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Multiphase Modelling of Thermomechanical Behaviour of Early-Age Silicate Composites

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1. Introduction

The reliable prediction of thermomechanical behaviour of early-age silicate composites is a complicated multiphysical and multiscale problem, containing a lot of open questions. However, silicate mixtures, namely fresh concrete, are the most commonly used materials in building constructions throughout the world, thus such prediction is of great practical significance. The most important modelling outputs are the macroscopic effective strain, stress, temperature, moisture etc. time evolutions, driven by chemical reactions of particular clinker minerals with water. Every realistic model is then expected to include thermo-, chemo- and hygromechanical processes and phase changes, involving all available microstructural information related to the real porous medium.

The deformation of a material sample or a building construction made from silicate composites has to be analyzed at least as the superposition of

- reversible elastic deformation,
- viscous material flow,
- volume changes, unlike remaining contributions independent of external loads.

The crucial external and internal influences are:

- internal hydration heat, generated by the hydration hydraulic processes,
- ambient temperature variation, connected with ambient humidity variation (natural or artificial ones),
- external mechanical loads.

The significant physical (and chemical) processes are:

- a) thermal deformation,
- b) autogenous shrinkage,
- c) carbonation,
- d) elastic and creep deformation,
- e) additional thermal deformation,
- f) drying shrinkage and swelling.

In the first period of intense hydration a), accompanied by b), is dominant. In the later period the role of a) decreases, but the effect of c) has to be taken into account. The external mechanical loads cause d) (creep especially in the earliest age), the external temperature changes simultaneously force e), modified by f).

The traditional approach to the modelling of such complex physical and technical problems is the phenomenological one, as discussed in (Bažant, 2001): the effect of changes of density, porosity, permeability, compressive strength, etc. on material behaviour is lumped together to some model parameters, which must be identified by long-lasting tests in the whole range of model applicability. On the contrary, the so-called CCBM ("Computational Cement-Based Material") approach, suggested in (Maruyama et al., 2001), develops the original idea of (Tomosawa, 1997): the slight generalization of its (seemingly simple) form

$$\dot{\epsilon} = \Phi(\epsilon, \epsilon_*), \quad \dot{\epsilon}_* = \Psi(\epsilon, \epsilon_*)$$

where ϵ is the radius of an unhydrated cement particle, ϵ_* its total radius including hydrate, dot symbols refer (everywhere in this chapter) to derivatives with respect to the time $t \geq 0$ and Φ, Ψ are (in general rather complicated) material characteristics with hidden ϵ, ϵ_* (but not with their time derivatives) again. The analysis of (Maruyama et al., 2001) assumes ideal spherical particles, hydration products adherent to such particles (whose size distribution is approximated by a special Rosin-Ramler function), water diffusing through the hydrate layer and chemically reacting with cement, up to interparticle contact effects; the amount of water is controlled by the pore structure, modified by hydration reactions of cement constituents and corresponding heat generation. Particular cement constituents, namely alite (C_3S , typically 65 % of the total mass in the Portland cement), belite (C_2S , 15 %), aluminate phase (C_3A , 7 %), ferrite phase (C_4AF , 8 %), etc., have their own densities and hydration reactions, generating hydration heat.

For various types of cement we have different hydration degree Γ , introduced as

$$\Gamma := \frac{\mu^h}{\mu_\infty^h}$$

where μ^h denotes the (usually increasing) mass of skeleton (and corresponding sink of liquid water mass) and μ_∞^h the final mass of hydrated (chemically combined) water in a volume unit; alternatively (cf. (Gawin et al., 2006a), p. 309)

$$\Gamma := \frac{Q^h}{Q_\infty^h}$$

in terms of the heat Q^h released during hydration and of its final value Q_∞^h . However, it is difficult to guarantee above sketched model assumption in building practice, applying also (not single-sized) additional aggregate; thus Γ is usually quantified from macroscopic experiments (as adiabatic calorimetric or isothermal strength evolution tests) not from such microstructural considerations. Consequently Γ can be evaluated by (Gawin et al., 2006a), p. 309, from an auxiliary evolution problem of type

$$\dot{\Gamma} = A(\Gamma, \phi, T)$$

with an a priori known real function A .

During the same hydration process the non-negligible vapour mass source μ^e , caused by the liquid water evaporation or desorption, occurs, too. Unfortunately, unlike μ^h , no reasonable constitutive relation is available for the direct evaluation of μ^e .

Clearly, the reliable prediction of material behaviour applicable to real building objects during hydration needs some multiscale analysis. The mechanistic approach (Pichler et al., 2007) makes it possible to consider above sketched effects explicitly because they appear directly in the model equations, distinguishing between 4 length scales, characterized as

- I) anhydrous-cement scale (typical length of a representative volume element from 10^{-8} to 10^{-6} m), in more details decomposed into 3 subscales, where the qualitative estimate of activity of four main clinker phases, water and air requires the detailed micromechanical evaluation of corresponding chemical reactions,
- II) cement-paste scale (from 10^{-6} to 10^{-4} m),
- III) mortar scale (about 10^{-2} m),
- IV) macroscale (about 10^{-1} m).

The analysis of capillary depression at scale I) (considering membrane forces on solid/liquid, solid/gas and liquid/gas interfaces), of ettringite formation at scale II), of autogenous deformation at scales II) and III), referring to the Hill homogenization lemma (see (Dormieux et al., 2006), p.105), must be completed by the interpretation of such multiscale results at scale IV). However, different physical and chemical processes studied at particular scales do not admit proper and physically transparent mathematical analysis of two- and more-scale convergence, as discussed in (Cioranescu & Donato, 1999), (Vala, 2006) or (Efendiev et al., 2009), including its non-periodic (formally complicated) generalization, introduced in (Nguentseng, 2003-4).

The approach (Gawin et al., 2006a) applies certain mechanistic-type method to obtain the governing equations only, using the averaging hybrid mixture theory: the developments starts at the micro-scale and balance equations for particular phases and interfaces are introduced at this level and then averaged for obtaining macroscopic balance equations. Four phases are distinguished: solid skeleton, liquid water, vapour and dry air, whose densities are considered (under the passive air assumption) as constants; the whole hygro-thermo-chemo-mechanical process is then studied as the time evolution of capillary pressure, gas pressure, temperature and displacement of points related to the reference (initial) configuration, driven by balance equations of classical thermodynamics and conditioned by corresponding constitutive laws. The detailed geometrical analysis (Sanavia et al., 2002) (without phase changes) offers the possibility to extend such considerations beyond the assumption of small deformations and involve some elements of fracture mechanics.

The development, laboratory testing and computational simulations of new materials, namely those for the application of advanced engineering structures, belong to the research priorities of the Faculty of Civil Engineering of Brno University of Technology. Moreover, these activities should be intensified thanks to the proposed complex research institution AdMaS ("Advanced Materials and Structures") in the near future. The long-time behaviour of massive structures, especially its bearing value, durability and user properties, is typically conditioned by the early-age heat, moisture, etc. treatment, modified by foundations, subgrades, reinforcement and connecting members; thus the aim is to design the whole building process to minimize the development of significant tensile stresses to avoid the the danger of cracking, or even to force volume changes and corresponding final stresses appropriate for the future use of a structure. The deeper understanding of decisive

processes in early-age materials that effects volume changes is therefore needed, although no closed physical and mathematical models are available and all simplified calculations contain empirical parameters and functions, whose identification, supported by laboratory measurements or in situ observations, generates separate non-trivial problems, not discussed in details here. However, we shall demonstrate how the thermomechanical analysis of balance of mass, (linear and angular) momentum and energy for computational HAM ("heat, air and moisture") models in civil engineering is able to be extended to a complex computational model, including the mass source or solid skeleton related to the hydration process (and corresponding sink of liquid water mass), as well as the vapour mass source caused by the liquid water evaporation or desorption, using some micromechanical arguments from the theory of porous media.

2. Mixture components

To analyze the phase changes in an early-age silicate composite, we shall consider four material phases:

- solid material, identified by an index s ,
- liquid water, identified by an index w ,
- water vapour, identified by an index v ,
- dry air, identified by an index a .

In addition to partial derivatives of scalar quantities ψ with respect to time, i. e.

$$\dot{\psi} := \partial\psi/\partial t,$$

we shall introduce also the partial derivatives of such quantities with respect to x_i , $i \in \{1, 2, 3\}$, $x = (x_1, x_2, x_3)$ being a Cartesian coordinate system in the three-dimensional Euclidean space \mathcal{R}^3 ,

$$\psi_{,i} := \partial\psi/\partial x_i.$$

In the case of real vector variables with values in \mathcal{R}^3 we shall write ψ briefly instead of (ψ_1, ψ_2, ψ_3) . Even in the case of matrix variables with values in $\mathcal{R}^{3 \times 3}$, the space of real matrices of the third order, we shall write ψ only instead of ψ_{ij} , $i, j \in \{1, 2, 3\}$. Consequently, due to the preceding notation, unlike the matrix elements ψ_{ij} from $\psi \in \mathcal{R}^{3 \times 3}$ with $i, j \in \{1, 2, 3\}$, we have e. g. for $\psi \in \mathcal{R}^3$

$$\psi_{i,j} := \partial\psi_i/\partial x_j.$$

We shall assume that the scale bridging between particular scales (if relevant scale material data are available) can be done by means of the averaging of model variables. The basic (averaged) variables in our model, related to a representative volume element, are:

- 4 intrinsic phase densities $R = (\rho^s, \rho^w, \rho^v, \rho^a)$,
- 12 components of phase velocities $V = (v_i^s, v_i^w, v_i^v, v_i^a)$ with $i \in \{1, 2, 3\}$,
- 3 fluid pressures $P = (p^w, p^v, p^a)$,
- 1 (absolute) temperature ϑ .

Intrinsic phase densities evidently do not reflect the amount of particular phases in a volume unit; thus it is useful to define (real) phase densities

$$\rho_\varepsilon := \eta^\varepsilon \rho^\varepsilon$$

formally for any phase index $\varepsilon \in \{s, w, v, a\}$ where

$$\begin{aligned} \eta^s &= (1 - n), \\ \eta^w &= ns, \\ \eta^v &= n(1 - s), \\ \eta^a &= n(1 - s)(1 - \phi). \end{aligned}$$

Unfortunately it is not easy to evaluate the porosity n , the saturation degree s and the relative humidity (the volume fraction occupied by water vapour in the total gaseous phase) ϕ . Nevertheless, similarly to $\rho_\varepsilon, \varepsilon \in \{s, v, w, a\}$, being motivated by the Dalton law by (Bermúdez de Castro, 2005), p. 111, we can also introduce pressures

$$p_\varepsilon := \eta^\varepsilon p^\varepsilon.$$

We can evaluate also the “macroscopic” mixture density

$$\rho := \rho_s + \rho_w + \rho_v + \rho_a.$$

Let us also remark that, from the point of view of solid phase, fluid pressures P are accompanied by a (partial) Cauchy stress tensor compound from components τ_{ij} with $i, j \in \{1, 2, 3\}$, whose (indirect) relation to V will be discussed later.

The porosity can be evaluated from the finite strain analysis by (Sanavia et al., 2002), p. 139. The multiphase medium at the macroscopic level can be described as the superposition of all phases ε , whose material point with coordinates $x_i^{\varepsilon 0}$ in the reference configuration Ω in R^3 occupies a point with coordinates $x_i^\varepsilon(t)$; zero indices are related to the reference configuration, here in the initial time $t = 0$. In the Lagrangian description of the motion the position of each material point can be expressed as

$$x_i^\varepsilon(t) = x_i^{\varepsilon 0} + u_i^\varepsilon(x_i^{\varepsilon 0}, t)$$

where $u_i^\varepsilon(x_i^{\varepsilon 0}, t)$ denotes the displacement at chosen time and zero indices are related to a reference configuration, here in time $t = 0$. Thus

$$F_{ij}^\varepsilon(x^{\varepsilon 0}, t) := \frac{\partial x_i^\varepsilon(x^{\varepsilon 0})}{\partial x_j^{\varepsilon 0}} = \delta_{ij} + \frac{\partial u_i^\varepsilon(x^{\varepsilon 0}, t)}{\partial x_j^{\varepsilon 0}}$$

can be taken as a deformation characteristic, δ being a Kronecker symbol, consequently

$$n = 1 - (1 - n_0) (\det F^s)^{-1}$$

where $n_0(x^{s0})$ denotes the porosity in the reference configuration. In the linearized geometry this access is not available: e.g. (Gawin et al., 2006a), p. 310 presents an empirical (nearly linear) function $n(\Gamma)$, justified by the correlation analysis, exploiting the experimental database of (De Schutter, 2002) where hardening cement pastes with 5 different values of water/cement ratio are studied.

The saturation degree s comes from the microporomechanical considerations (cf. (Dormieux et al., 2006), p. 247); their usual result (verified by laboratory measurements) is the so-called sorption isotherm, a real function $s(p^c)$ where p^c is the capillary pressure, determined (in general) as

$$p^c = \Xi(p^w, p^v, p^a)$$

for certain real function Ξ . For temperatures normally encountered in building structures and for capillary saturation range (Gawin et al., 2006a), pp. 305 and 311, recommends the simplified relation

$$p^c = p^v + p^a - p^w,$$

justified by an exploitation of the entropy inequality by means of the Coleman-Noll method; for more details and substantial generalizations see (Gray, 2000), p. 482.

To formulate the basic balance laws of classical thermodynamics, consequently the announced system of partial differential or integral equations of evolution, let us introduce the simple notation of (Vala, 2006), p. 33, applied to particular phases identified by indices $\varepsilon \in \{s, w, v, a\}$. If ω^ε is a source corresponding to a scalar quantity ψ^ε then the conservation of a scalar quantity ψ^ε reads

$$\dot{\psi}^\varepsilon + (\psi^\varepsilon v_i^\varepsilon)_{,i} = \omega^\varepsilon; \quad (1)$$

this will be exploited in the following three sections.

3. Mass balance

For an arbitrary $\varepsilon \in \{s, w, v, a\}$ let us insert a scalar quantity

$$\psi^\varepsilon = \rho_\varepsilon$$

and a corresponding source term ω^ε into (1) where

$$\begin{aligned} \omega^s &= -\dot{\mu}^h, \\ \omega^w &= \dot{\mu}^h - \dot{\mu}^e, \\ \omega^v &= \dot{\mu}^e, \\ \omega^a &= 0. \end{aligned}$$

To simplify our notations, we shall apply the Einstein summation convention for indices from the set $\{1, 2, 3\}$ without additional explanations, e. g. in the following equation the sum over $j \in \{1, 2, 3\}$ is omitted formally. The resulting system of partial differential equations of evolution is

$$\begin{aligned} \dot{\rho}_s + (\rho_s v_j^s)_{,j} &= -\dot{\mu}^h, \\ \dot{\rho}_w + (\rho_w v_j^w)_{,j} &= \dot{\mu}^h - \dot{\mu}^e, \\ \dot{\rho}_v + (\rho_v v_j^v)_{,j} &= \dot{\mu}^e, \\ \dot{\rho}_a + (\rho_a v_j^a)_{,j} &= 0. \end{aligned} \quad (2)$$

Let us notice (here and similarly for other balance laws, too, without explicit comments) that the system (2) contains the standard left-hand-side additive terms, well-known e. g. from (Bermúdez de Castro, 2005), p. 4 (for one phase), and from (Dormieux et al., 2006), p. 9 (for

more phases), supplied by the additional right-hand-side additive terms, containing variables μ^h , determined from the hydration degree Γ , and μ^e , a priori unknown. For the effective numerical calculations, finite element techniques (cf. (Efendiev et al., 2009), p. 47) or finite volume ones (cf. (Efendiev et al., 2009), p. 52) should be applied. Therefore we need to rewrite (2) (and analogous equations in the following sections) into the integral form, able to include boundary conditions in a simple way. Let $\partial\Omega$ be the boundary of a domain Ω in R^3 . Let us introduce the additional notation

$$\begin{aligned}(\zeta, \psi) &:= \int_{\Omega} \zeta(x) \psi(x) \, dx, \\ \langle \zeta, \psi \rangle &:= \int_{\partial\Omega} \zeta(x) \psi(x) \, ds(x)\end{aligned}$$

for any functions ζ and ψ (integrable in the needed sense) where dx refers to the standard Lebesgue measure and $ds(x)$ to the surface Hausdorff measure. The integration by parts (based on the Green-Ostrogradskii theorem) then gives

$$\begin{aligned}(\zeta, \dot{\rho}_s) + \langle \zeta, \rho_s v_j^s v_j \rangle - (\zeta_{,j}, \rho_s v_j^s) &= -(\zeta, \dot{\mu}^h), \\ (\zeta, \dot{\rho}_w) + \langle \zeta, \rho_w v_j^w v_j \rangle - (\zeta_{,j}, \rho_w v_j^w) &= (\zeta, \dot{\mu}^h - \dot{\mu}^e), \\ (\zeta, \dot{\rho}_v) + \langle \zeta, \rho_v v_j^v v_j \rangle - (\zeta_{,j}, \rho_v v_j^v) &= (\zeta, \dot{\mu}^e), \\ (\zeta, \dot{\rho}_a) + \langle \zeta, \rho_a v_j^a v_j \rangle - (\zeta_{,j}, \rho_a v_j^a) &= 0\end{aligned}\tag{3}$$

for any test function ζ (more precisely: sufficiently smooth, otherwise only in sense of distributions, from an appropriate function space which may be problem-specific);

$$\nu(x) = (\nu_1(x), \nu_2(x), \nu_3(x))$$

means the local unit outward normal vector on (sufficiently smooth) $\partial\Omega$.

4. Momentum balance

The momentum balance includes the linear balance and the angular balance. Since we consider a non-polar continuum, the second one forces only the symmetry of any Cauchy stress tensor τ . It remains to apply the first one. For an arbitrary $\varepsilon \in \{s, w, v, a\}$ and (step-by-step) for particular $i \in \{1, 2, 3\}$ let us insert a scalar quantity

$$\psi^\varepsilon = \rho_\varepsilon v_i^\varepsilon$$

and a corresponding source term

$$\omega^\varepsilon = \sigma_{ij,j}^\varepsilon + \rho_\varepsilon (g_i - a_i^\varepsilon + \theta_i^\varepsilon)$$

into (1) where

$$\sigma_{ij}^s = \tau_{ij}$$

for the solid phase and

$$\sigma_{ij}^\varepsilon = -\delta_{ij} p_\varepsilon$$

for all other phases with $\varepsilon \in \{w, v, a\}$, the acceleration $g = (g_1, g_2, g_3)$ generates $\rho_\varepsilon g$, the volume density of a gravitational force, the acceleration $a^\varepsilon = (a_1^\varepsilon, a_2^\varepsilon, a_3^\varepsilon)$, corresponding to the velocity

$v^\varepsilon = (v_1^\varepsilon, v_2^\varepsilon, v_3^\varepsilon)$, generates the volume density of an inertia force, and the acceleration $\theta_i^\varepsilon = (\theta_1^\varepsilon, \theta_2^\varepsilon, \theta_3^\varepsilon)$ generates the volume density due to mechanical interaction with other phases. The total Cauchy stress, introduced (unlike the partial Cauchy stress τ) as

$$\sigma := \sigma^s + \sigma^w + \sigma^v + \sigma^a,$$

then has the components

$$\sigma_{ij} = \tau_{ij} - \delta_{ij}(p_w + p_v + p_a).$$

The Clapeyron law (see (Gawin et al., 2006a), p. 305) enables us to evaluate both gas pressures p^v and p^a (consequently p_v and p_a , too) as certain functions $p^v(\rho^v, \vartheta^v)$ and $p^a(\rho^a, \vartheta^a)$. Unfortunately, for the remaining pressure p^w (or p_w) we do not know such constitutive relation.

In the linear momentum balance equations we need to calculate all velocities v^ε and accelerations a^ε from corresponding displacements u^ε , $\varepsilon \in \{s, w, v, a\}$. By the chain rule we have

$$\begin{aligned} v_i^\varepsilon(x^{\varepsilon 0}, t) &= \dot{u}_i^\varepsilon(x^{\varepsilon 0}, t) + u_{i,j}^\varepsilon(x^{\varepsilon 0}, t) v_j^\varepsilon(x^{\varepsilon 0}, t), \\ a_i^\varepsilon(x^{\varepsilon 0}, t) &= \ddot{u}_i^\varepsilon(x^{\varepsilon 0}, t) + \dot{v}_{i,j}^\varepsilon(x^{\varepsilon 0}, t) v_j^\varepsilon(x^{\varepsilon 0}, t). \end{aligned}$$

The terms $u_{i,j}^\varepsilon v_j^\varepsilon$ and $\dot{v}_{i,j}^\varepsilon v_j^\varepsilon$, can be understood in the sense of scalar products $\text{grad } u^\varepsilon \cdot v^\varepsilon$, $\text{grad } v^\varepsilon \cdot v^\varepsilon$ by (Sanavia, 2001), p. 139 (though the construction of such general grad-operator is not quite trivial). More precisely, the geometry of structured continua is described using fiber bundles and Riemannian manifold in (Yavari & Marsden, 2009), p. 8. Another approach, explained in (Bermúdez de Castro, 2005), p. 195, results in the ALE ("Arbitrary Lagrangian-Eulerian") formulations by (Bermúdez de Castro, 2005), p. 195. Nevertheless, both such generalizations lead to complicated, reader-unfriendly expressions.

The classical constitutive relation for the solid phase between τ , u^s , v^s , etc., considers a linearized sufficiently small strain tensor and its additive decomposition into several parts, typically to the linear elastic and the power-law viscoelastic (creep) ones, containing facultative corrections due to microcracking, as in (Gawin et al., 2006a), p. 343, and (in more details) in (Gawin et al., 2006b), p. 519, with help of special mechanical and chemical damage parameters. The finite deformation theory needs some multiplicative decomposition of F^s in the form

$$F^s = F^{s1} F^{s2} \dots F^{sM}$$

into a finite number $M > 1$ of matrix components; the constitutive relation is then characterized by a function

$$\tau(F^{s1}, \dots, F^{sM}, \dot{F}^{s1}, \dots, \dot{F}^{sM}, \dots).$$

Especially in the case $M = 2$ (Sanavia et al., 2002), p. 143 combines the first standard reversible elastic component with the second irreversible one from the Drucker-Prager plasticity model with linear isotropic hardening, Neff (2008) combines elasticity with nonlocal linear kinematic hardening due to dislocation interaction, etc. Recently Majorana (2010) suggests even $M = 9$, taking into account i) elastic deformation, ii) plastic deformation, iii) damage, iv) cracking, v) creep, vi) shrinkage, vii) lits, viii) thermal strain, ix) autogenous strain, covering most items a)-e) from *Introduction*. However, for all simulation of real processes the theoretical extent of such decomposition must be supported by the competence in the laboratory identification

of needed material characteristics and in the estimate of their uncertainty, imported into constitutive relations.

The evaluation of θ_i^s , θ_i^w , θ_i^v and θ_i^a for all $i \in \{1, 2, 3\}$ comes from the Darcy law, whose general (nonlinear) form, following (Dormieux et al., 2006), p. 50, based on the knowledge of certain material functions F_1 , F_2 and F_3 , valid for each $\varepsilon \in \{w, v, a\}$, is

$$v_i^\varepsilon - v_i^s = F_i^\varepsilon(\theta_1^\varepsilon, \theta_2^\varepsilon, \theta_3^\varepsilon, p^\varepsilon, \eta^\varepsilon).$$

The special (linear) form of these relations, suggested in (Sanavia, 2001), p. 9 (this part of (Sanavia, 2001) contains much more technical details than its later revision (Sanavia et al., 2002)), is

$$K_{ij}^\varepsilon(\rho_\varepsilon \theta_j^\varepsilon - p_{,j}^\varepsilon) + \kappa^\varepsilon \eta^\varepsilon (v_i^\varepsilon - v_i^s) = 0$$

where, for a fixed $\varepsilon \in \{w, v, a\}$, K_{ij}^ε are components of a symmetric permeability matrix and κ^ε is a (positive) dynamic viscosity. Such constitutive relations have to be supplied by the constraint by (Sanavia, 2001), p. 8,

$$\theta_i^s + \theta_i^w + \theta_i^v + \theta_i^a = 0.$$

The resulting system of partial differential equations of evolution, unified (for brevity) for all $\varepsilon \in \{w, v, a\}$ and $i \in \{1, 2, 3\}$ is

$$(\rho_\varepsilon v_i^\varepsilon)' + (\rho_\varepsilon v_i^\varepsilon v_{j,j}^\varepsilon) = -p_{,i}^\varepsilon + \rho_\varepsilon (g_i - a_i^\varepsilon + \theta_i^\varepsilon). \quad (4)$$

For the solid phase we receive similarly for all $i \in \{1, 2, 3\}$

$$(\rho_s v_i^s)' + (\rho_s v_i^s v_{j,j}^s) = \tau_{ij,j} + \rho_s (g_i - a_i^s + \theta_i^w + \theta_i^v + \theta_i^a). \quad (5)$$

We can see that for negligible values of all components of v^s and θ^s (5) this result degenerates to classical Cauchy equilibrium conditions, well-known in building statics (with zero a^s) and dynamics (with nonzero a^s),

$$\rho_s a_i^s + \tau_{ij,j} = -\rho_s g_i.$$

Let us repeat the approach with a test function ς from the previous section and apply it to (4) and (5). For any $i \in \{1, 2, 3\}$ the integration by parts with $\varepsilon \in \{w, v, a\}$ gives

$$\begin{aligned} & (\varsigma, (\rho_\varepsilon v_i^\varepsilon)) + \langle \varsigma, \rho_\varepsilon v_i^\varepsilon v_j^\varepsilon v_j \rangle - (\varsigma_{,j}, \rho_\varepsilon v_i^\varepsilon v_j^\varepsilon) \\ & = -\langle \varsigma, p^\varepsilon v_i \rangle + (\varsigma_{,i}, p^\varepsilon) + (\varsigma, \rho_\varepsilon (g_i - a_i^\varepsilon + \theta_i^\varepsilon)), \end{aligned} \quad (6)$$

whereas for the solid phase the analogous result is

$$\begin{aligned} & (\varsigma, (\rho_s v_i^s)) + \langle \varsigma, \rho_s v_i^s v_j^s v_j \rangle - (\varsigma_{,j}, \rho_s v_i^s v_j^s) \\ & = \langle \varsigma, \tau_{ij} v_j \rangle - (\varsigma_{,j}, \tau_{ij}) + (\varsigma, \rho_s (g_i - a_i^s - \theta_i^w - \theta_i^v - \theta_i^a)) \end{aligned} \quad (7)$$

for any test function ς .

5. Energy balance

Let us introduce four (in general temperature-variable) heat capacities $c^\varepsilon(\vartheta)$ as prescribed material characteristics and four heat fluxes $q^\varepsilon = (q_1^\varepsilon, q_2^\varepsilon, q_3^\varepsilon)$ as additional variables. Similarly to the mass balance, for an arbitrary $\varepsilon \in \{s, w, v, a\}$, let us insert a scalar quantity

$$\psi^\varepsilon = \frac{1}{2} \rho_\varepsilon (v_i^\varepsilon)^2 + \rho_\varepsilon c^\varepsilon \vartheta$$

and a corresponding source term

$$\omega^\varepsilon = (\sigma_{ij,j}^\varepsilon + q_i^\varepsilon)_{,i} + (\rho_\varepsilon (g_i - a_i^\varepsilon + \theta_i^\varepsilon))_{,i} + \omega^\varepsilon$$

into (1) where the exchange of energy between phases is accounted using the additive terms

$$\begin{aligned}\omega^s &= -\dot{\mu}^h \zeta^h, \\ \omega^w &= \dot{\mu}^h \zeta^h - \dot{\mu}^e \zeta^e, \\ \omega^v &= \dot{\mu}^e \zeta^e, \\ \omega^a &= 0\end{aligned}$$

with specific enthalpies ζ^h and ζ^e (introduced in (Bermúdez de Castro, 2005), p. 110): ζ^h that of hydration (related to the mass unit of chemically bound water) and ζ^e that of evaporation, following (Gawin et al., 2006a), p. 303. The resulting system of partial differential equations of evolution is

$$\begin{aligned}& (\rho_s v_i^s v_i^s + 2\rho_s c^s \vartheta)_{,i} + ((\rho_s v_i^s v_i^s + 2\rho_s c^s \vartheta) v_j^s)_{,j} \\&= 2\tau_{ij,ij} - 2q_{i,i}^s + 2(\rho_s (g_i - a_i^s - \theta_i^w - \theta_i^v - \theta_i^a))_{,i} - 2\dot{\mu}^h \zeta^h, \\& (\rho_w v_i^w v_i^w + 2\rho_w c^w \vartheta)_{,i} + ((\rho_w v_i^w v_i^w + 2\rho_w c^w \vartheta) v_j^w)_{,j} \\&= -2p_{i,i}^w - 2q_{i,i}^w + 2(\rho_w (g_i - a_i^w + \theta_i^w))_{,i} + 2\dot{\mu}^h \zeta^h - 2\dot{\mu}^e \zeta^e, \\& (\rho_v v_i^v v_i^v + 2\rho_v c^v \vartheta)_{,i} + ((\rho_v v_i^v v_i^v + 2\rho_v c^v \vartheta) v_j^v)_{,j} \\&= -2p_{i,i}^v - 2q_{i,i}^v + 2(\rho_v (g_i - a_i^v + \theta_i^v))_{,i} + 2\dot{\mu}^e \zeta^e, \\& (\rho_a v_i^a v_i^a + 2\rho_a c^a \vartheta)_{,i} + ((\rho_a v_i^a v_i^a + 2\rho_a c^a \vartheta) v_j^a)_{,j} \\&= -2p_{i,i}^a - 2q_{i,i}^a + 2(\rho_a (g_i - a_i^a + \theta_i^a))_{,i}.\end{aligned}\tag{8}$$

All heat fluxes can be computed using the Fourier law by (Bermúdez de Castro, 2005), p. 42: in general we have

$$q_i^\varepsilon + \lambda_{ij}^\varepsilon \vartheta_{,j} = 0$$

for every $\varepsilon \in \{s, w, v, a\}$ and $i \in \{1, 2, 3\}$ and prescribed material characteristics

$$\lambda_{ij}^\varepsilon(\vartheta, \vartheta_{,1}, \vartheta_{,2}, \vartheta_{,3}).$$

Supposing that all these characteristics are independent of derivatives of ϑ , in the linearized case the elements λ_{ij} generate certain symmetrical matrix of real factors, allowed to be functions of ϑ . Under the assumption of isotropy material we obtain moreover $\lambda_{ij} = \lambda_* \delta_{ij}$ for some real factor $\lambda_*(\vartheta)$; this is just the crucial simplification of (Gawin et al., 2006a), p. 313,

$$q_i^\varepsilon = -\lambda_*^\varepsilon \vartheta_{,i}.$$

Repeating the approach with some test function ς again and applying it to (8), from the integration by parts we obtain

$$\begin{aligned}
 & (\varsigma, (\rho_s v_i^s v_i^s + 2\rho_s c^s \vartheta)) \\
 & + \langle \varsigma, (\rho_s v_i^s v_i^s + 2\rho_s c^s \vartheta) v_j^s v_j^s \rangle - (\varsigma, j, (\rho_s v_i^s v_i^s + 2\rho_s c^s \vartheta) v_j^s) \\
 = & 2\langle \varsigma, (\tau_{ij,j} - 2q_i^s) v_i \rangle - 2(\varsigma, i, \tau_{ij,j} - 2q_i^s) \\
 & + 2\langle \varsigma, \rho_s (g_i - a_i^s - \theta_i^w - \theta_i^v - \theta_i^a) v_i \rangle - 2(\varsigma, i, \rho_s (g_i - a_i^s - \theta_i^w - \theta_i^v - \theta_i^a)) - 2(\varsigma, \dot{\mu}^h \zeta^h), \\
 & (\varsigma, (\rho_w v_i^w v_i^w + 2\rho_w c^w \vartheta)) \\
 & + \langle \varsigma, (\rho_w v_i^w v_i^w + 2\rho_w c^w \vartheta) v_j^w v_j^w \rangle - (\varsigma, j, (\rho_w v_i^w v_i^w + 2\rho_w c^w \vartheta) v_j^w) \\
 = & -2\langle \varsigma, (p_i^w + q_i^w) v_i \rangle + 2(\varsigma, i, p_i^w + q_i^w) \\
 & + 2\langle \varsigma, (\rho_w (g_i - a_i^w + \theta_i^w)) v_i \rangle - 2(\varsigma, i, \rho_w (g_i - a_i^w + \theta_i^w)) + 2(\varsigma, \dot{\mu}^h \zeta^h - \dot{\mu}^e \zeta^e), \quad (9) \\
 & (\varsigma, (\rho_v v_i^v v_i^v + 2\rho_v c^v \vartheta)) \\
 & + \langle \varsigma, (\rho_v v_i^v v_i^v + 2\rho_v c^v \vartheta) v_j^v v_j^v \rangle - (\varsigma, j, \rho_v v_i^v v_i^v + 2\rho_v c^v \vartheta) v_j^v) \\
 = & -2\langle \varsigma, (p_i^v + q_i^v) v_i \rangle + 2(\varsigma, i, p_i^v + q_i^v) \\
 & + 2\langle \varsigma, \rho_v (g_i - a_i^v + \theta_i^v) v_i \rangle - 2(\varsigma, i, \rho_v (g_i - a_i^v + \theta_i^v)) + 2(\varsigma, \dot{\mu}^e \zeta^e), \\
 & (\varsigma, (\rho_a v_i^a v_i^a + 2\rho_a c^a \vartheta)) \\
 & + \langle \varsigma, (\rho_a v_i^a v_i^a + 2\rho_a c^a \vartheta) v_j^a v_j^a \rangle - (\varsigma, j, \rho_a v_i^a v_i^a + 2\rho_a c^a \vartheta) v_j^a) \\
 = & -2\langle \varsigma, (p_i^a + q_i^a) v_i \rangle + 2(\varsigma, i, p_i^a + q_i^a) \\
 & + 2\langle \varsigma, \rho_a (g_i - a_i^a + \theta_i^a) v_i \rangle - 2(\varsigma, i, \rho_a (g_i - a_i^a + \theta_i^a)).
 \end{aligned}$$

for any test function ς .

6. Initial and boundary conditions

Since the class of admissible problems (moreover, not defined properly yet) is rather large, we shall not try to create a list of all physically reasonable types boundary conditions. However, the following considerations demonstrate the methods of implementation of boundary conditions into above derived systems of evolution.

Let us remind the boundary integrals occurring in the integral forms of evolution equations. Those from (3) contain functions

$$\rho_s v_j^s v_j^s, \quad \rho_w v_j^w v_j^w, \quad \rho_v v_j^v v_j^v, \quad \rho_a v_j^a v_j^a,$$

those from (6) and (7), in addition to functions

$$\rho_s v_i^s v_j^s v_j^s, \quad \rho_w v_i^w v_j^w v_j^w, \quad \rho_v v_i^v v_j^v v_j^v, \quad \rho_a v_i^a v_j^a v_j^a$$

also functions

$$\tau_{ij} v_j, \quad p^w v_i, \quad p^v v_i, \quad p^a v_i,$$

finally those from (9) functions in addition to functions

$$\rho_s v_i^s v_i^s v_j^s v_j^s, \quad \rho_s v_i^w v_i^w v_j^w v_j^w, \quad \rho_s v_i^v v_i^v v_j^v v_j^v, \quad \rho_s v_i^a v_i^a v_j^a v_j^a$$

still other functions

$$\begin{aligned} &\rho_s c^s \vartheta v_j^s v_j, \quad \rho_w c^w \vartheta v_j^w v_j, \quad \rho_v c^v \vartheta v_j^v v_j, \quad \rho_a c^a \vartheta v_j^a v_j, \\ &\tau_{ij,j} v_i, \quad p_i^w v_i, \quad p_i^v v_i, \quad p_i^a v_i, \\ &q_i^s v_i, \quad q_i^w v_i, \quad q_i^v v_i, \quad q_i^a v_i, \\ &\rho_s g_i v_i, \quad \rho_w g_i v_i, \quad \rho_v g_i v_i, \quad \rho_a g_i v_i, \\ &\rho_s a_i^s v_i, \quad \rho_w a_i^w v_i, \quad \rho_v a_i^v v_i, \quad \rho_a a_i^a v_i, \\ &(\rho_w - \rho_s) \theta_i^w v_i, \quad (\rho_v - \rho_s) \theta_i^v v_i, \quad (\rho_a - \rho_s) \theta_i^a v_i. \end{aligned}$$

Solutions of the resulting system of equations (3), (6), (7) and (9), supplied by needed constitutive equations, should be included in certain spaces of abstract functions, mapping each time $t \geq 0$ to some Sobolev, Lebesgue, etc. function space \mathcal{S} . Initial values of all independent variables (whose appropriate choice will be discussed later) are supposed to be prescribed in time $t = 0$. Boundary conditions on $\partial\Omega$ or its part for the resulting system of equations (3), (6), (7) and (9), supplied by needed constitutive equations, can be then divided into three groups:

- conditions built in the definition of spaces V , usually prescribed values of abstract functions from V on $\partial\Omega$ (in sense of traces) at any admissible time,
- conditions exploiting the knowledge of above listed functions or their linear combinations,
- other conditions.

All subsequent examples work with any x from $\partial\Omega$ or its certain part and with arbitrary time $t \geq 0$. The typical example of a) is

$$\vartheta = \vartheta_*$$

for the a priori known temperature $\vartheta_*(x, t)$. Another (technically more complicated, but homogeneous) example of a) can be

$$\rho v_i v_i = 0$$

with the carefully defined “effective” velocity

$$v_i := (\rho_s v_i^s + \rho_w v_i^w + \rho_a v_i^a) / \rho.$$

The classical example of b), known even from elementary statics, is

$$\sigma_{ij} v_j = f_i$$

with $i \in \{1, 2, 3\}$ for the prescribed surface load

$$f(x, t) = (f_1(x, t), f_2(x, t), f_3(x, t)).$$

Indirectly this is a boundary condition for u (or v , etc.), due to stress-strain constitutive relations. Its analogy for heat transfer

$$q_i v_i = q_*$$

works with the total heat flux vector

$$q := \rho_s q^s + \rho_w q^w + \rho_v q^v + \rho_a q^a$$

for the prescribed heat flux $q_*(x, t)$.

One could expect a similar result for the total diffusive flux vector

$$r := \rho_w(v_i^w - v_i^s) + \rho_v(v_i^v - v_i^s) + \rho_a(v_i^a - v_i^s),$$

as applied in (Gawin et al., 2006a), p. 316, but this is limited by the facultative nonlinearity of the Darcy law. If the form of F_i^ε with $i \in \{1, 2, 3\}$ and $\varepsilon \in \{w, v, a\}$ does not admit the explicit evaluation of all corresponding vectors θ^ε as linear combinations of $v^\varepsilon - v^s$, we must refer to c). In general, to satisfy such boundary conditions properly, additional techniques, as the application of Lagrange multipliers, Kuhn-Tucker conditions, etc., are necessary.

7. Exact solutions and iterative algorithms

The mathematical solvability of engineering problems, whose formulation comes from physically reasonable and transparent considerations, depends critically on the choice:

- of the set of primary variables,
- of the choice spaces \mathcal{S} of functions, abstract functions, etc.,
- of the proper formulation of boundary and initial conditions.

Nevertheless, our problem of early-age time-dependent behaviour of silicate composites is rather complicated, thus most authors bring new versions of a), applying different mathematical, physical and technical simplifications. From the most simple algebraic relations, avoiding differential and integral calculus completely, referring to empirical relations and selected statistical techniques, as presented in (Moon et al., 2005) or in (Bentz, 2008), through one evolution equation, usually of heat conduction, supplied by a lot of empirical dependencies, justified by extensive experimental works, it is possible to trace the development to such advanced physical and mathematical models, as to the system of 10 differential equations of evolution with 10 primary variables and numerous constitutive relations in (Gawin et al., 2006b), p. 519.

To reduce the number of empirical relations, typically motivated by some micromechanical considerations, but not fully compatible with quantitative lower-scale computations, we are ready to work with 20 primary variables. In *Mixture components* we have introduced 20 variables \mathcal{R} , \mathcal{V} , \mathcal{P} and ϑ . Only 2 of these variables, p^v and p^a , can be evaluated outside the system of (differential or integral) equations of evolution. On the other hand, regardless of the fact that the proper evaluation of Γ forces solution of an additional ordinary differential equation, no constitutive relations are available just to μ^e and φ . This motivates us to reorder our set of variables slightly, introducing

$$\mathcal{T} = (\theta, p^w, \mu^e, \varphi).$$

Therefore we can take \mathcal{R} , \mathcal{V} and \mathcal{T} as primary variables; finally we have 20 primary variables and 20 equations in evolution: (2), (4) with (5) and (8), or (3), (6) with (7) and (9), alternatively. We have noticed that the second version is much more frequently used for numerical computations.

Because of the complexity of the problem, the mathematical verification of existence, uniqueness, regularity etc. of solutions of initial and boundary problems, corresponding in the case of weak solutions to (3), (6) with (7) and (9), or in the case of strong (classical) solutions to (2), (4) with (5) and (8), due to admissible classes of initial and boundary conditions, contains a lot of open questions. The crucial problem seems to be just in b), i.e. in the definition of some spaces of (generalized) functions with the good properties, expected for the solutions.

Even a very special case with a liquid phase only, whose some important additive terms are neglected, derived directly from (2), (4) and (8), namely

$$\begin{aligned}\dot{\rho}_w + (\rho_w v_j^w)_{,j} &= 0, \\ (\rho_w v_1^w) + (\rho_w v_1^w v_j^w)_{,j} &= -p_{,1}^w + \rho_w (g_1 - a_1^w), \\ (\rho_w v_2^w) + (\rho_w v_2^w v_j^w)_{,j} &= -p_{,2}^w + \rho_w (g_2 - a_2^w), \\ (\rho_w v_3^w) + (\rho_w v_3^w v_j^w)_{,j} &= -p_{,3}^w + \rho_w (g_3 - a_3^w), \\ (\rho_w v_i^w v_i^w) + ((\rho_w v_i^w v_i^w) v_j^w)_{,j} &= -2p_{,i}^w + 2(\rho_w (g_i - a_i^w))_{,i},\end{aligned}$$

generates (with standard constitutive relations) the so-called Navier-Stokes existence and smoothness problem, one of the *Millenium Prize Problems*, formulated by the Clay Mathematics Institute; for its complete definition see www.claymath.org/millennium/Navier-Stokes_Equations/Official_Problem_Description.pdf.

Although the formal solvability of Navier-Stokes equations is not clear, various methods have been developed successfully to analyze their approximate solutions. This can motivated us to the design of an iterative algorithm for numerical simulation of our much more complex physical (and chemical) process, clearly with expected difficulties in any convergence analysis. The precise form of such iterative algorithm, constructing, step-by-step in time, a finite-dimensional approximation of solution of (3), (6) with (7) and (9), depends substantially on c), discussed briefly in the previous section. However, the main idea, coming from some finite element or finite volume technique and from the Rothe method of discretization in time, at least at a finite time interval, can be:

1. set \mathcal{R} , \mathcal{V} and \mathcal{T} by the initial conditions at $t = 0$,
2. add a time step length to t , preserving \mathcal{R} , \mathcal{V} and \mathcal{T} ,
3. solve \mathcal{R} from some linearized version of (3), evaluate the correction $\varepsilon_{\mathcal{R}}$ of \mathcal{R} ,
4. solve \mathcal{V} from the linearized version of (6 and 7), evaluate the correction $\varepsilon_{\mathcal{V}}$ of \mathcal{V} ,
5. solve \mathcal{T} from the linearized version of (9), evaluate the correction $\varepsilon_{\mathcal{T}}$ of \mathcal{T} ,
6. if $\varepsilon_{\mathcal{R}}$, $\varepsilon_{\mathcal{V}}$ and $\varepsilon_{\mathcal{T}}$ are sufficiently small, return to 3,
7. if the final time is reached, stop the computation, otherwise return to 2.

Evidently, preconditioning, mesh adaptivity, stabilization techniques and other technical manipulations are useful to be implemented into such algorithm to force its robustness and effectivity.

8. Computational simulations

Most non-trivial physical and technical studies of the problems of early-age behaviour of silicate composites, or (in particular) of concrete, of mortar pastes, etc., include or refer to some numerical experiment, modelling or simulation, applying finite element or finite (control) volume (rarely finite difference or meshless) techniques together with methods for time discretization, as that of lines, of characteristics or of discretization in time, including some microstructural data. However, no specialized commercial or research software code concentrated to such problems is available; one could expect that the complete development of such a code (in such languages for scientific computing as Fortran or C++) would be expensive and time-consuming and would require a team of specialists in many fields of

knowledge, including those outside information technologies. This results in the following rough classification of typically applied software packages:

- commercial software for HAM analysis as WUFI (Fraunhofer Institut Holzkirchen) or DELPHIN (Technische Universität Dresden),
- large commercial software systems as ANSYS, ABAQUS, etc. (not very flexible, offering only weak support for specific properties of silicate composites)
- specialized software for computations in civil engineering, namely ATHENA (Červenka Consulting Prague) for calculations of strain and stress distributions in concrete structures at various stages of their existence, including the concrete/reinforcement cooperation, the prediction of fracture and the behaviour under extreme loads, or CESAR-LCPC (Ram Caddsys Chennai, India) for mechanical, structural and geotechnical calculations involving even certain analysis of phenomena associated with young hardening concrete,
- user-friendly environment MATLAB/COMSOL for the support of development of original software.

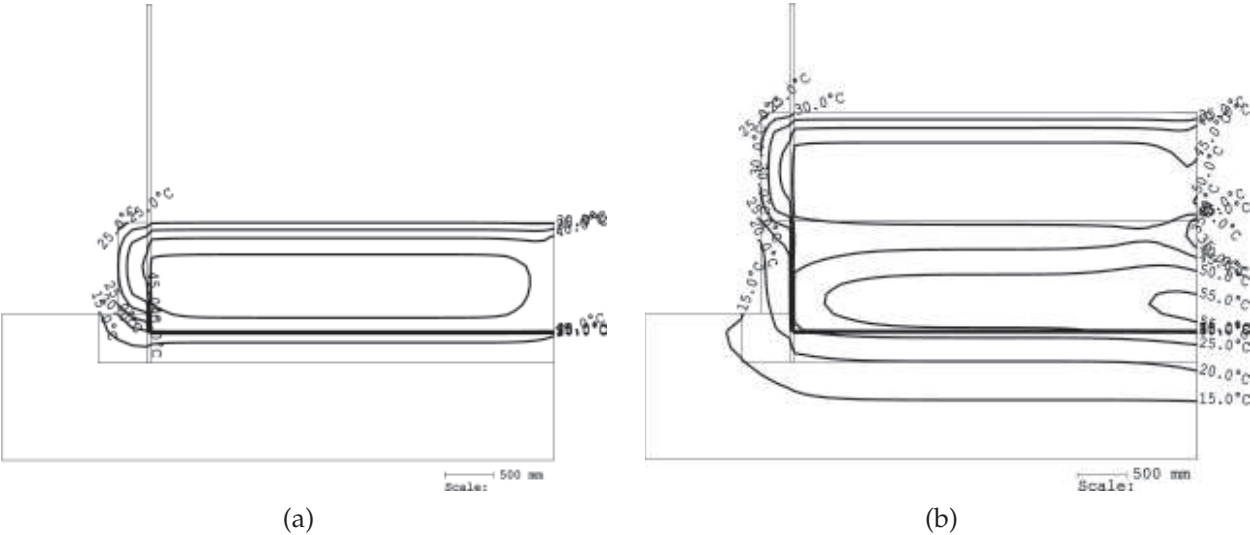


Fig. 1. Distribution of: (a) $\vartheta(x_1, x_2)$ for fixed x_3 at $t = 24$ s, (b) $\vartheta(x_1, x_2)$ for fixed x_3 at $t = 96$ s.

The attempts to predict long-time properties of concrete and other silicate mixtures from the proper analysis of physical and chemical processes during their hardening at the Faculty of Civil Engineering of Brno University of Technology have its own history, involving all above sketched approaches. The original software is in progress, being still far from covering all above discussed micro- and macrostructural aspects. For illustration see (Vala et al., 2009) with numerical simulation of the time-variable thermomechanical behaviour of a massive concrete bridge structure in the Czech Republic (2.5 m thick slab has been formed in 5 layers in 5 time periods) during first 45 hours of its existence; the thermochemical evaluation of hydration heats corresponds to 9 dominant minerals included in the Portland cement.

Another practical example (not published yet) refers to a massive concrete foundation, prepared for the vibrational compactor. Fig. 1-3 document the temperature development in time, using the isotherms for $t \in \{24, 96, 144, 312, 408\}$ s (where their redistribution seems to be most interesting) in one half of a typical cut through such structure, built in successive time steps.

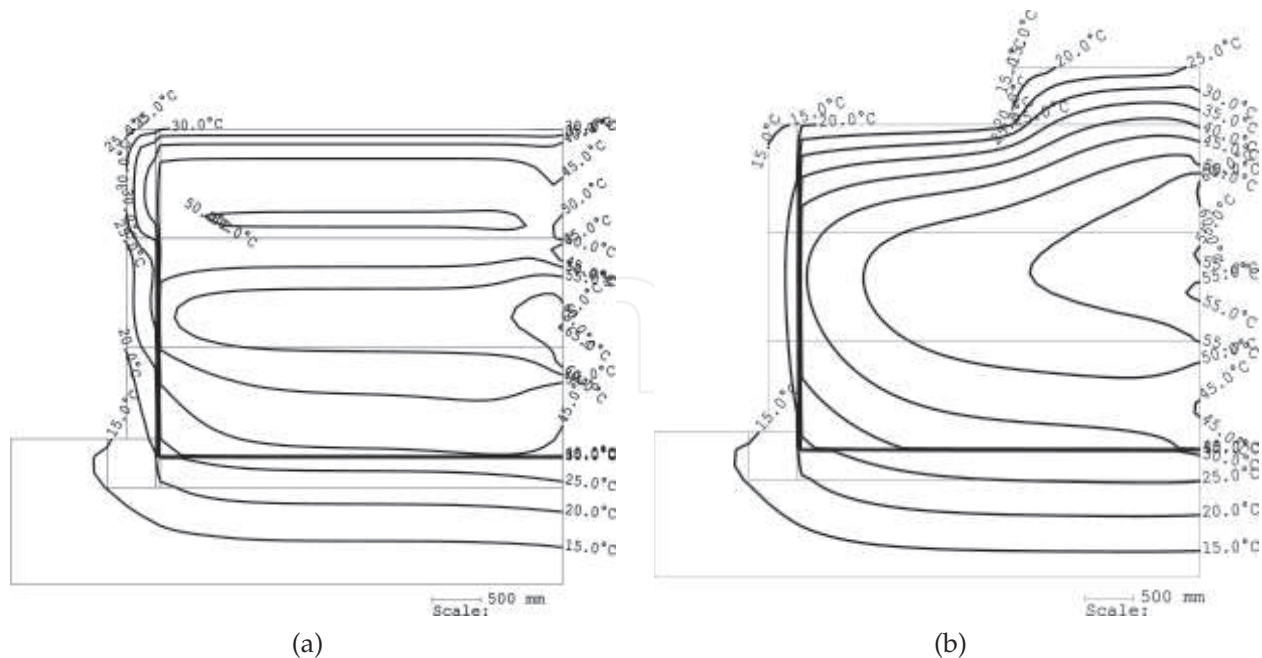


Fig. 2. Distribution of: (a) $\vartheta(x_1, x_2)$ for fixed x_3 at $t = 144$ s, (b) $\vartheta(x_1, x_2)$ for fixed x_3 at $t = 312$ s.

9. Conclusion

We have derived a rather general (but physically transparent) model of thermomechanical behaviour of early-age silicate composites, including four phases, their interactions and phase changes. The related software experiments, motivated from building practice, exploit, up to now, only a minor part of this model.

We have mentioned some mathematical and numerical difficulties, reflected in the intricacy of software codes. From the practical point of view, even more unpleasant complication are connected with the (often unstable and ill-conditioned) inverse problems of identification of material characteristics, typically as nonlinear functions of several variables, in their reliability and correlation with (often only qualitative) microstructural information – cf. (Aly & Sanjayan, 2009) and Chap. 15 of (Kosmatka et al., 2002), called *Volume Changes of Concrete*. Simultaneously still other generalization, not built in our theory explicitly, are needed in practically motivated technical calculation, as thermal radiation of buildings, discussed in (Štastník, 2007), or nonlocal modelling of micro- and macrocracking and damage by (Kozák & Vlček, 2005). Continued research seems to require more expensive both laboratory equipments and computer hardware and software, thus its extent depends on the grant support of some complex research project, as that mentioned in *Introduction*, in the near future.

10. Acknowledgement

This research has been partially supported by the Ministry of Education, Youth and Sports of Czech Republic No. MSM 0021630511, and by the project of specific research of Brno University of Technology No. FAST-S-10-17.

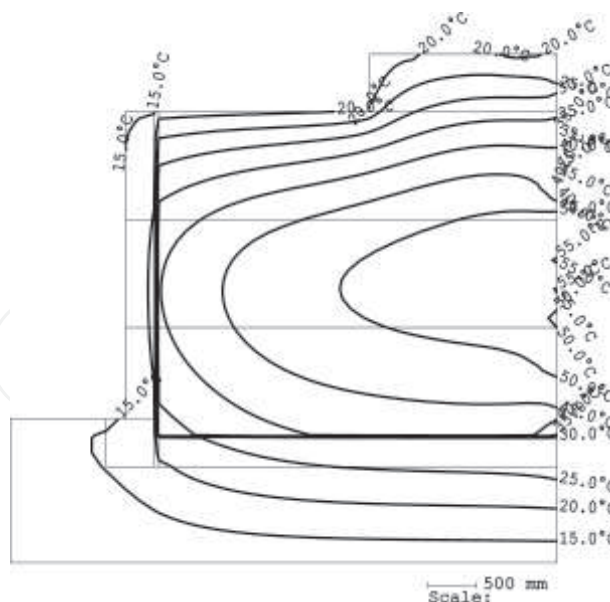
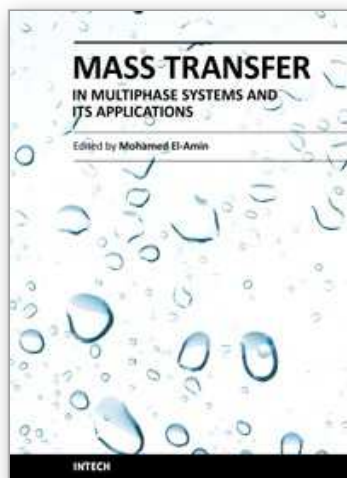


Fig. 3. Distribution of $\theta(x_1, x_2)$ for fixed x_3 at $t = 408$ s

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Mass Transfer in Multiphase Systems and its Applications

Edited by Prof. Mohamed El-Amin

ISBN 978-953-307-215-9

Hard cover, 780 pages

Publisher InTech

Published online 11, February, 2011

Published in print edition February, 2011

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Jiri Vala (2011). Multiphase Modelling of Thermomechanical Behaviour of Early-Age Silicate Composites, Mass Transfer in Multiphase Systems and its Applications, Prof. Mohamed El-Amin (Ed.), ISBN: 978-953-307-215-9, InTech, Available from: <http://www.intechopen.com/books/mass-transfer-in-multiphase-systems-and-its-applications/multiphase-modelling-of-thermomechanical-behaviour-of-early-age-silicate-composites>

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