

Modeling of leaching-mechanical coupling in concrete

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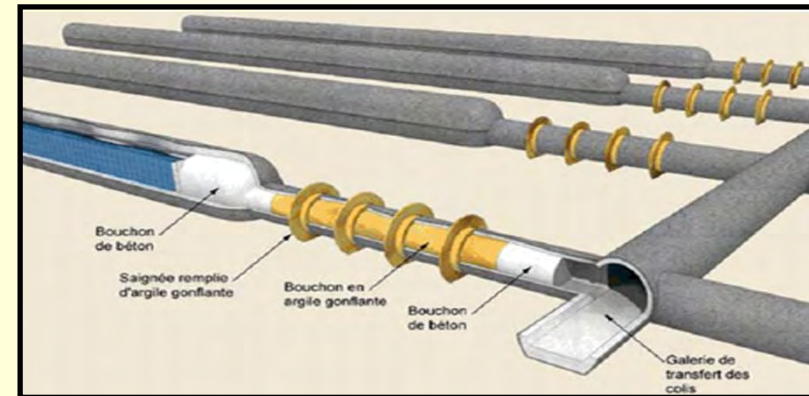
Plan

- Background and problem
- Mechanical model
- Leaching
- Coupling model
- Conclusions and perspectives

Background

Where is the studied concrete?

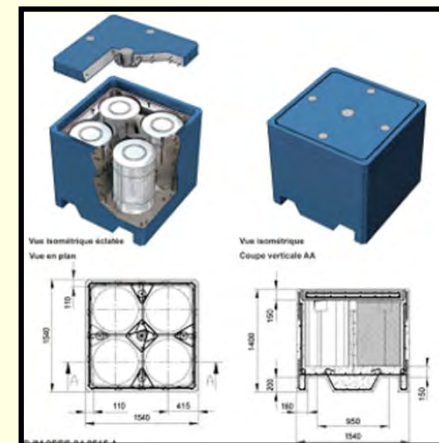
- Structures;
- Seal material;
- Stock cell of nuclear waste B.



Representation of closed tunnel [ANDRA]

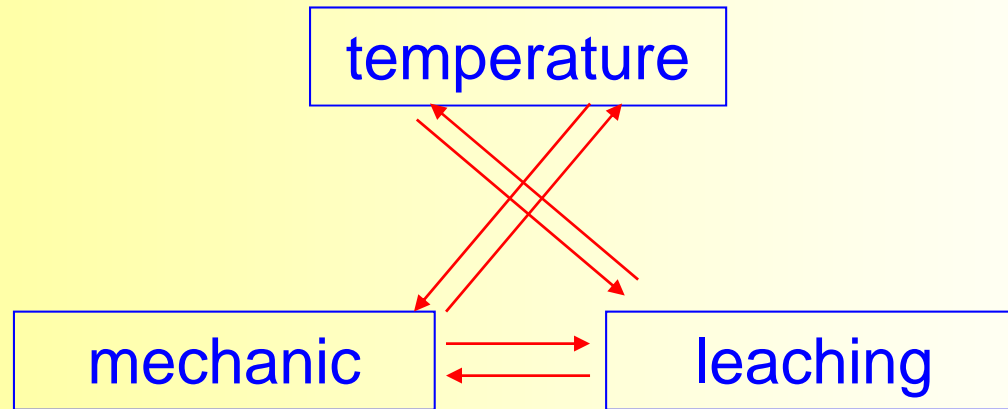
Which is the concrete subjected?

- Thermal load;
- Mechanical evolution;
- Chimical degradation.



Representation of stock cell of nuclear waste B [ANDRA]

Problem



Implemented models in COMSOL for concrete

- ✓ Mechanical
- ✓ Leaching
- ✓ Leaching-mechanical coupling

Mechanical model

1) Plastic damage modeling

- Plastic characterization

Criterion of Drucker-Prager

$$f_p(\sigma_{ij}, \gamma^p, d_m) = q + \eta p - \alpha(\gamma^p, d_m) K = 0$$

$$\alpha(\gamma^p, d_m) = (1 - d_m) \left[\alpha_0 + (\alpha_m - \alpha_0) \frac{\gamma^p}{b_1 + \gamma^p} \right]$$

$$\eta = \frac{1}{\sqrt{3}} \left(\frac{2Rc}{Rt + Rc} - 1 \right)$$

Rc : Uniaxial compression strength

$$K = \frac{2}{\sqrt{3}} \left(\frac{Rt \cdot Rc}{Rt + Rc} \right)$$

Rt : Tension strength

Mechanical model

1) Plastic damage modeling

- Associated plasticity

$$d\varepsilon_{ij}^p = d\lambda \frac{\partial f_p}{\partial \sigma_{ij}}$$

- Damage characterization

$$d_m = \bar{d}_{mc} \left[1 - \exp\left(-b_2 \gamma^p\right) \right]$$

- Effective modulus

$$\sigma_{ij} = \left[(1 - d_m) C_{ijkl}^0 \right] : \varepsilon_{kl}^e$$

Mechanical model

1) Plastic damage modeling

- Plane stress module for plastic damage modeling subdomain settings

The image shows a software interface with two overlapping dialog boxes. The background dialog is titled "Subdomain Settings - Plane Strain (smpn)" and has tabs for "Material", "Constraint", "Load", "Damping", "Initial Stress and Strain", "Init", and "E". The "Material" tab is active, showing "Material settings" with fields for "Library material", "Material model" (set to "Elasto-plastic"), and "Coordinate system" (set to "Global coordinate system"). There is a checkbox for "Use mixed U-P formulation (nearly incompressible material)". A table lists material properties:

Quantity	Value/Expression	Unit	Description
E	Ed	Pa	Young's modulus
v	nu		Poisson's ratio
alpha	1.2e-5	1/K	Thermal expansion coefficient
rho	7850	kg/m ³	Density
thickness	1	m	Thickness

The foreground dialog is titled "Elasto-Plastic Material Settings" and has a "Hardening model" dropdown set to "Perfectly plastic". It contains a table for material parameters:

Quantity	Value/Expression	Unit	Description
Yield function	User defined		
σ_{yfunc}	F	Pa	Yield function
σ_{ys}	K	Pa	Yield stress level
Kinematic hardening			
E_{Tkin}	-d*E	Pa	Kinematic tangent modulus
Isotropic hardening			
<input checked="" type="radio"/> Tangent data			
E_{Tiso}	Ed	Pa	Isotropic tangent modulus
<input type="radio"/> Hardening function data			
$\sigma_{yhard}(\epsilon_p)$	2.0e10[Pa]/(1-2.0e1	Pa	Hardening function

Buttons for "OK", "Cancel", "Apply", and "Help" are visible at the bottom of the "Subdomain Settings" dialog.

Mechanical model

1) Plastic damage modeling

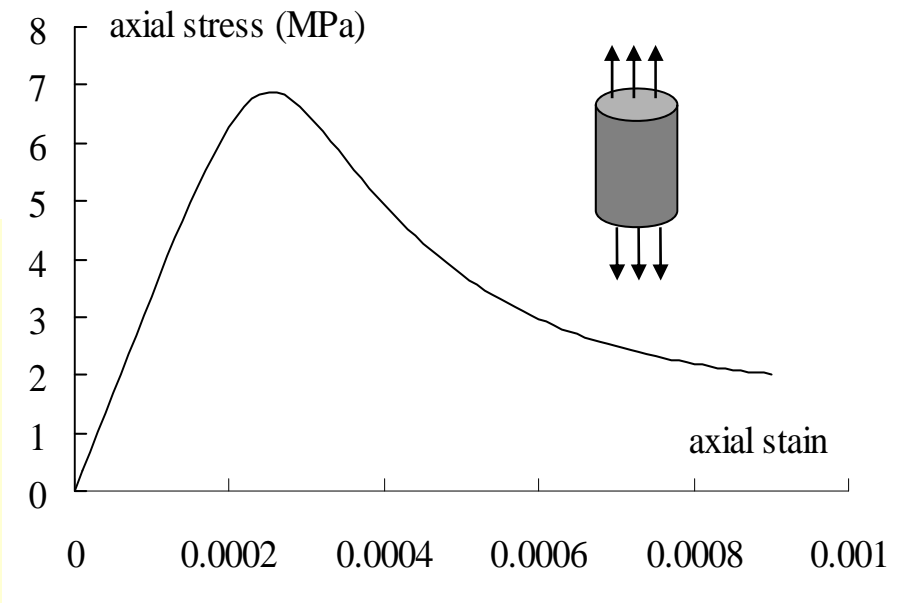
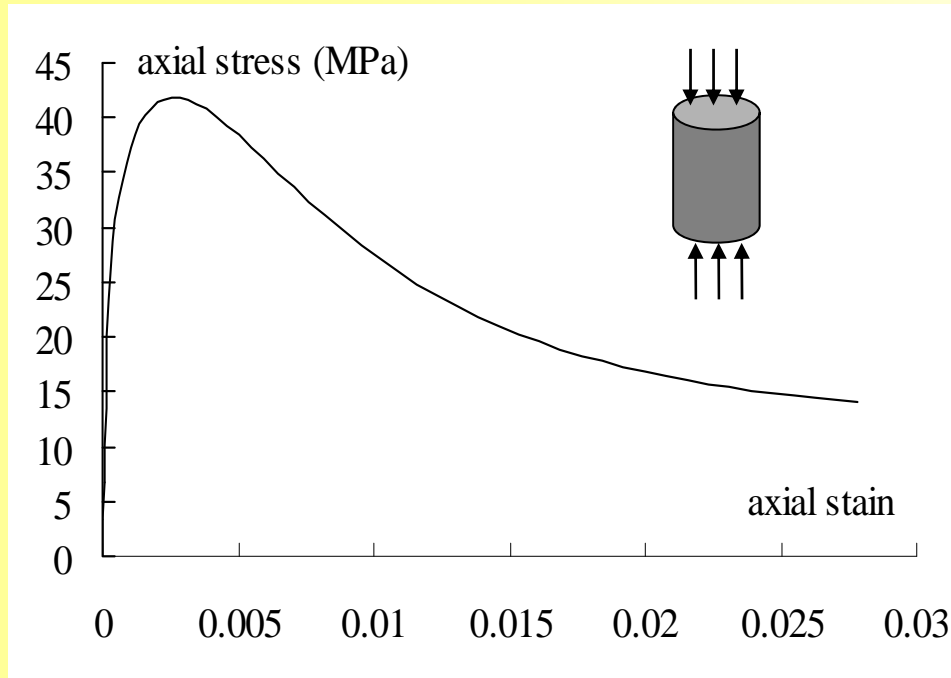
- Plane stress module for plastic damage damage scalar expressions

Name	Expression	Unit	Description
ALPHA	$(1/\sqrt{3}) * (2 * R_c / (R_c + R_t) - 1)$	1	
K	$(2/\sqrt{3}) * (R_t * R_c / (R_t + R_c)) * \eta$	Pa	
I1	$(s_x_{smpn} + s_y_{smpn} + s_z_{smpn}) / 3$	Pa	first stress invariant
dsx	$s_x_{smpn} - I1$	Pa	
dsy	$s_y_{smpn} - I1$	Pa	
dsz	$s_z_{smpn} - I1$	Pa	
TOEQ	$\sqrt{0.5 * (dsx^2 + dsy^2 + dsz^2) + s_{xy_smpn}^2}$	Pa	equivalent deviatoric stress
F	$1.45 * ALPHA * I1 + TOEQ$	Pa	plastic yield function
eta	$(1 - d) * (0.5 + (1 - 0.5) * e_{pe_smpn} / (b1 + e_{pe_smpn}))$	1	
d	$w_c * (1 - \exp(-b * e_{pe_smpn}))$		damage evolution law
Ed	$(1 - d) * E$	Pa	effective modulus

Mechanical model

1) Plastic damage simulation

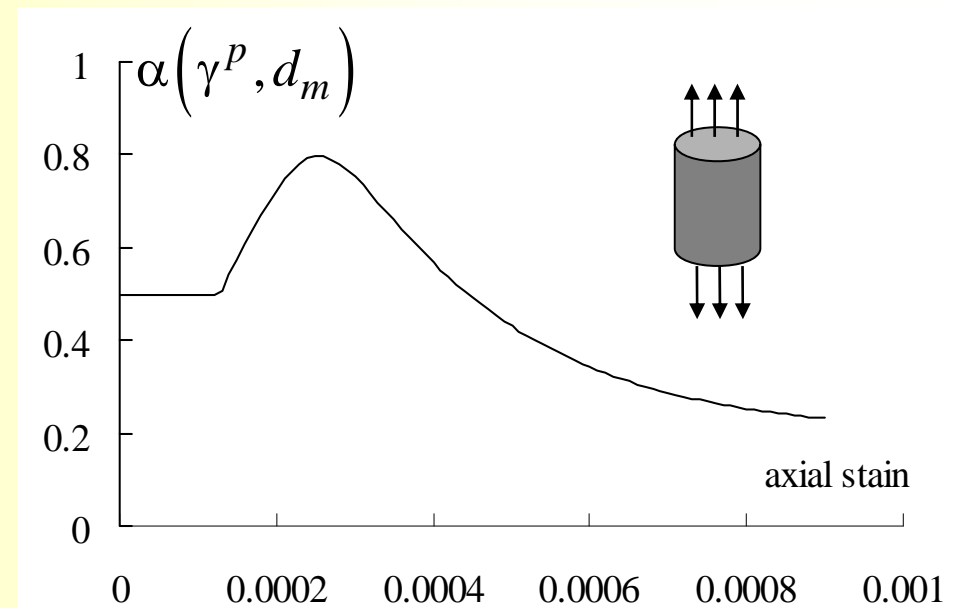
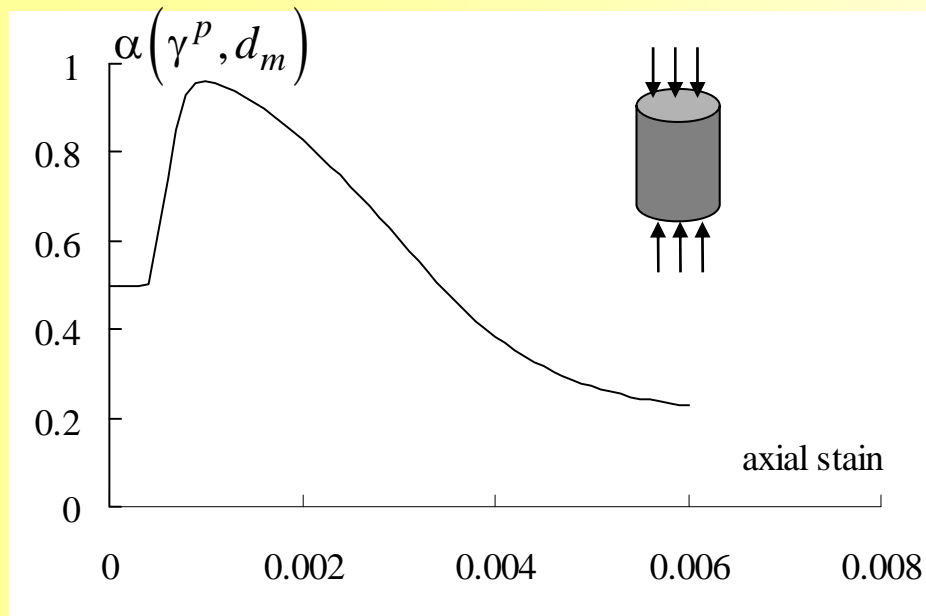
Simulation of uniaxial compression and tension



Mechanical model

1) Plastic damage simulation

Evolution of plastic hardening and softening function



Mechanical model

2) Creep characterization

- Creep strain
in compression

$$\dot{\epsilon}^{cpc} = A_c \left(\underbrace{A_1 m t^{m-1}}_{\text{First creep}} + \underbrace{A_2}_{\text{Second creep}} \right) \sigma, 0 < m < 1$$

First creep

Second creep

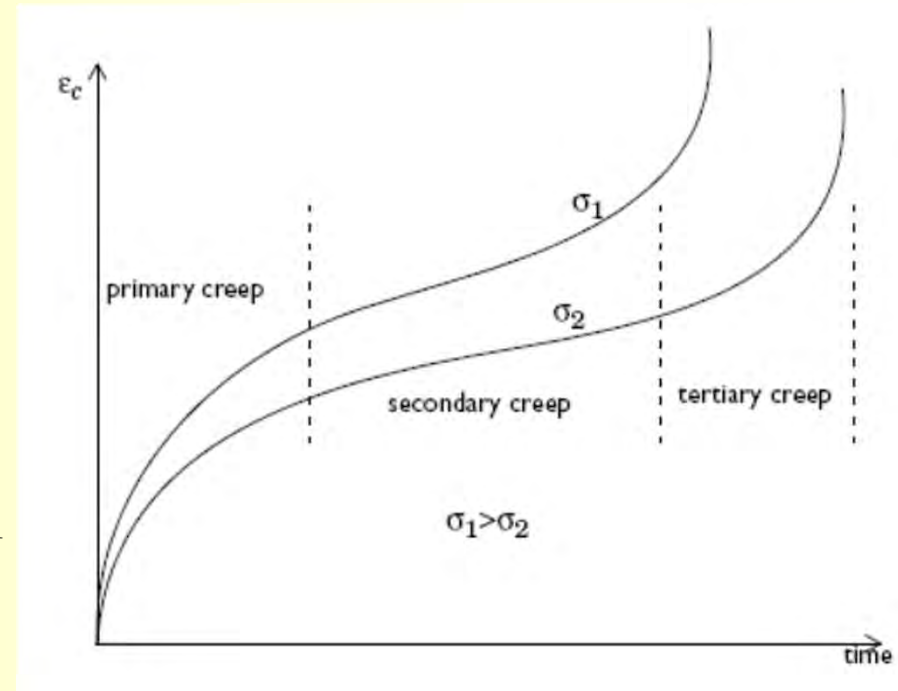
In tension

$$\dot{\epsilon}^{cpt} = A_t \left(A_1 m t^{m-1} + A_2 \right) \sigma, 0 < m < 1$$

- Total strain

Elastic + Plastic + Creep

$$\epsilon_{ij} = \epsilon_{ij}^e + \epsilon_{ij}^p + \epsilon_{ij}^{cp}$$



Mechanical model

2) Creep characterization

- PDE module for creep

Subdomain Settings - PDE, Coefficient Form (fluage_spherique_irreversible)

Equation

$$e_a \partial^2 w_s / \partial t^2 + d_a \partial w_s / \partial t + \nabla \cdot (-c \nabla w_s - a w_s + \gamma) + a w_s + \beta \cdot \nabla w_s = f$$

Subdomains Groups

Subdomain selection

1

Group:

Select by group

Active in this domain

Coefficients Init Element Weak Color

PDE coefficients

Coefficient	Value/Expression	Description
c	0	Diffusion coefficient
a	0	Absorption coefficient
f	sigma_mean	Source term
e _a	0	Mass coefficient
d _a	creepate	Damping/Mass coefficient
α	0 0	Conservative flux convection coeff.
β	0 0	Convection coefficient
γ	0 0	Conservative flux source term

OK Cancel Apply Help

Leaching model

1) Leaching characterization

- Mass balance equation

$$\frac{\partial Ca^{solid}}{\partial Ca^{2+}} \frac{\partial Ca^{2+}}{\partial t} = \nabla \cdot \left[\underline{D(Ca^{2+})} \nabla Ca^{2+} \right]$$

Hydric source of calcium ion

Diffusion coefficient of calcium ion

- Diffusion coefficient with ammonium nitrate

$$D(Ca(NO_3)_2) = \lambda \underline{D_e(Ca^{2+})} \nabla^2 Ca^{2+}$$

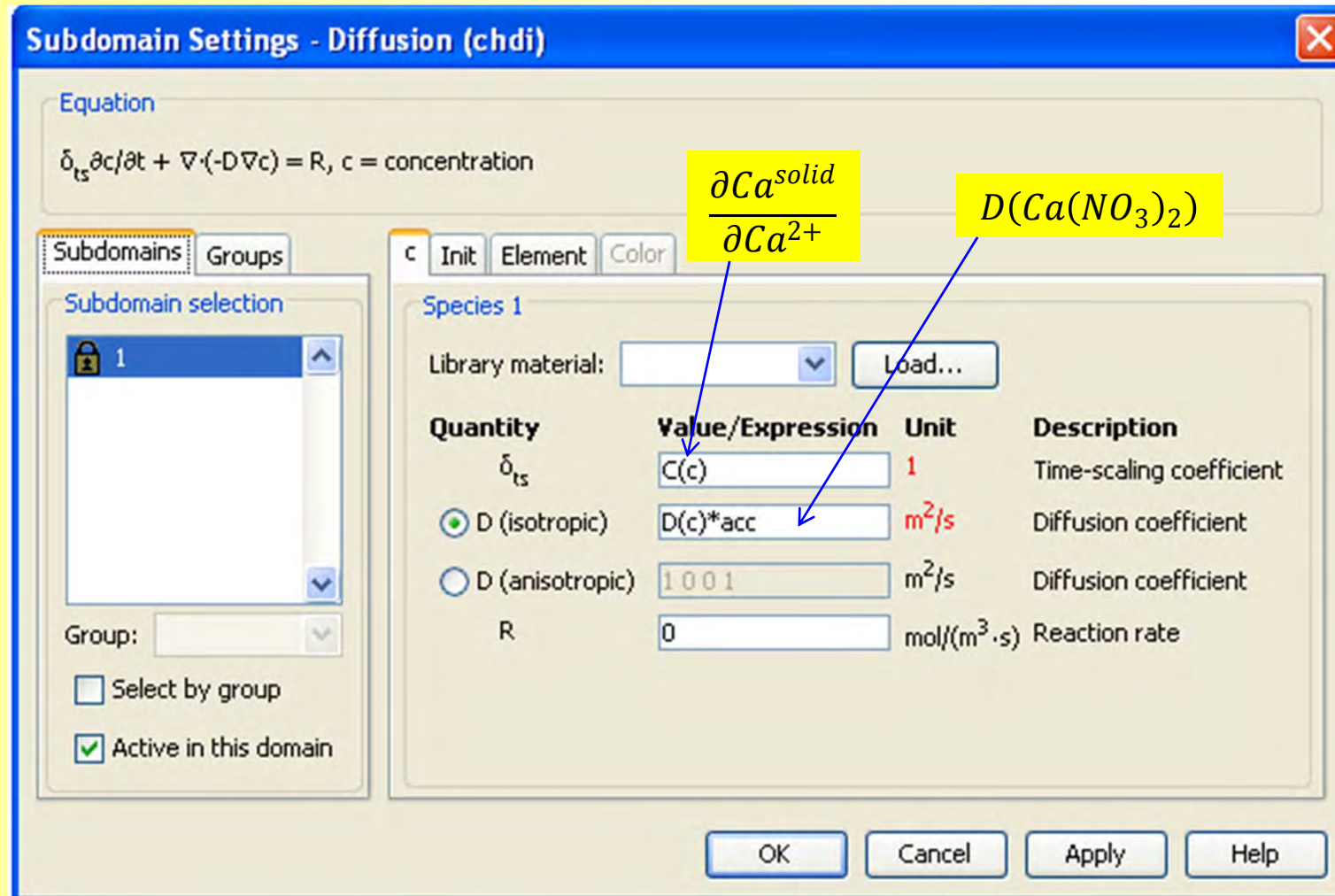
Acceleration parameter

Diffusion coefficient of calcium ion

Leaching model

1) Leaching characterization

- Diffusion module for leaching



Leaching model

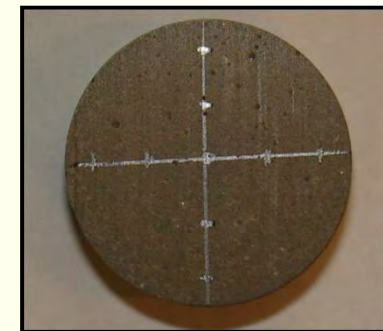
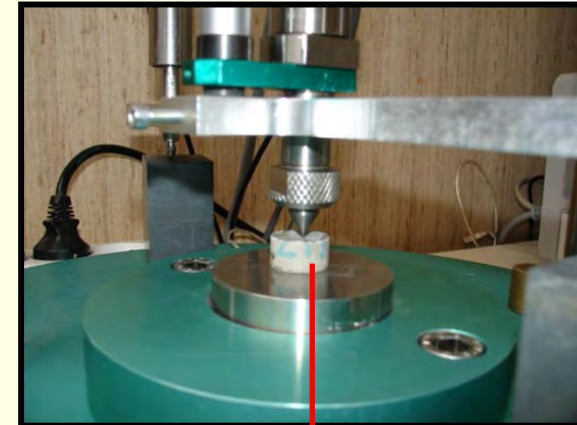
2) Leaching-plastic damage coupling

- Chemical damage

$$d_c = d_{c\max} \left[1 - \exp\left(Ca^{2+} - Ca^{2+} \Big|_0 \right) \right]$$

- Chemical damage-mechanical parameters

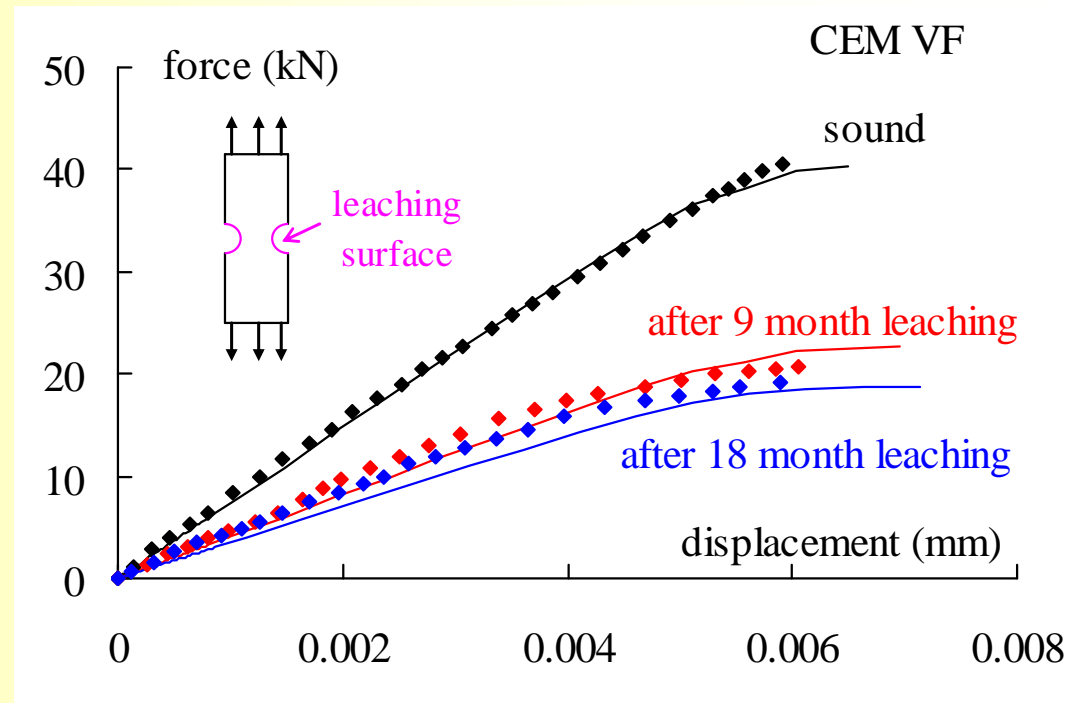
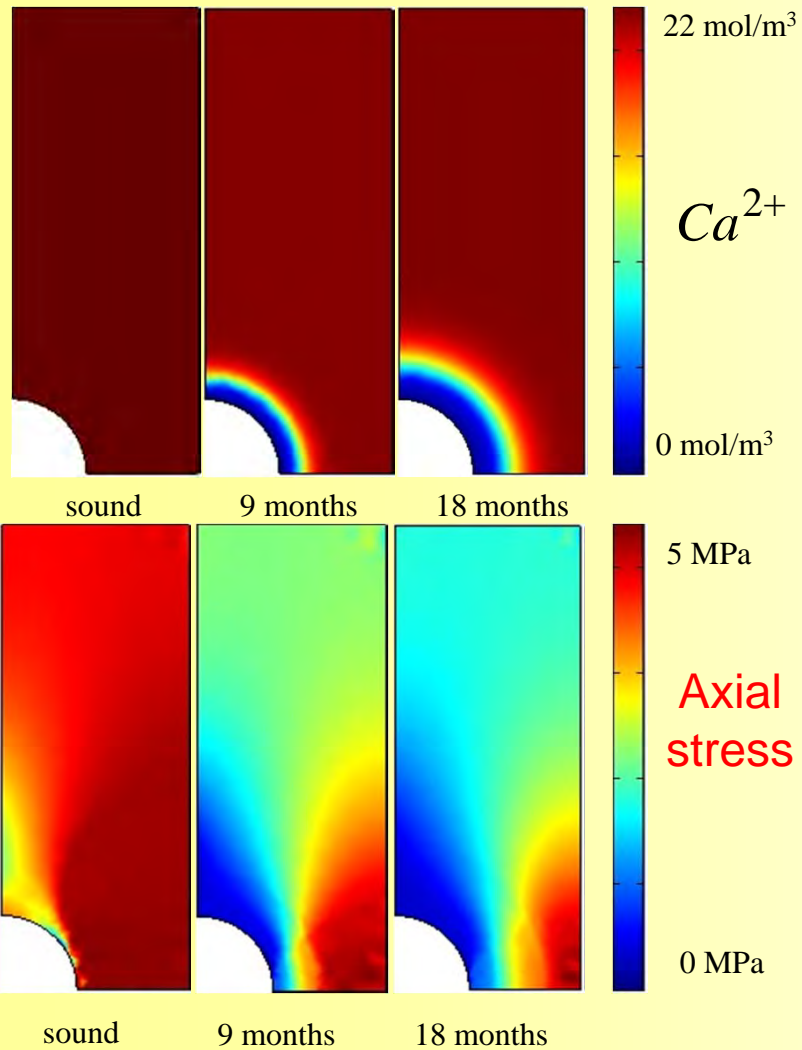
$$\begin{cases} E = E_0 (1 - d_c) \\ R_c = R_{c0} (1 - d_c) \\ R_t = R_{t0} (1 - d_c) \end{cases}$$



Test of micro indentation

Leaching model

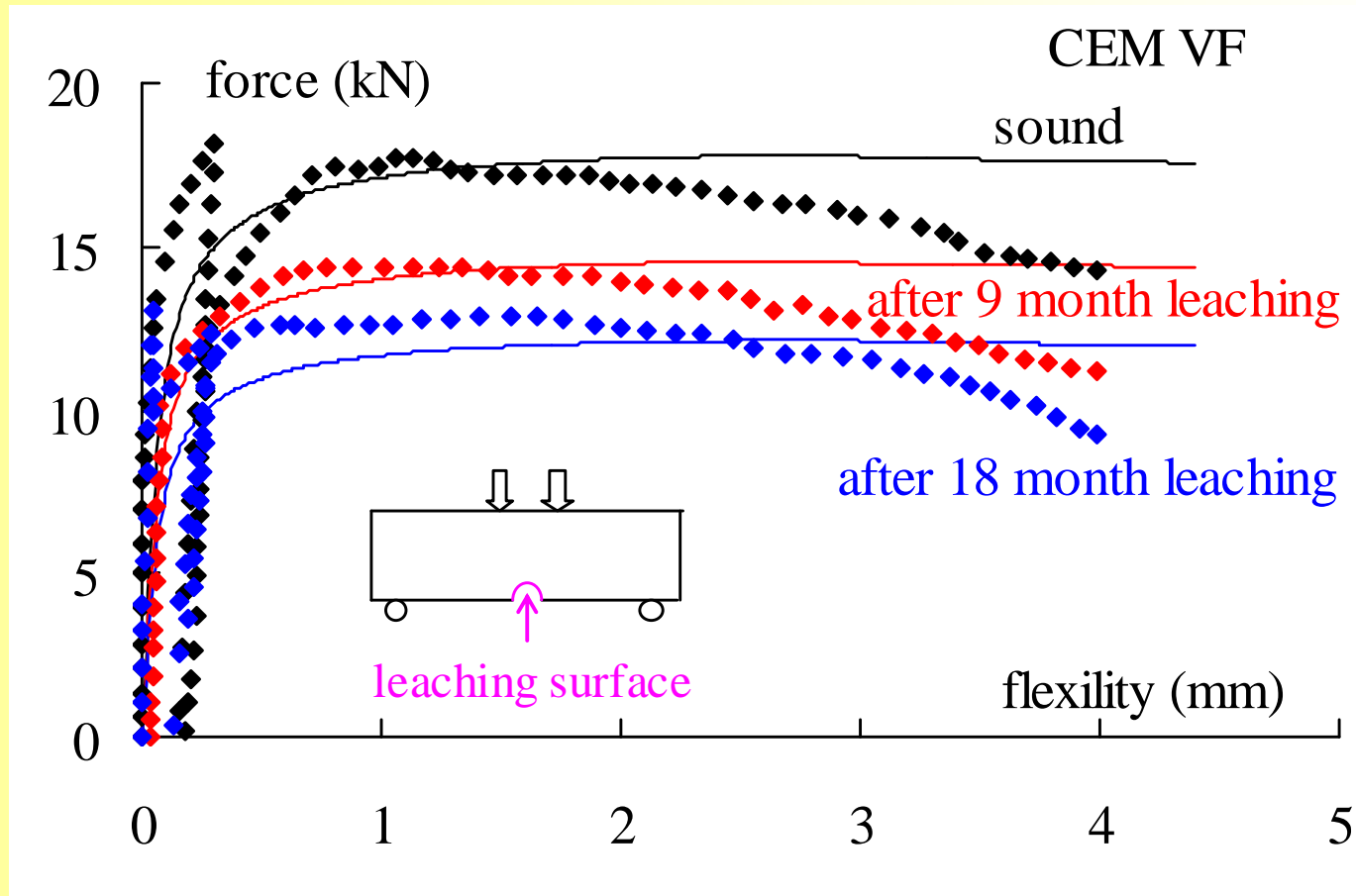
2) Leaching-plastic damage simulation



Directe tension test after different degradation times (data after Camps 2008)

Leaching model

2) Leaching-plastic damage simulation



Flexion test after different degradation times
(data after Camps 2008)

Coupling Model

1) Leaching-creep coupling characterization

- Variation of diffusion coefficient with plastic damage

$$D(d_m) = \lambda D_e (1 + \alpha_D d_m)$$

- Variation of creep strain rate with chemical damage

$$\begin{cases} \dot{\epsilon}^{cpc} = A_c \left(A_1 m t^{m-1} + A_2 \right) (1 + \alpha_{dc} d_c) \sigma, & \text{compressive stress} \\ \dot{\epsilon}^{cpt} = A_t \left(A_1 m t^{m-1} + A_2 \right) (1 + \alpha_{dc} d_c) \sigma, & \text{tensive stress} \end{cases}$$

Coupling Model

1) Leaching-creep coupling characterization

➤ Plane stress module

The image shows two overlapping dialog boxes from a finite element software interface. The background dialog is 'Subdomain Settings - Plane Stress (smps)' and the foreground dialog is 'Elasto-Plastic Material Settings'.

Subdomain Settings - Plane Stress (smps)

- Subdomains: 1 (default)
- Material settings:
 - Library material: [] Load...
 - Material model: Elasto-plastic
 - Coordinate system: Global coordinate system
 - Use mixed U-P formulation (nearly incompressible material)
- Material properties table:

Quantity	Value/Expression	Unit
E	E1*Coeffdc*(1-d)	Pa
ν	nu1	
α	1.2e-5	1/K
ρ	rho1	kg/m ³
thickness	0.1	m
- Buttons: OK, Cancel, Apply, Help

Elasto-Plastic Material Settings

- Hardening model: Perfectly plastic
- Yield function: User defined
- Yield function parameters:

Quantity	Value/Expression	Unit	Description
σ_{yfunc}	F	Pa	Yield function
σ_{ys}	K	Pa	Yield stress level
- Kinematic hardening:
 - E_{Tkin} : 2.0e10 Pa (Kinematic tangent modulus)
- Isotropic hardening:
 - Tangent data
 - E_{Tiso} : 2.0e10 Pa (Isotropic tangent modulus)
 - Hardening function data
 - $\sigma_{yhard}(\epsilon_p)$: 2.0e10[Pa]/(1-2.0e1) Pa (Hardening function)
- Buttons: OK, Cancel

Coupling Model

1) Leaching-creep coupling characterization

- PDE module for creep

Subdomain Settings - PDE, Coefficient Form (fluage_spherique_irreversible)

Equation

$$e_a \partial^2 w_s / \partial t^2 + d_a \partial w_s / \partial t + \nabla \cdot (-c \nabla w_s - \alpha w_s + \gamma) + \alpha w_s + \beta \cdot \nabla w_s = f$$

Subdomains Groups

Subdomain selection

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PDE coefficients

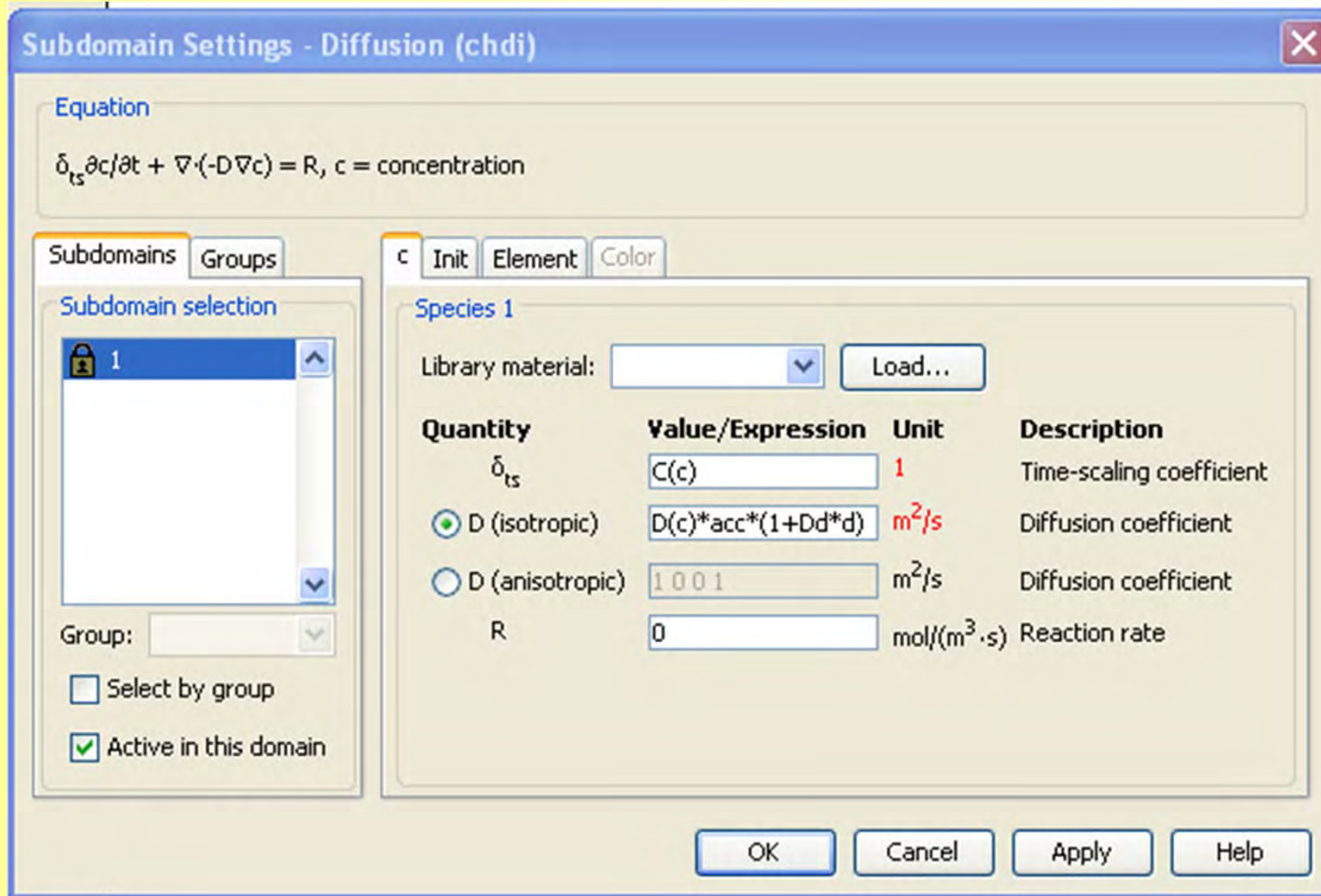
Coefficient	Value/Expression	Description
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d _a	creepate*Coeffdc	Damping/Mass coefficient
α	0 0	Conservative flux convection coeff.
β	0 0	Convection coefficient
γ	0 0	Conservative flux source term

OK Cancel Apply Help

Coupling Model

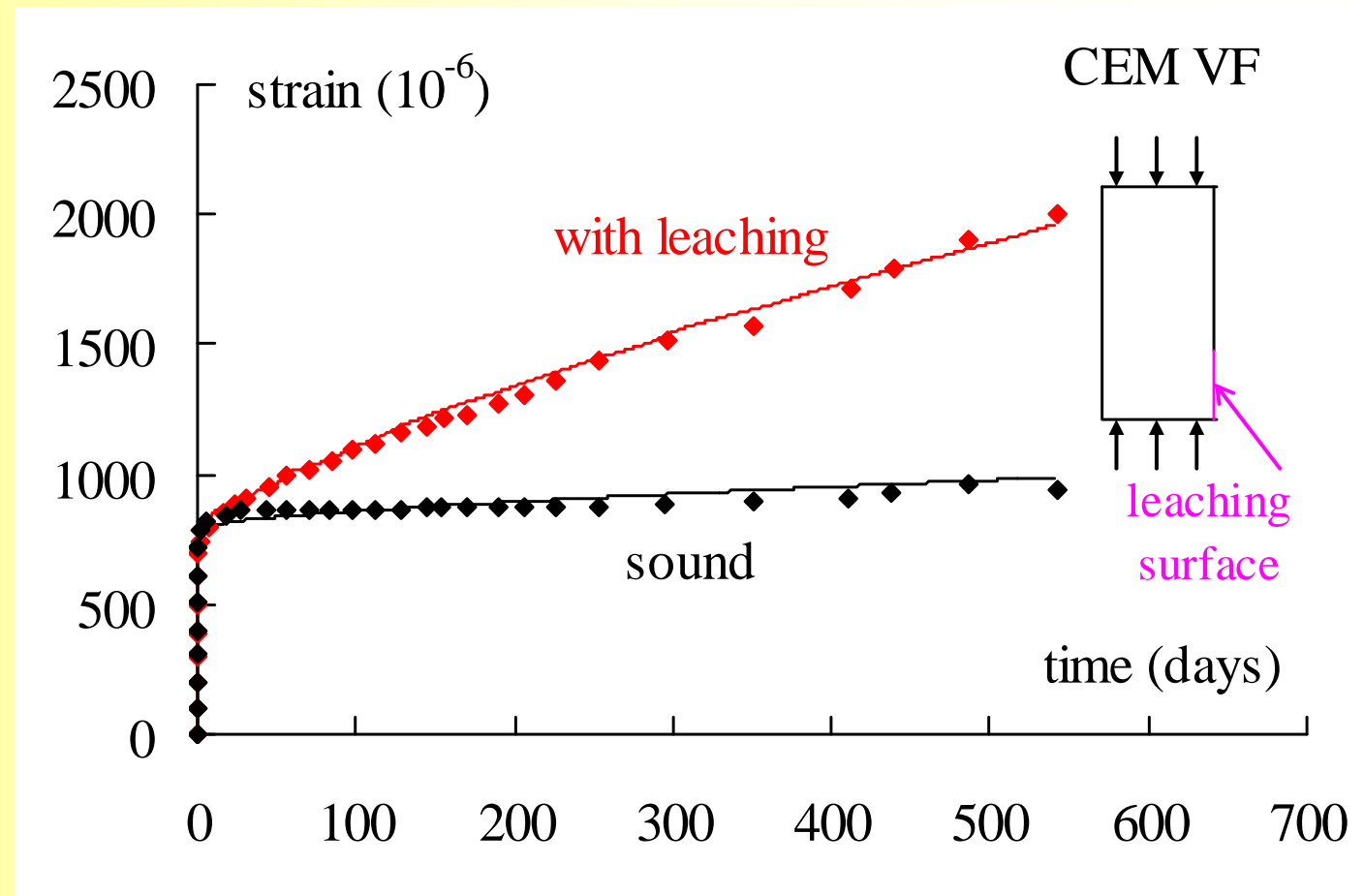
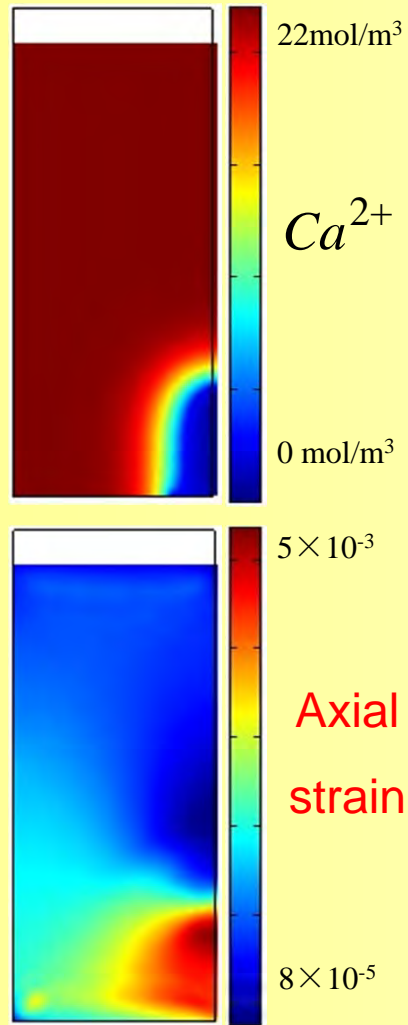
1) Leaching-creep coupling characterization

- Diffusion module for leaching



Coupling Model

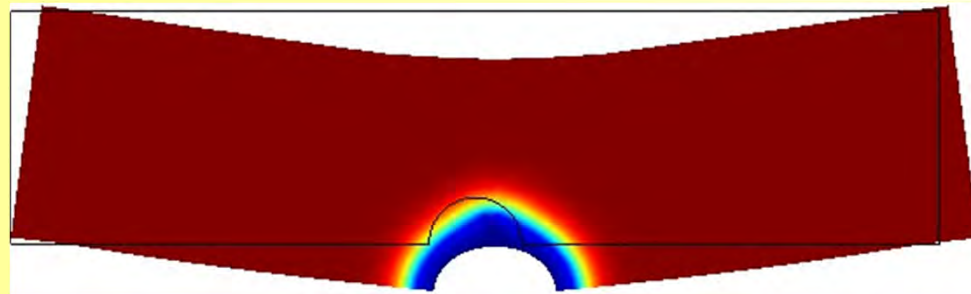
2) Leaching-creep simulation



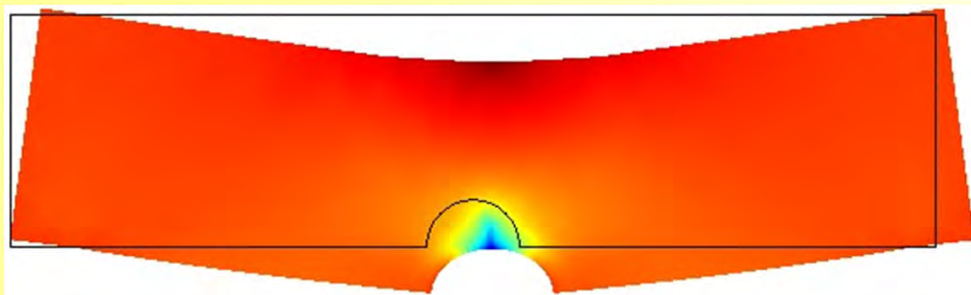
Creep compression test with degradation
(data after Camps 2008)

Coupling Model

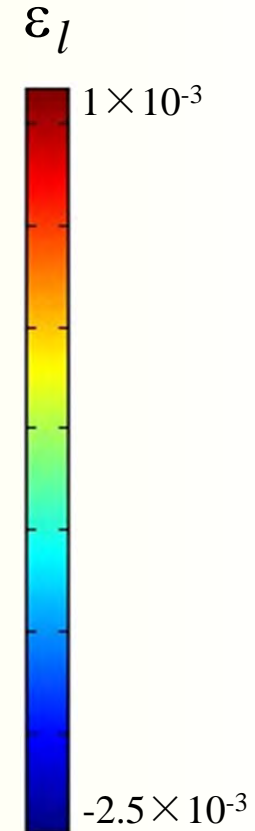
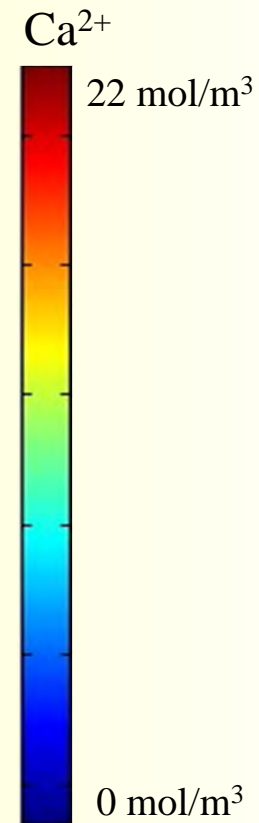
2) Leaching-creep simulation



Concentration of calcium ion



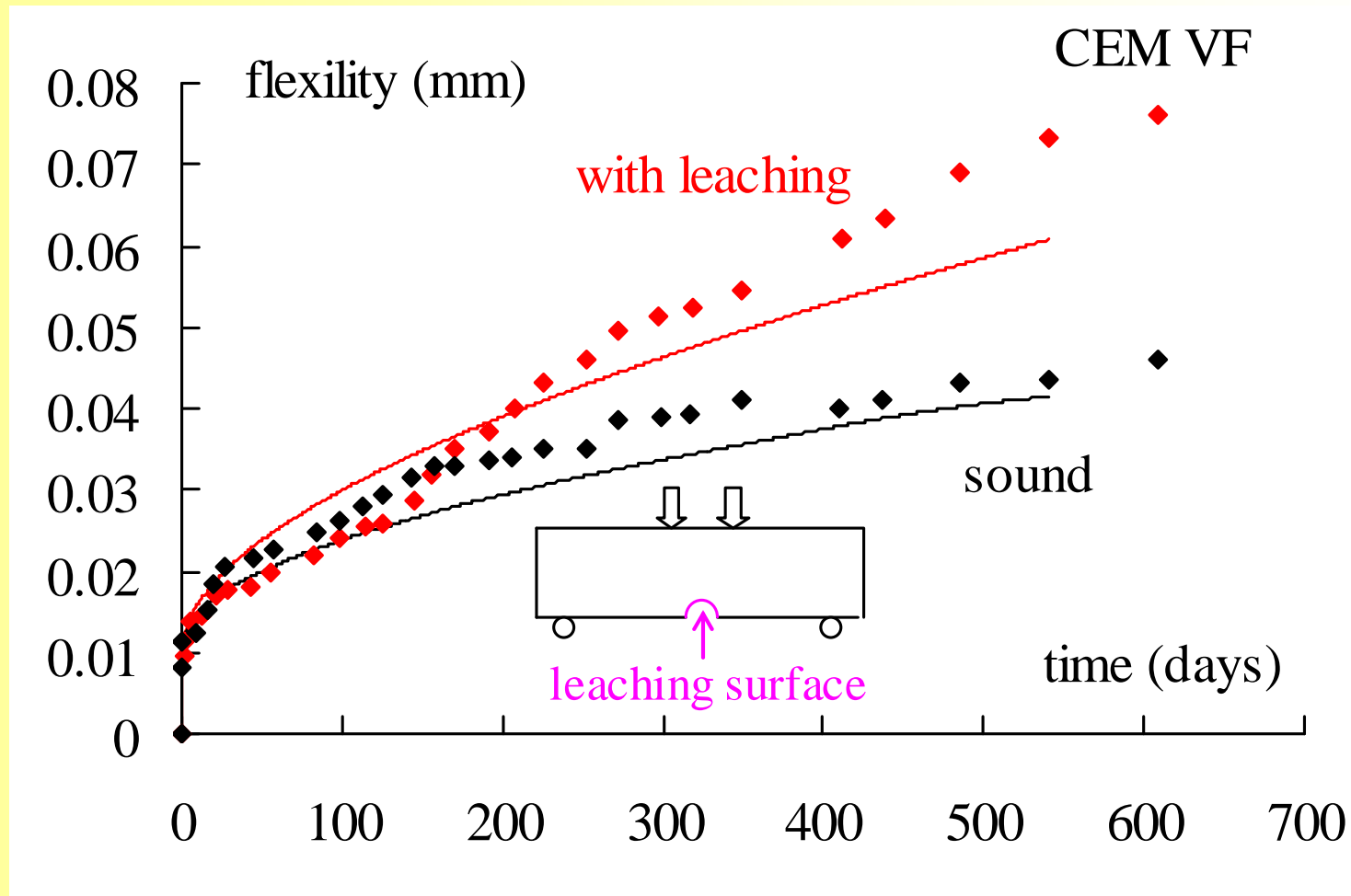
Longitudinale strain



Creep flexion test with degradation (data after Camps 2008)

Coupling Model

2) Leaching-creep simulation



Creep flexion test with degradation
(data after Camps 2008)

Conclusions and perspectives

Conclusions

- Elastoplastic damage model and creep model can describe the mechanical behavior of concrete in short and long term.
- The coupling of mechanical and leaching can describe the mechanical behavior subjected to chimic degadation in long term .

Perspectives

- Temperature-leaching-mechanical coupling

Thank you for your attention!