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Finite element simulation of chemo-mechanical damage under cyclic loading conditions

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ABSTRACT: A model for the coupled analysis of chemo-mechanical deterioration of concrete is developed within the theory of mixtures. As a particular example for corrosive mechanisms, the material degradation due to coupled calcium leaching and mechanical damage is investigated. The coupling of the calcium dissolution-diffusion and the elasto-damage process is based on the definition of the total porosity as the sum of the initial porosity, the porosity caused by calcium dissolution and the apparent porosity due to mechanical damage. The evolution of the mechanically and chemically induced porosities is controlled by internal parameters and related evolution laws. This enables the modeling of cyclic mechanical as well as cyclic chemical loadings. The suitability of the model is investigated by means of a finite element simulation of a beam subjected to combined mechanical loading and chemical attack.

1 INTRODUCTION

Durability of concrete structures is not exclusively affected by damage induced by mechanical loads. The life-time of such structures may significantly depend also on environmental conditions. This paper is focusing on moist environmental conditions where the life-time of the structure is mainly restricted by two interacting processes. These are the mechanically induced damage and the calcium leaching resulting in the opening and propagation of micro-cracks and the dissolution of the cement matrix. The relevant interactions of the mechanical and the chemical problem are the acceleration of the calcium ion diffusion and consequently the calcium dissolution process by mechanical induced damage and the stiffness and strength degradation of the cement based material caused by the increasing pore space as result of the calcium dissolution-diffusion process, see (Gérard 1996), (Carde and François 1997) and (Trägårdh and Lagerblad 1998). For the simulation of this long-term deterioration process of concrete, a constitutive model has been developed within the theory of mixtures (Bowen 1976) taking coupled chemical and mechanical damage mechanisms into account (Kuhl et al. 2000). In this reference, the coupling of the elasto-damage and the calcium dissolution-diffusion process is based on the definition of the total porosity as the sum of the initial porosity, the porosity caused by calcium dissolution and the apparent porosity due to mechanical damage. The evolution of the mechanically and chemically induced porosities are both controlled by internal parameters. This enables the modeling of cyclic loadings and allows a consistent thermodynamic formulation of the coupled field problems. The mechanical and the chemical damage processes are both formulated on a phenomenological level. On the one hand a strain based damage formulation (Simo and Ju 1987) is adapted for the modeling of concrete by means of the equivalent strain formulation proposed by (de Vree et al. 1995). On the other hand the chemical equilibrium model by (Gérard 1996) is applied to describe the relation between the calcium concentration in the pore fluid and the cement skeleton. As far as the numerical formulation is concerned, the implicit time integration and the finite element discretization are used in order to solve the coupled chemo-mechanical problem. The ability of the chemo-mechanical model to capture chemical loading and unloading processes is demonstrated by means of a representative example.

2 PHENOMENOLOGICAL DESCRIPTION OF THE CHEMO-MECHANICAL PROBLEM

2.1 Mechanical elasto-damage problem

Material degradation due to mechanical actions is characterized by the loss of stiffness and strength. For the modeling of mechanically induced damage the continuum damage theory, proposed by (Kachanov 1958), is employed. Among the wide variety of different material models, in the context of the present paper an isotropic damage model with a single internal damage parameter d_m, which can be interpreted as the ratio of the damaged cross section and the initial cross section, is used. The effective stress concept in conjunction with a strain based description of the damage evolution as proposed by (Simo and Ju 1987) is extended to model damage in porous materials, which is assumed to consist of an ideal mixture of the skeleton and the pore space. Mechanically induced damage in porous media is restricted to the skeleton. Therefore, the extension of the classical continuum damage model to porous media can be accomplished by using the theory of mixtures together with the description of the material properties in terms of the pure matrix material and the porosity. The pore space, represented by the initial porosity ϕ_0, is assumed to have no stiffness. Consequently the macroscopically measured initial stiffness of the material represents the stiffness of the skeleton multiplied by the volume fraction of the skeleton $(1-\phi_0)$. If the skeleton is damaged by mechanical actions, the initial macroscopic stiffness is reduced according to the classical damage formulation.

2.2 Chemical dissolution-diffusion problem

The matrix dissolution-diffusion problem describes the chemical solution of skeleton material which produces an increase of the porosity and the transport of the solute through the pore structure of the remaining material. In the case of the calcium dissolution by dissociation of portlandite, ettringite and C-S-H phases and the transport of calcium ions (Ca^{2+}) within the pore liquid, denoted as calcium leaching, the following characteristics of the fundamental processes are observed, see e.g. (Gérard 1996), (Carde and François 1997), (Trägårdh and Lagerblad 1998), (Torrenti et al. 1998) and (Mainguy et al. 2000). Firstly, the amount of calcium leaching in time depends almost linearly upon the square root of time. Secondly, two dissolution fronts, representing the dissolution of portlandite and the C-S-H phases can be distinguished due to the discontinuous change of the porosity. The above mentioned observations indicate a diffusion controlled leaching process with different chemical equilibrium states for the dissolution of the main constituents of the cement paste. Consequently the calcium leaching is modeled by a transient non-linear diffusion equation, assuming instantaneous matrix dissolution, whereby the calcium concentration s in the skeleton and the calcium concentration c in interstitial solution represent a chemical equilibrium state, which is described by a smooth function $s(c)$. A plot of this function proposed by (Gérard 1996) is given in Figure 1.

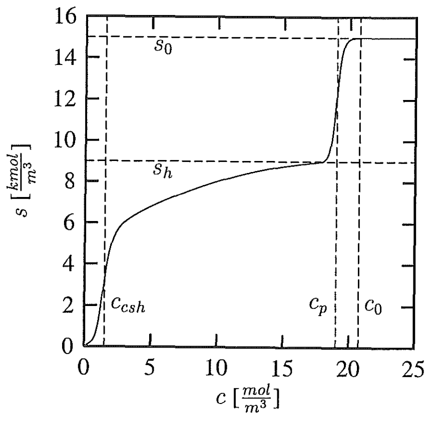

Figure 1: Phenomenological chemical equilibrium function $s(c)$ (Gérard 1996)

Based on the related function $s(c)$, the rate of matrix dissolution $\dot{s}$, the chemically induced porosity ϕ_c and the conductivity $(\phi_0+\phi_c)D_0$ for the calcium ion diffusion are modeled within the framework of the mixture theory (Bowen 1976). Furthermore, in analogy to the mechanical damage model, the dissolution-diffusion model is supplemented by an internal variable to account for the irreversible character of the matrix dissolution process.

In accordance with a hypothesis proposed by (Ulm et al. 1999), the model is restricted to diffusion dominated transport of calcium ions. The convective transport is not considered due to the assumption of a vanishing mass transfer of the pore fluid across the boundary of the representative elementary volume. In existing models it is customary to treat the diffusion coefficient of ions D_0 as being independent of its local concentration in its solution. As shown e.g. by (Robinson and Stokes 1959) this is only correct in the infinitely diluted state because ionic reactions reduce the conductivity with an increasing amount of ions. In particular, these are the relaxation and the electrophoretic effects depending on the permittivity and the viscosity of the pore fluid, respectively. Both effects are approximately a function of the square root of the calcium ion concentration. For this reason in the presented model the microscopic diffusion coefficient D_0 is related to the calcium concentration c in the pore solution by the macroscopic representation of Kohlrausch's law (Kohlrausch 1900).

2.3 Chemo-mechanical couplings

The interactions of calcium dissolution-diffusion and material damage have been investigated e.g. by (Gérard 1996), (Gérard et al. 1998), (Pijaudier-Cabot et al. 1998) and (Le Béllego et al. 2000). In these papers two main interactions of both field problems are addressed: The dissolution of calcium in the cement paste leads to a decrease of mechanical material properties, namely the stiffness and strength. Vice versa, mechanical damage results in an increasing permeability for the calcium ions in the fluid phase.

In order to consider the described interaction phenomena of chemical and mechanical material degradation, the material is formulated as an ideal mixture of the pore space and the skeleton. Consequently, the substantial link between the mechanical and the chemical field equations is given by the definition of the total porosity ϕ as the sum of the initial porosity ϕ_0, the porosity due to matrix dissolution ϕ_c and the apparent mechanical porosity ϕ_m:

$$\phi = \phi_0 + \phi_c + \phi_m \,. \tag{1}$$

The chemical porosity $\phi_c(s)$ depends on the calcium concentration s in the skeleton. The porosity ϕ_m represents the influence of mechanically induced micro pores and micro cracks onto the macroscopic material properties of the porous material. It is obtained by multiplying the scalar damage parameter d_m by the current volume fraction of the skeleton

$$\phi_m = [1 - \phi_0 - \phi_c]\, d_m \,. \tag{2}$$

It is worth to note, that the mechanical induced porosity ϕ_m is an apparent porosity. It effects measurable the chemical and mechanical material properties but not the mass balance of the porous material. With equation (2), the apparent volume fraction of the pore space and the skeleton can be formulated in the following manner:

$$\begin{aligned} \phi \quad &= [\phi_0 + \phi_c]\,[1 - d_m] + d_m \,, \\ 1 - \phi &= [1 - \phi_0 - \phi_c]\,[1 - d_m] \,. \end{aligned} \tag{3}$$

3 GOVERNING EQUATIONS

The coupled system of calcium diffusion-dissolution, mechanical deformation and damage is characterized by the concentration field c of calcium ions in the pore solution and the displacement field $\boldsymbol{u}$ as external variables and a set of internal variables concerning the irreversible material behavior.

The deformation field $\boldsymbol{u}$ is described by the macroscopic balance of linear momentum. In the quasi-static, geometrically linear theory, disregarding volume forces, the momentum balance is given by the vanishing divergence of the macroscopic stress tensor:

$$\operatorname{div} \boldsymbol{\sigma} = \boldsymbol{0} \,. \tag{4}$$

The matrix dissolution-diffusion problem is governed by the macroscopic balance of the calcium ion mass in the pore space

$$\operatorname{div} \boldsymbol{q} + [[\phi_0 + \phi_c]\, c]^{\cdot} + \dot{s} = 0 \,, \tag{5}$$

whereby $\boldsymbol{q}$ is the mass flux of the solute. The term $[[\phi_0 + \phi_c]\, c]^{\cdot}$ accounts for the change of the calcium mass due to the temporal change of the porosity and the concentration. The rate $\dot{s}$ denotes the calcium mass production due to the dissolution of the skeleton.

According to (Gérard 1996), the term $[[\phi_0 + \phi_c]\, c]^{\cdot}$ in the mass balance (5) can be neglected compared to the dissolution rate $\dot{s}$. In contrast to previous models, e.g. by (Delagrave et al. 1997), (Torrenti et al. 1998) and (Gérard 2000), in the present paper this term is taken into account in order to qualify the model for the description of chemical unloading conditions ($\dot{s} = 0$).

The system of differential equations (4)-(5) is completed by boundary and initial conditions on the boundary $\Gamma = \Gamma_q \cup \Gamma_c = \Gamma_\sigma \cup \Gamma_u$ and in the domain Ω

$$\begin{aligned} \boldsymbol{u}(t=0) &= \boldsymbol{u}_0^\star \text{ in } \Omega \,, & c(t=0) &= c_0^\star \text{ in } \Omega \,, \\ \boldsymbol{\sigma} \cdot \boldsymbol{n} &= \boldsymbol{t}^\star \text{ on } \Gamma_\sigma \,, & \boldsymbol{q} \cdot \boldsymbol{n} &= q^\star \text{ on } \Gamma_q \,, \\ \boldsymbol{u} &= \boldsymbol{u}^\star \text{ in } \Gamma_u \,, & c &= c^\star \text{ in } \Gamma_c \,, \end{aligned} \tag{6}$$

where $\boldsymbol{n}$ is the normal vector on the boundary surface, $\boldsymbol{q}^\star$ is the calcium ion mass flux across the boundary, $c^\star$ is the prescribed concentration, $\boldsymbol{t}^\star$ is the traction vector and $\boldsymbol{u}^\star$ are prescribed displacements.

4 CONSTITUTIVE LAWS

4.1 State equations

The elasto-damage constitutive law is characterized by the free energy function Ψ_m:

$$\Psi_m = \frac{1 - \phi}{2}\, \boldsymbol{\varepsilon} : \boldsymbol{\mathcal{C}}_0 : \boldsymbol{\varepsilon} \,. \tag{7}$$

Herein, $\boldsymbol{\varepsilon}$ denotes the linearized strain tensor

$$\boldsymbol{\varepsilon} = \frac{1}{2}[\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u}] \tag{8}$$

and $\boldsymbol{\mathcal{C}}_0$ is the fourth order elasticity tensor of the the skeleton, defined in terms of the Young's modulus E_0, the Poisson's ratio ν_0, the second order identity tensor $\boldsymbol{1}$ and the symmetric fourth order identity tensor $\boldsymbol{\mathcal{I}}$ as

$$\boldsymbol{\mathcal{C}}_0 = \frac{E_0}{1 + \nu_0}\, \boldsymbol{\mathcal{I}} + \frac{E_0\, \nu_0}{[1 + \nu_0][1 - 2\nu_0]}\, \boldsymbol{1} \otimes \boldsymbol{1} \,. \tag{9}$$

The derivative of the free energy function Ψ_m with respect to the strain tensor $\boldsymbol{\varepsilon}$ yields the stress tensor $\boldsymbol{\sigma}$:

$$\boldsymbol{\sigma} = \frac{\partial \Psi_m}{\partial \boldsymbol{\varepsilon}} = (1 - \phi)\, \boldsymbol{\mathcal{C}}_0 : \boldsymbol{\varepsilon} \,. \tag{10}$$

The diffusion-dissolution problem is defined by the potential energy Ψ_c of the calcium ions in the pore space

$$\Psi_c = \frac{\phi\, D_0}{2}\, \boldsymbol{\gamma} \cdot \boldsymbol{\gamma} \,, \tag{11}$$

where $\boldsymbol{\gamma}$ is the negative gradient of the concentration field c:

$$\boldsymbol{\gamma} = -\nabla c \,. \tag{12}$$

D_0 denotes the isotropic conductivity of the pore fluid, which depends on the calcium concentration c. The conductivity can be calculated by the macroscopic representation of Kohlrausch's law

$$D_0 = D_{00} - D_{0c} \sqrt{c} \,. \tag{13}$$

The derivative of the potential energy Ψ_c with respect to the negative concentration gradient γ results in the calcium ion mass flux vector $\boldsymbol{q}$

$$\boldsymbol{q} = \frac{\partial \Psi_c}{\partial \gamma} = \phi \, D_0 \, \gamma \, . \tag{14}$$

4.2 Evolution laws

The mechanically induced material degradation is described by an isotropic damage model. According to (Simo and Ju 1987) the evolution of the damage parameter $d_m(\kappa_m)$ is described by the damage criterion

$$\Phi_m = \eta(\varepsilon) - \kappa_m \leq 0 \, , \tag{15}$$

where η and κ_m are the equivalent strain function and the internal variable defining the current damage threshold. From the Kuhn-Tucker loading/unloading conditions and the consistency condition

$$\Phi_m \leq 0 \, , \quad \dot{\kappa}_m \geq 0 \, , \quad \Phi_m \, \dot{\kappa}_m = 0 \, , \quad \dot{\Phi}_m \, \dot{\kappa}_m = 0 \, , \tag{16}$$

follows, that κ_m is unchanged for $\Phi_m < 0$ and calculated by $\kappa_m = \eta$ otherwise.

In order to complete the description of the elasto-damage material model, the equivalent strain η and the damage function d_m must be defined. Here the equivalent strain measure proposed by (de Vree et al. 1995) is used

$$\eta = \frac{k_0 - 1}{2k_0[1-\nu_0]} I_1 + \frac{1}{2k_0} \sqrt{\frac{[k_0-1]^2}{[1-2\nu_0]^2} I_2 + \frac{12 k_0}{[1+\nu_0]^2} J_2} \, , \tag{17}$$

in which $I_1 = \text{tr}[\varepsilon]$, $I_2 = [\text{tr}^2[\varepsilon] - \varepsilon : \varepsilon]/2$ and $J_2 = [\varepsilon^{dev} : \varepsilon^{dev}]/2$ are the first and the second invariant of the strain tensor ε and the second invariant of the strain deviator ε^{dev}, respectively. The parameter k_0 denotes the ratio of tensile to compressive strength of the skeleton. The exponential damage function is given by

$$d_m = 1 - \frac{\kappa_m^0}{\kappa_m} \left[1 - \alpha_m + \alpha_m \exp[\beta_m(\kappa_m^0 - \kappa_m)] \right] \, , \tag{18}$$

where κ_m^0 is the initial damage threshold and α_m, β_m are material parameters.

The state of the chemically induced degradation of the porous material is characterized by the chemical porosity $\phi_c(s)$. Starting from a chemical equilibrium state between the calcium solved in the pore fluid and the calcium bounded in the skeleton, the dissolution process requires a decreasing concentration c in the pore fluid. Otherwise, if c is increased, the structure of the skeleton is unchanged. In order to describe this chemical induced degradation similarly to the elasto-damage problem, an internal variable κ_c is introduced, which corresponds to the current equilibrium calcium concentration in the pore solution. Based on this internal variable κ_c the chemical reaction criterion Φ_c is formulated as

$$\Phi_c = \kappa_c - c \leq 0 \, . \tag{19}$$

According to the Kuhn-Tucker conditions and the consistency condition

$$\Phi_c \leq 0 \, , \quad \dot{\kappa}_c \leq 0 \, , \quad \Phi_c \, \dot{\kappa}_c = 0 \, , \quad \dot{\Phi}_c \, \dot{\kappa}_c = 0 \, , \tag{20}$$

the process of matrix dissolution is associated with a decreasing chemical equilibrium calcium concentration ($\dot{\kappa}_c \leq 0$). The dissolution threshold κ_c is unchanged for $\Phi_c < 0$ and equal to the current calcium concentration of the pore fluid ($\kappa_c = c$) otherwise.

As already mentioned, the current state of the calcium concentration in the skeleton s is controlled by the spontaneous calcium dissolution. It can be described as a function of the chemical equilibrium threshold κ_c (Gérard 1996):

$$s = s_0 - (1 - \alpha_c) \, s_h \left[1 - \frac{1}{10} \kappa_c + \frac{1}{400} \kappa_c^2 \right] - \frac{s_0 - s_h}{1 + \left(\frac{\kappa_c}{c_p} \right)^n} - \frac{\alpha_c s_h}{1 + \left(\frac{\kappa_c}{c_{csh}} \right)^m} \, . \tag{21}$$

Herein α_m, n and m are model parameters. c_0 and s_0 are the equilibrium concentrations of the sound material, c_p and c_{csh} are material constants related to the averaged fluid calcium concentration of the progressive dissolution of the portlandite and the C-S-H phases, s_h is the solid calcium concentration related to the portlandite-free cement matrix. A plot of function (21) and an illustration of the material parameters are given in Figure 1.

If equation (21) is taken as basis to determine the current calcium concentration in the skeleton, the chemically induced porosity can be calculated by multiplying the amount of dissolved calcium $s_0 - s$ by the molar volume of the skeleton constituents. In order to simplify the present model, the averaged molar volume $\mathcal{M}/\rho$ is used:

$$\phi_c = \frac{\mathcal{M}}{\rho} [s_0 - s] \, . \tag{22}$$

The matrix dissolution rate $\dot{s}$, required in equation (5), can be determined by application of the chain rule as

$$\dot{s} = \frac{\partial s}{\partial \kappa_c} \frac{\partial \kappa_c}{\partial c} \, \dot{c} \, . \tag{23}$$

The derivative $\partial \kappa_c / \partial c$ is equal to one in the case of active matrix dissolution and zero otherwise.

4.3 Linearization

As the stress tensor $\boldsymbol{\sigma}$ and the molar flux vector $\boldsymbol{q}$ depend non-linearly on both field variables, namely the calcium concentration c in the pore fluid and the displacement vector $\boldsymbol{u}$, they have to be linearized with respect to the increments of both primary variables. The linearization of equations (10) and (14) yields the following expressions:

$$\begin{aligned} \Delta\boldsymbol{\sigma} &= \frac{\partial\boldsymbol{\sigma}}{\partial\boldsymbol{\varepsilon}} : \Delta\boldsymbol{\varepsilon} + \frac{\partial\boldsymbol{\sigma}}{\partial c}\,\Delta c\,, \\ \Delta\boldsymbol{q} &= \frac{\partial\boldsymbol{q}}{\partial\boldsymbol{\varepsilon}} : \Delta\boldsymbol{\varepsilon} + \frac{\partial\boldsymbol{q}}{\partial c}\,\Delta c\,. \end{aligned} \tag{24}$$

In particular, the linearization of the stress tensor

$$\begin{aligned} \Delta\boldsymbol{\sigma} &= [1-\phi_0-\phi_c]\,\boldsymbol{C}_0^{ed} : \Delta\boldsymbol{\varepsilon} \\ &\quad - [1-d_m]\,\boldsymbol{C}_0 : \boldsymbol{\varepsilon}\,\frac{\partial\phi_c}{\partial s}\,\frac{\partial s}{\partial\kappa_c}\,\frac{\partial\kappa_c}{\partial c}\,\Delta c\,, \end{aligned} \tag{25}$$

including the consistent tangent operator of the pure mechanical problem

$$\boldsymbol{C}_0^{ed} = (1-d_m)\,\boldsymbol{C}_0 - (\boldsymbol{C}_0 : \boldsymbol{\varepsilon}) \otimes \frac{\partial d_m}{\partial\kappa_m}\,\frac{\partial\kappa_m}{\partial\eta}\,\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\,, \tag{26}$$

and the linearization of the molar flux vector

$$\begin{aligned} \Delta\boldsymbol{q} &= [1-\phi_0-\phi_c] D_0 \left[\boldsymbol{\gamma} \otimes \frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\right] \frac{\partial d_m}{\partial\kappa_m}\frac{\partial\kappa_m}{\partial\eta} : \Delta\boldsymbol{\varepsilon} \\ &\quad + [1-d_m]\left[\frac{\partial\phi_c}{\partial s}\frac{\partial s}{\partial\kappa_c}\frac{\partial\kappa_c}{\partial c} D_0\boldsymbol{\gamma} + \phi\,\frac{\partial D_0}{\partial c}\boldsymbol{\gamma}\right]\Delta c \\ &\quad - \phi\, D_0\, \nabla\Delta c \end{aligned} \tag{27}$$

are obtained.

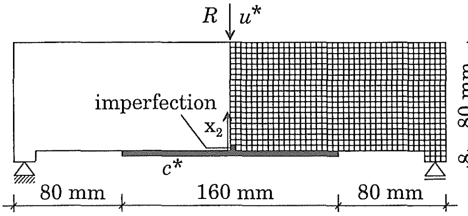

Figure 2: Geometry, finite element mesh and boundary conditions of the numerical example

5 NUMERICAL APPLICATION

The numerical solution of the coupled chemo-mechanical problem is accomplished by a combination of common techniques in computational mechanics, including the weak formulation, the finite difference time discretization by the second order accurate mid-point rule, the consistent linearization and the finite element discretization. Finally the resulting discrete algebraic system of equations is solved by a Newton-Raphson procedure using the consistent tangent operator. For a detailed description of the numerical solution procedure, see (Kuhl et al. 2001).

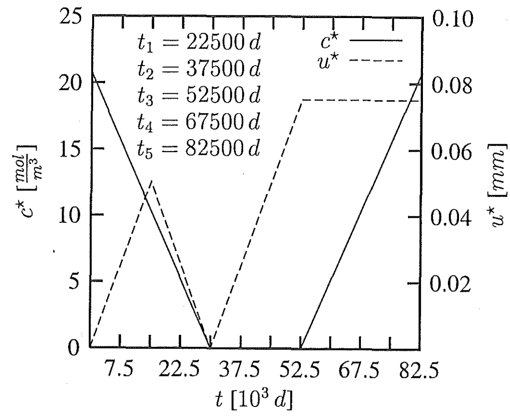

Figure 3: Loading history of the numerical example

As a representative example for coupled chemo-mechanical degradation, a beam of unit thickness, which is subjected to cyclic mechanical loading and to cyclic chemical attack is investigated by means of the proposed material model. Two-dimensional plane strain finite elements with bilinear shape functions are used. Figure 2 illustrates the geometry, the finite element discretization and the boundary conditions, respectively. The initial conditions are given by $\boldsymbol{u}_0^\star = 0$ and $c_0^\star = c_0$. A displacement driven point load is prescribed in the center of the beam. At the bottom of the beam, the calcium concentration $c^\star$ of the solute is prescribed starting from an initial value $c^\star = c_0$ corresponding to the initial equilibrium state. The time histories of the mechanical and the chemical loading are given in Figure 3.

Table 1: Material and model parameters of the numerical example

$E_0 = 4.375 \cdot 10^{10}$	$\frac{N}{m^2}$	$\kappa_m^0 = 1.1 \cdot 10^{-4}$	
$\nu_0 = 0.2$		$\alpha_m = 0.96$	
$\phi_0 = 0.2$		$\beta_m = 400$	
$k_0 = 10$			
$n = 85$		$m = 5$	
$c_0 = 20.7378$	$\frac{mol}{m^3}$	$s_0 = 15$	$\frac{kmol}{m^3}$
$c_p = 19$	$\frac{mol}{m^3}$	$s_h = 9$	$\frac{kmol}{m^3}$
$c_{csh} = 1.5$	$\frac{mol}{m^3}$	$\alpha_c = 0.565$	$\frac{m^3}{mol}$
$D_{00} = 7.9 \cdot 10^{-10}$	$\frac{m^2}{s}$	$D_{0c} = 9.7 \cdot 10^{-11}$	$\sqrt{\frac{m^7}{s^2\,mol}}$
$\frac{\mathcal{M}}{\rho} = 3.5 \cdot 10^{-10}$	$\frac{m^3}{mol}$	$\Delta t = 150$	d

Table 1 contains the material and model parameters used for the fully coupled simulation. In order to initiate just on single crack along the axis of symmetry, which propagates from the bottom to the top, a slight imperfection within one element at the bottom side is introduced ($0.8\ \kappa_m^0$), see Figure 2.

Figure 4 illustrates the distribution of the calcium concentration c in the solute, the remaining concentration s of the calcium in the skeleton, the matrix dissolution rate $\dot{s}$ and the scalar damage parameter d_m at five stages of the loading history. Since the ill-posed elasto-damage problem is not regularized, damage is restricted to one column of elements. As expected, damage propagates from the bottom to the top of the beam. At time t_1 the chemical attack has penetrated approximately 1/3 of the height of the beam. Two dissolution fronts, indicated by higher values of the rate $\dot{s}$, are visible. The upper one corresponds to the dissolution of portlandite ($\kappa_c \approx c_p$), while the second front at the bottom side of the beam is associated to the dissolution of the C-S-H phases ($\kappa_c \approx c_{csh}$). Between these fronts other constituents like ettringite are dissolved at a much lower rate. Along the axis of symmetry the chemical degradation is accelerated by mechanical damage. The next two stages t_2 and t_3 show the progression of the dissolution process, while the concentration at the bottom of the beam is kept constant at $c^\star = 0$. At time t_3 the dissolution front of the C-S-H phases is not visible anymore. The reason for this observation is, that the concentration rate $\dot{c}$ near the bottom side with the prescribed boundary condition decreases with time. As a consequence, the dissolution process in this region decelerates. Stages t_4 and t_5 correspond to chemical unloading. While the calcium concentration in the solute slowly increases according to the prescribed boundary condition $c^\star = c_0$, the state of the skeleton characterized by the concentration s does not change. The local chemical degradation process stops ($\dot{s} = 0$), if c is increased. Consequently no dissolution occurs at the end of the simulation, since in the whole structure the initial calcium concentration $c = c_0$ is recovered.

To obtain a deeper insight into the interactions between mechanical and chemical material degradation, an uncoupled analysis with the same loading history (Figure 3) is performed in addition to the fully

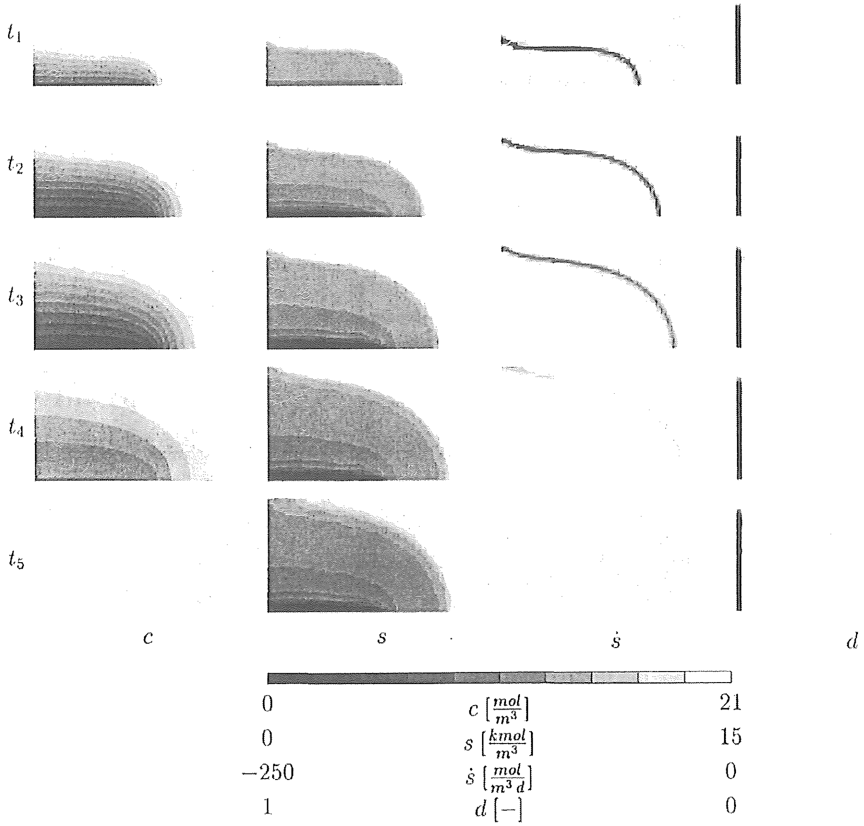

Figure 4: Evolution of concentrations c, s and of the matrix dissolution rate $\dot{s}$ at five stages of the loading history

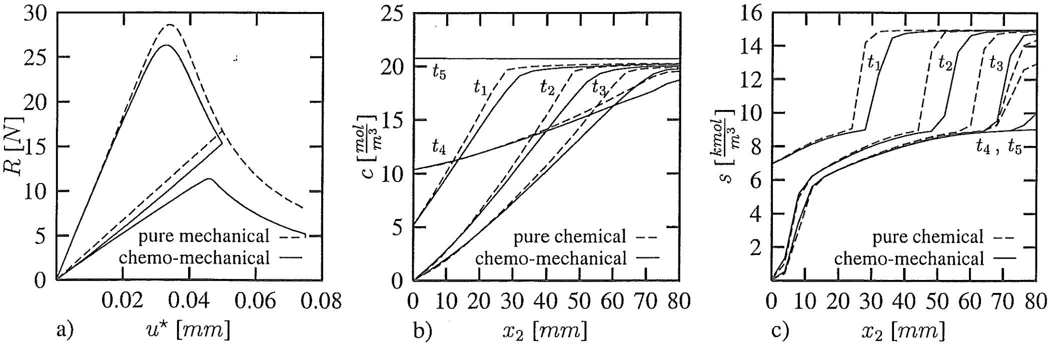

Figure 5: a) Load-displacement relation; b), c) Evolution of the calcium concentration c in the pore fluid and s in the skeleton along the axis of symmetry

coupled analysis. Therefore the stress-strain relation (10) and the molar flux vector (14) are rewritten with $\phi_c = 0$ and $\phi_m = 0$, respectively.

The load-displacement relations obtained from the pure mechanical and the coupled chemo-mechanical simulation shown in Figure 5a illustrate the influence of chemical damage on the stiffness and strength of the material. Both material properties are reduced due to chemical degradation. Due to the matrix dissolution the mechanical unloading and reloading path are no longer identical in the coupled chemo-mechanical analysis.

In Figures 5b and 5c the profiles of the solute calcium concentration c and the skeleton calcium concentration s along the axis of symmetry (Figure 2) are plotted. It can be observed, that the c-profiles are smooth, whereas the s-profiles show the dissolution fronts of the portlandite and the C-S-H phases. It is quite obvious, that the dissolution and diffusion of calcium is accelerated by mechanical damage.

6 SUMMARY AND CONCLUSIONS

A constitutive model describing the coupled chemo-mechanically induced damage of porous materials was developed within the framework of the theory of mixtures, where the material is characterized by the superposition of the pore space and the skeleton. A scalar damage formulation was used for the description of the mechanically induced deterioration of the skeleton. For the chemical part, a phenomenological chemical equilibrium model for the calcium dissociation of cementitious materials was used. The proposed model was applied to the mathematical description of calcium leaching in concrete, taking the interactions between the irreversible chemical and the mechanical processes into account. Full coupling between both fields was accomplished by the definition of a chemically and a mechanically induced portion of the total porosity. The chemo-mechanical model considers the interactions between mechanical damage and calcium transport as well as the decrease of stiffness and strength of concrete due to matrix dissolution. In contrast to previous models, the proposed formulation accounts for cyclic chemical loading conditions. It was demonstrated by a numerical example, that the present model is able to describe the relevant characteristics of the coupled mechanisms of calcium leaching and mechanical damage.

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