T= 38°C;

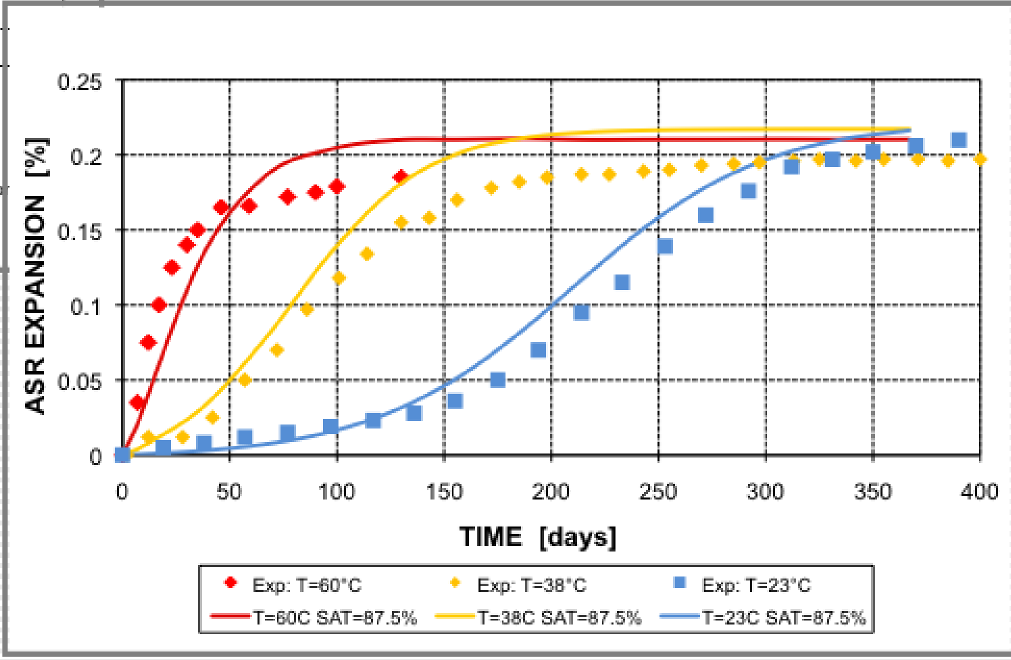
Modelling Silica Alkali Reaction

Validation of the model



Influence of saturation degree

(Steffens, 2003 after Larive, 1998)



Influence of temperature

(Larive, 1998)

Modelling Silica Alkali Reaction

Experimental - numerical results comparison

Poyet's 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, Univ. de Marne la Vallée, **2003**.

- ✓ Size of the specimens:

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

27

- ✓ Boundary conditions:

  - convective heat and mass exchange:

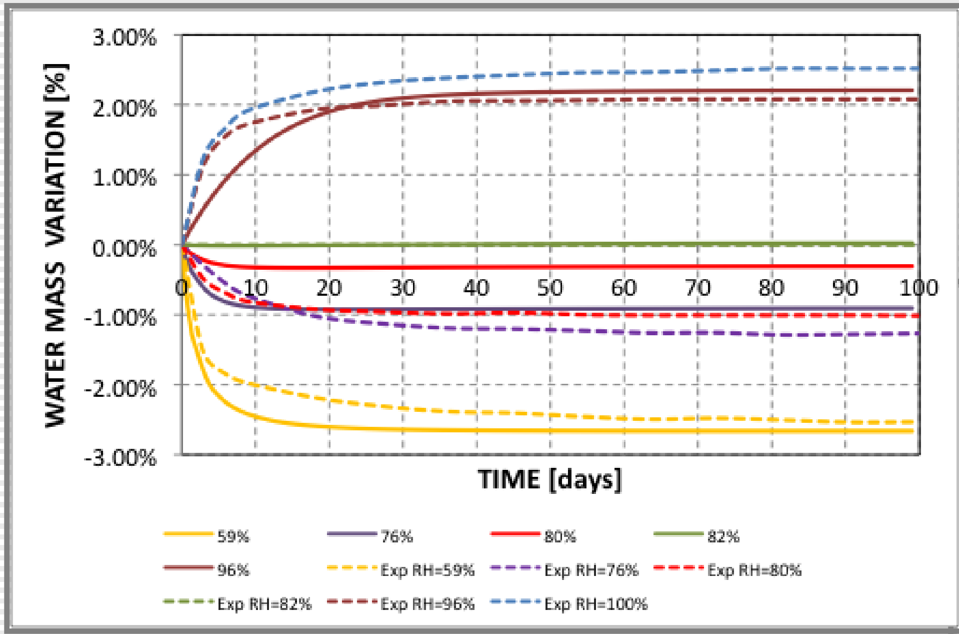
- RH_{∞}=82%, and then 59%, 76%, 82%, 96% or 100% kept constant in time with β_c=0.002 m/s (drying cases) and β_c=0.002 m/s (swelling cases)
- T=60°C with α_c=5 W/Km^2

  - surface mechanical load: unloaded

Modelling Silica Alkali Reaction

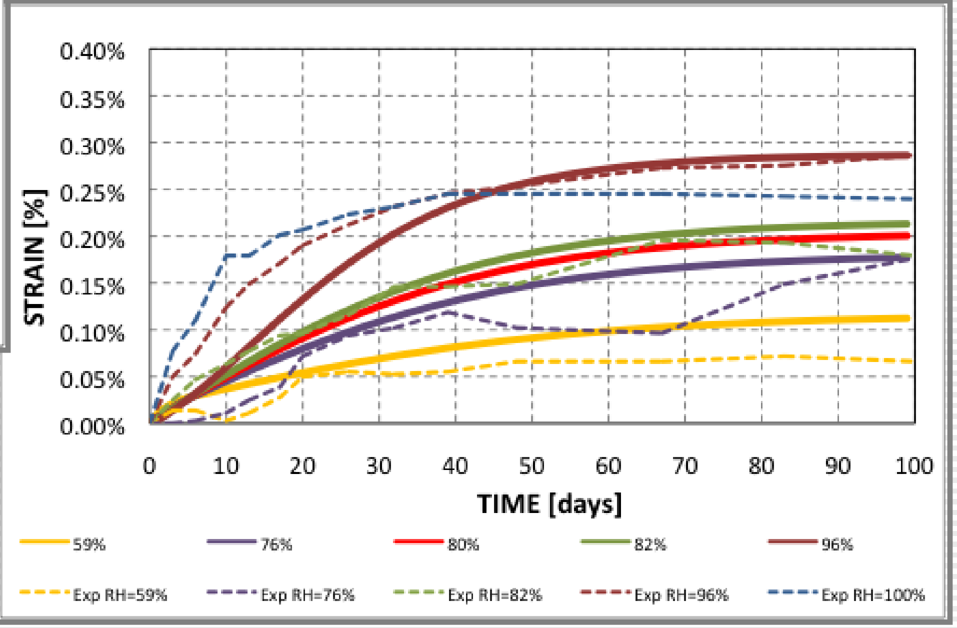
Experimental - numerical results comparison

Poyet's tests at constant relative humidity



Mass variation

ASR strain evolution



Modelling Silica Alkali Reaction

Experimental - numerical results comparison

Poyet's 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, Univ. de Marne la Vallée, **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)

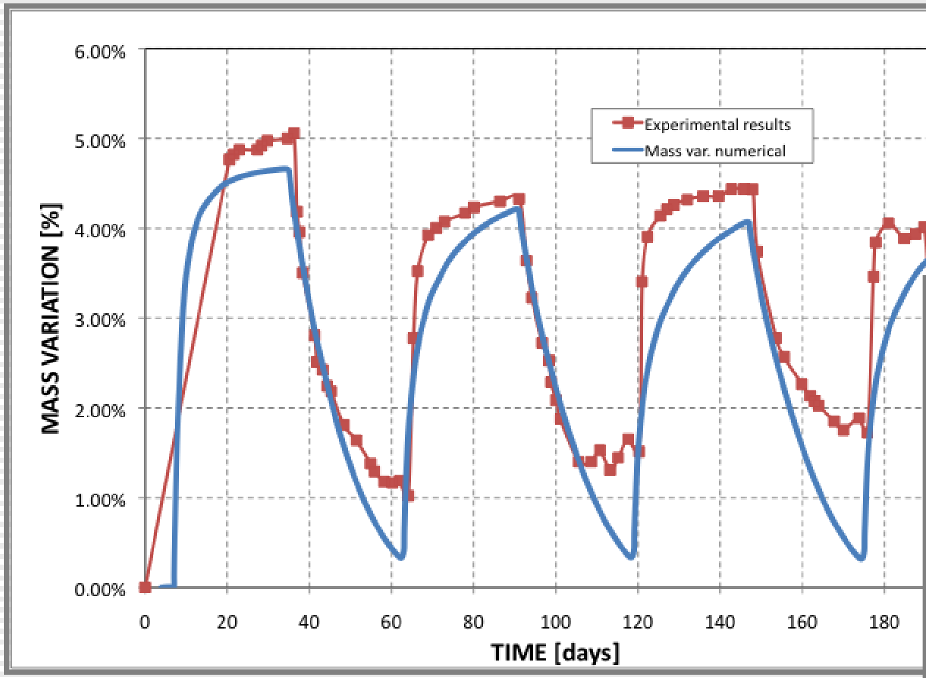
  β_c=0.002 m/s (drying phases) and β_c=0.002 m/s (swelling phases)

- T=60°C with α_c=5 W/Km^2

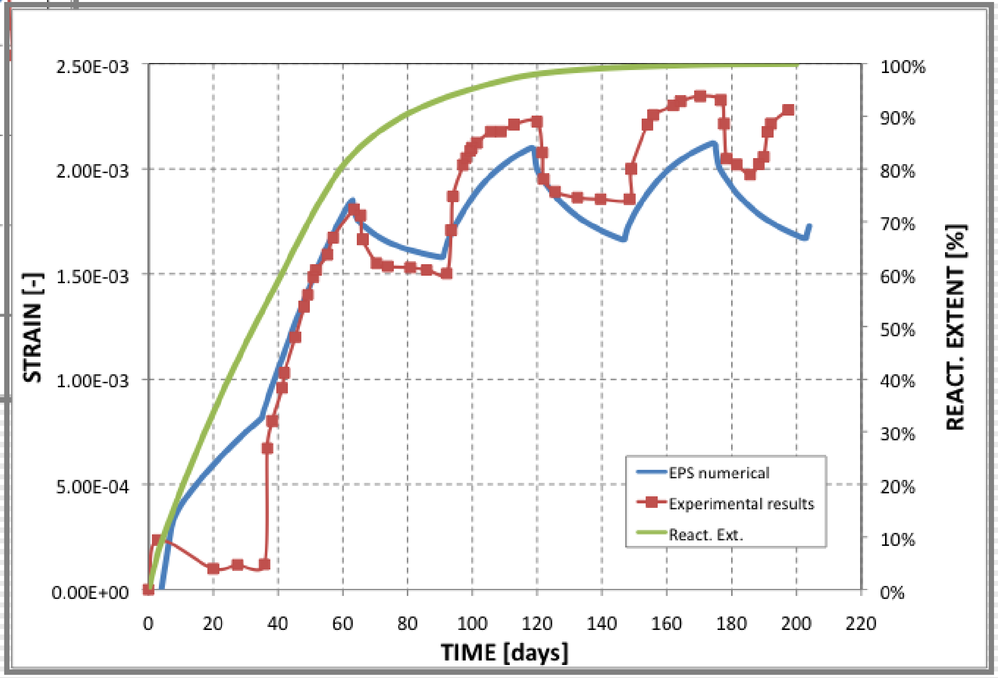
Modelling Silica Alkali Reaction

Experimental - numerical results comparison

Poyet's tests at variable relative humidity (long cycle)



Mass variation

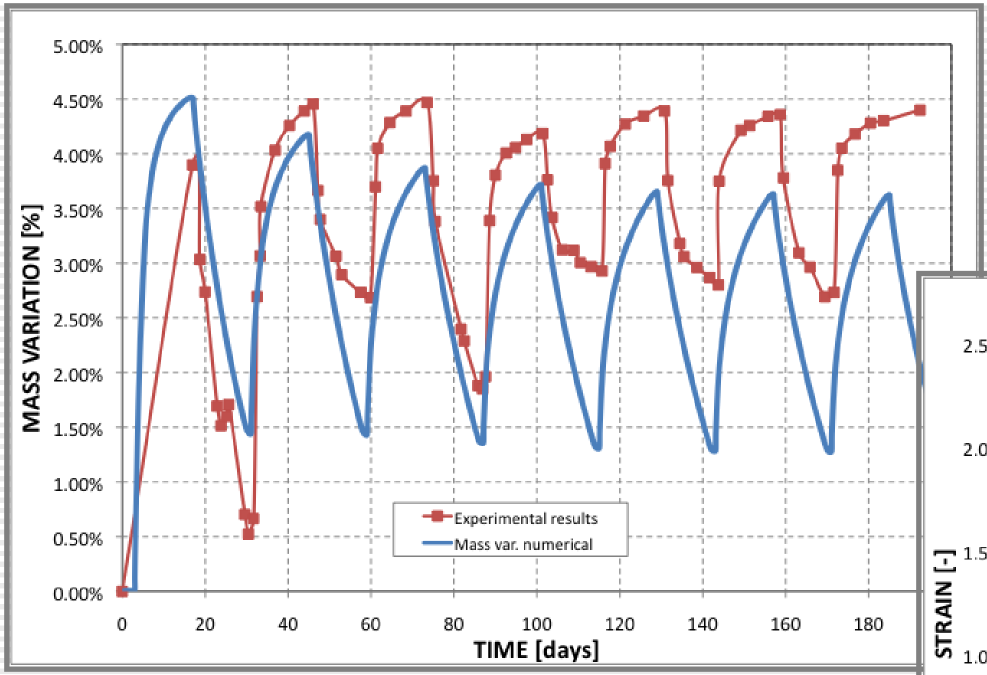


ASR strain and react. extent evolution

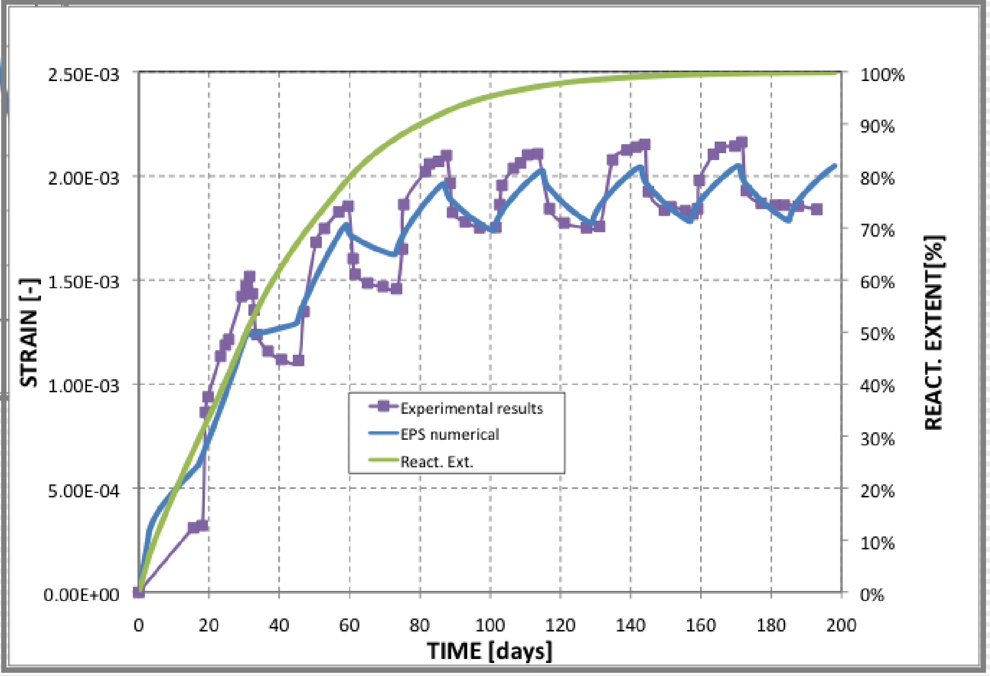
Modelling Silica Alkali Reaction

Experimental-Numerical results comparison

Poyet's tests at variable relative humidity (short cycle)



Mass variation



ASR strain and react. extent evolution

Final Remarks & Conclusions

- A general model based on the **mechanics of multiphase porous media** for the analysis of thermo-hygral processes, as well as chemical and mechanical degradation of concrete has been presented.
- The model accounts for both **variable water content** (saturation) and **temperature influence on the ASR reaction evolution** and the strain development
- The **rate type ASR model** has been presented and compared to available experimental results

Future research:

- Extension the ASR model for taking into account the anisotropy and the dependence of ASR strain on load level.
- Implementation of mechanical and chemical damage.
- 3-D computer code

Final Remarks & Conclusions

Modeling chemical reactions with a **kinetic (rate) approach** allows for taking into account the effect of variable temperature and moisture content on the chemical degradation processes .

Future research:

- Extension the ASR model for taking into account the anisotropy and the dependence of ASR strain on load level.
- Implementation of mechanical and chemical damage.
- 3-D computer code

Effect of variable hygro-thermal conditions on chemical degradation of concrete structures due to alkali – silica reaction

Thank you for your attention !

Questions ?

Modelling Silica Alkali Reaction

Multon's experimental tests

Description

- ✓ Material properties as in:

  S. Multon, F. Tiutlemonde, Effect of applied stress on alkali-silica reaction-induced expansion, Cement and Concrete Research, 36, 912-920, 2006

- ✓ Material tested: reacted and unreacted material

- ✓ Size of the specimens:

  Cylindrical specimens – diameter=130 mm, height=240 mm

- ✓ Boundary conditions:

  \- convective heat and mass exchange:

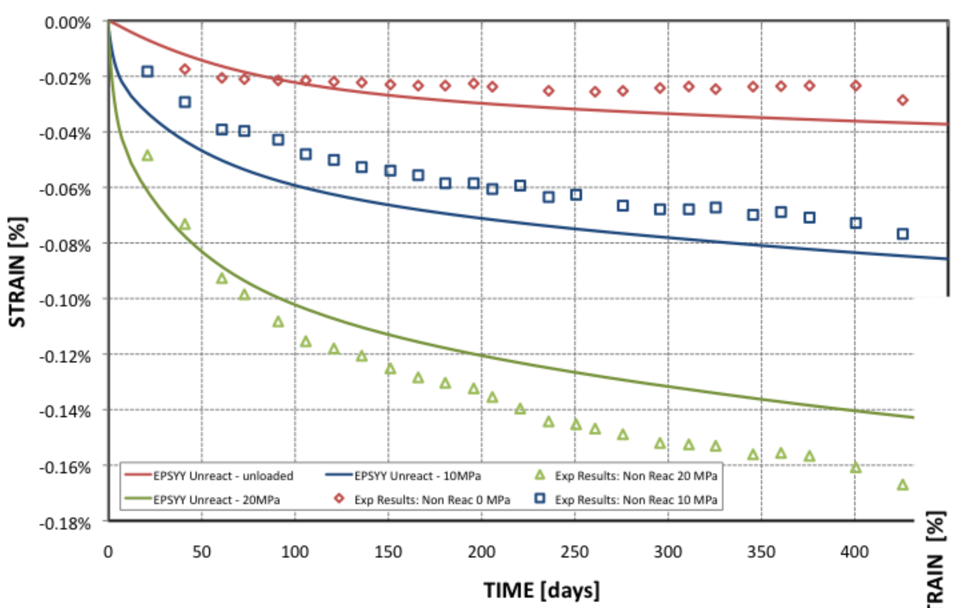
  - RH_∞=91% constant in time with β_c=0.000070 m/s
  - T=38°C with α_c=1 W/Km^2

  \- surface mechanical load: 0 MPa, 10 MPa, 20 MPa

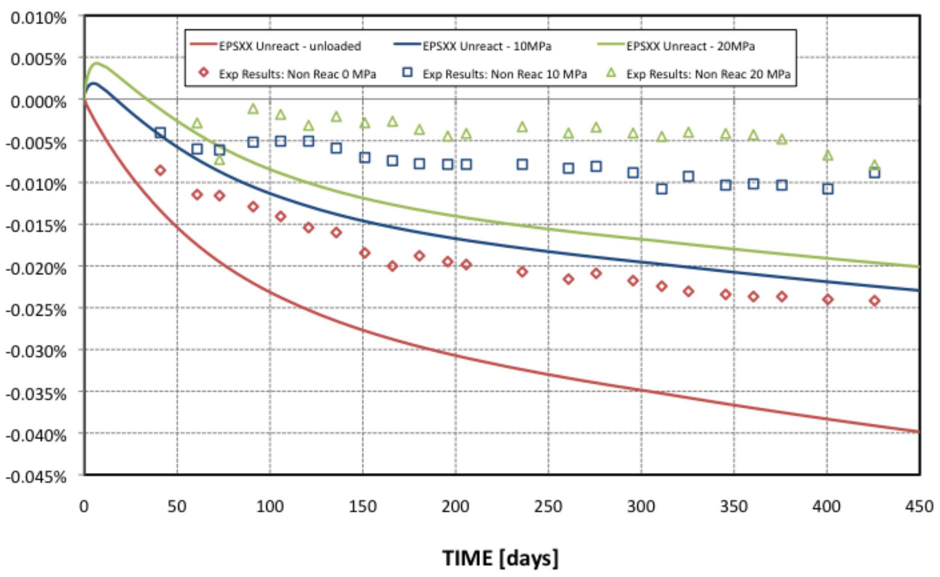
Modelling Silica Alkali Reaction

Multon's experimental tests

Results for the unreacted material



ASR axial strain evolution

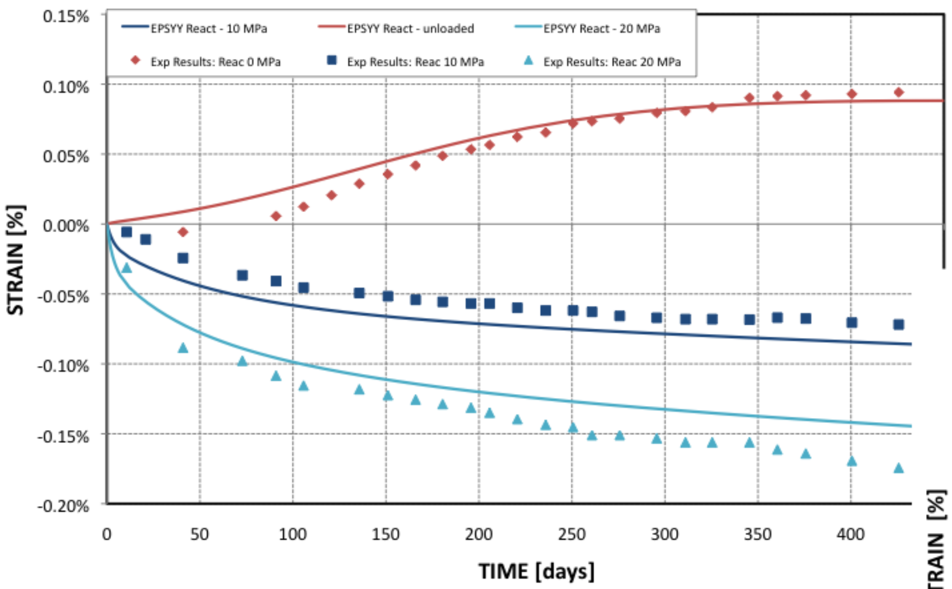


ASR radial strain evolution

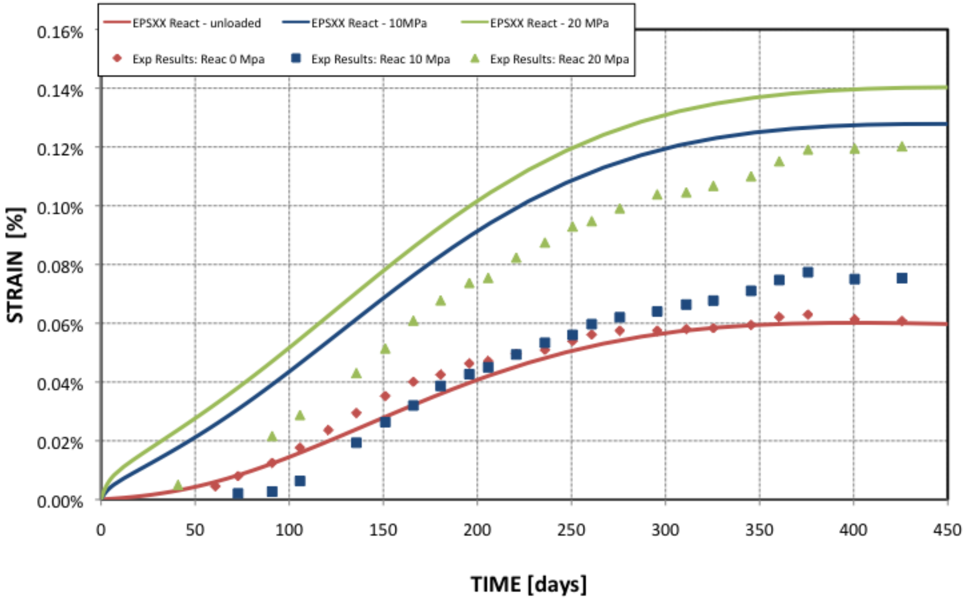
Modelling Silica Alkali Reaction

Multon's experimental tests

Results for the reacted material



ASR axial strain evolution



ASR radial strain evolution

Theoretical Model

Fundamental hypotheses

- Thermodynamical equilibrium state locally (slow phenomena)
- Concrete treated as a deformable, multiphase porous material
- Phase changes and chemical reactions (hydration, ASR) taken into account
- Full coupling: hygro-thermo-mechanical ⇒ chemical reaction *(ASR and strain development)*
- Various mechanisms of moisture- and energy- transport characteristic for the specific phases of concrete
- Evolution in time of material properties, e.g. densities, permeabilities, sorption isotherms, according to the reaction degree
- Non-linearity of material properties due to temperature, gas pressure, moisture content and material degradation

Theoretical Model

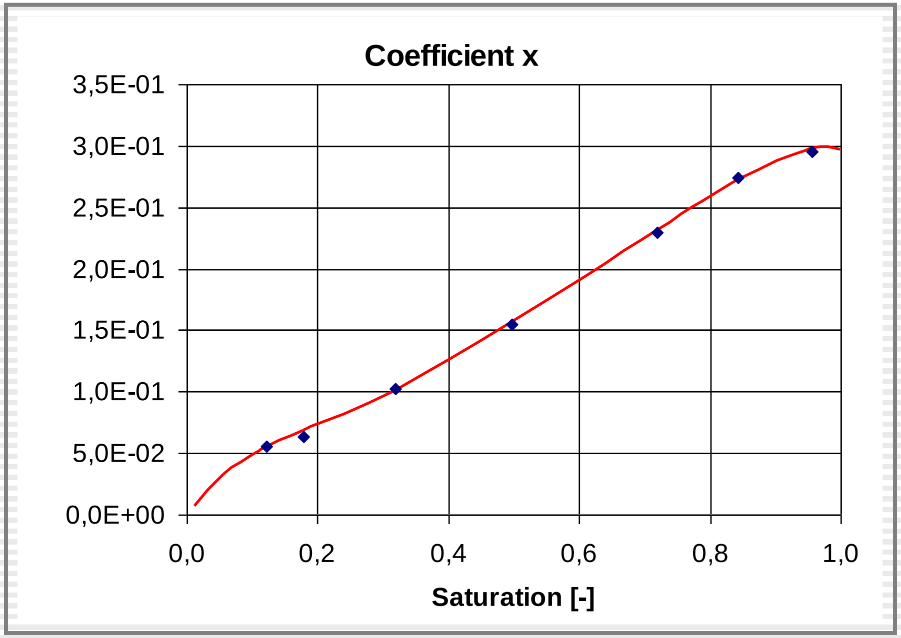
Shrinkage strains of concrete

Effective stress principle:

$$\boldsymbol{\sigma}_e^s = \boldsymbol{\sigma}^s + \alpha \mathbf{I} p^s$$

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

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



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

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

Layout

- Introduction
  - Existing models vs the model proposed
- General theoretical model
  - Mathematical model of concrete as multiphase porous material
- Modelling the alkali-silica reaction (ASR)
  - Chemical reaction evolution
  - Strain development
- Numerical solution of the model equations
- Validation of the model
  - Tests at various RH (constant temperature) - (Larive et al.)
  - Tests at various temperatures (RH constant) - (Larive et al.)
  - Tests at variabile relative humidity (Poyet et al.)
  - Tests at constant RH with various loads (Multon et al.)
- Conclusions and final remarks

Theoretical Model

Chemical material degradation

$$V = 1 - \frac{E_0(\Gamma_{ASR})}{E_0(\Gamma_{ASR} = 0)}$$

Joint effect of mechanical and chemical damage

[Pijaudier-Cabot, Gerard, Molez – 1998]

$$D = 1 - \frac{E(\Gamma_{ASR})}{E_0(\Gamma_{ASR} = 0)} = 1 - \frac{E(\Gamma_{ASR})}{E_0(\Gamma_{ASR})} \frac{E_0(\Gamma_{ASR})}{E_0(\Gamma_{ASR} = 0)} = 1 - (1 - d)(1 - V)$$

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