Prediction of Behaviour of Cementitious Composites Under Fire Conditions

JIŘÍ VALA
Brno University of Technology
Faculty of Civil Engineering
Veveří 95, 602 00 Brno
CZECH REPUBLIC
vala.j@fce.vutbr.cz

ANNA KUČEROVÁ
Brno University of Technology
Faculty of Civil Engineering
Veveří 95, 602 00 Brno
CZECH REPUBLIC
kucerova.a@fce.vutbr.cz

PETRA ROZEHNALOVÁ
Brno University of Technology
Faculty of Civil Engineering
Veveří 95, 602 00 Brno
CZECH REPUBLIC
rozehnalova.p@fce.vutbr.cz

Abstract: Prediction of non-stationary behaviour of cementitious composites as crucial materials of concrete building structures, at high temperatures, namely under fire conditions contains still a lot of difficulties, related to i) multiphysical analysis, dealing with the coupled heat and (liquid and vapour) mass transfer and related mechanical effects, ii) open questions of existence and uniqueness of formal mathematical solutions, including the convergence of numerical algorithms, iii) design and identification of suitable material characteristics, supportable by rather inexpensive experiments: the macroscopic mass, momentum and energy conservation equations need to exploit available information from micro-structural considerations. This paper discusses common traditional and advanced computational modelling and simulation approaches and shows a possible practical compromise between the model complexity and the reasonable possibility of identification of material characteristics of all components and their changes. An illustrative example confronts computational results from such a simplified model with experimental ones, performed in the specialized laboratory at the Brno University of Technology.

Key–Words: Cementitious composites, modelling of heat and mass transfer, fire simulation.

1 Introduction

Problems concerning cementitious composites, especially concrete both in its regular and more advanced forms, as high-strength, stamped, (ultra-)high-performance, self-consolidating, pervious or vacuum concrete, limecrete, shotcrete, etc., exposed to elevated and high temperatures are significant and wide ranging. The increasing interest of designers of building structures in this field in several last decades has been driven by the exploitation of advanced materials, structures and technologies, reducing the external energy consumption, whose thermal, mechanical, etc. time-dependent behaviour cannot be predicted using the simplified semi-empirical formulae from most valid European and national technical standards. Such models as that of one-dimensional heat conduction with (nearly) constant thermal conductivity and capacity, give no practically relevant results for refractory or phase change materials, thermal storage equipments, etc. – cf. [17]. Fortunately, in such cases the correlation between the predicted and measured quantities, e. g. of the annual energy consumption of a building, can be available, to help to optimize the design of both new and reconstructed building structures. This is not true for high temperatures leading to partial or total collapse of a structure, as those caused by thermal radiation during a fire.

A lot of historical remarks and relevant references for the analysis of structures exposed to fire can be found in [7]. The physical background for the evaluation of simultaneous temperature and moisture redistributions under such conditions is based on the balance law of classical thermodynamics. However, it is not trivial to supply a resulting system of evolution by reasonable effective constitutive relations, valid at the microstructural level, despite of the complicated (typically porous) material structures. Most classical approaches to evaluate temperature and moisture redistributions rely on the (semi-)empirical relations from [1]. The attempts to improve them can be seen in various directions, with still open problems and difficulties everywhere. The physical and/or mathematical homogenization approaches applied to a reference volume element seem to be useful. The process of cement hydration, distinguishing between anhydrous cement scale, cement-paste scale, mortar scale and macro-scale, handled by specific physical and mathematical formulations, with a posteriori scale bridging applying least squares arguments, has been described in details, evaluating the hydration of particular clinker phases, in [21]. However, the thermal gains and losses from chemical reactions cannot be con-

sidered as deterministic ones, moreover corresponding computations just in the case of dehydration must suffer from the lack of relevant data at some scales. The formal mathematical two-scale or similar homogenization, introduced in [5], needs to remove assumptions of periodicity using stochastic or abstract deterministic homogenization structures; this leads to physically non-transparent and mathematically very complicated formulations, whose applicability to the construction of practical algorithms for the analysis of engineering problems is not clear. From such point of view, the most promising approach of the last years seems to be that of [13] and (in a substantially generalized version) of [12], replacing the proper homogenization by some arguments from the mixture theory; this will be the principal idea even in our following considerations in this short paper.

2 Definitions of Function Spaces and Notation

Let us describe physical processes, which occur in concrete during fire. Concrete is non-combustible material with low thermal conductivity. Although concrete does not contribute to fire load of the structures significant changes occur in its structure during a fire exposure. Besides reduction of mechanical, deformation and material properties also chemical composition of concrete is varied during heating [2].

Concrete, as a porous material, contains a large amount of pores, which can be filled fully (saturated concrete) or just partially with water. The water occurred in the pores is evaporable water and starts to evaporate at early beginning of the fire. The first changes of concrete structure arise at 105 °C as stated in [16], when chemically bounded water is released from cement gel to the pores. Some small micro-cracks start to appear as the capillary porosity arises. The peak of the dehydration process is reached around 270 °C. The color of concrete is changed and a slight decrease of strength, modulus of elasticity and changes in material properties like thermal conductivity can be noted. Temperature of 300 °C is the extreme temperature beside which the concrete structure is irreversibly damaged [15]. In range of 400 °C - 600 °C calcium hydroxide decomposes into calcium oxide plus water (rise of amount of free water) and transition of and quartz, accompanied by increase in its volume, induces another creation of severe cracks in concrete.

Not only high temperature can affect adversely the load bearing capacity of concrete structures. Simultaneously with a temperature profile along a concrete member should be investigated also the change of mass of free water (mostly vapour) in concrete during fire and distributions of pore pressure. The pore pressure is one of the main reasons of concrete spalling (Figure 1 and 2), which happened at the beginning of heating (10 - 30 minutes) and is accidental. Small or grater (1 m wide and 1 m long) areas of concrete cover can be broken and cross section of member is reduced then. Furthermore in most cases the reinforcement is exposed directly to the fire and the member is heated faster, which can lead to loss of loadbearing capacity.

3 Mathematical considerations

Following [12] (unlike [21]), for the quantification of the dehydration process we shall work with the hydration degree Γ, a number between 0 and 1, as the part of hydrated (chemically combined) water m^w in its standard mass, constituted usually during the early-age treatment of a cementitious composite. Although the evaluation of Γ from a simple algebraic formula

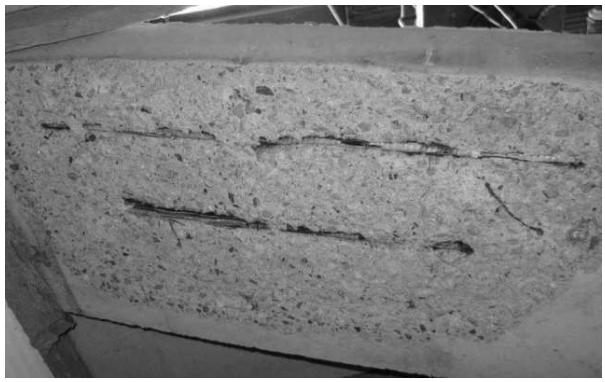

Figure 1: Areal spalling of concrete.

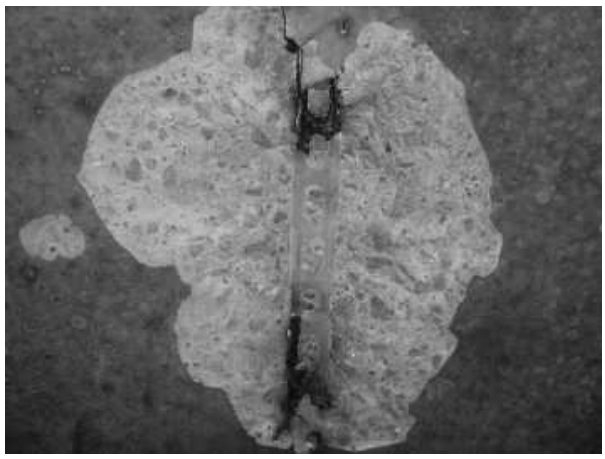

Figure 2: Local spalling of concrete.

is not available because it must take into account the chemical affinity and the fact that the accessibility of water for chemical reactions is controlled by the water content η^w inside the pores under certain temperature T, we shall apply Γ as a known function of such (or slightly transformed) variables.

The multiphase medium at the macroscopic level can be considered as the superposition of 4 phases: solid material, liquid water, water vapour and dry air, identified by their indices $\varepsilon \in \{s, w, v, a\}$. In the Lagrangian description of motion, following [24], the deformation tensor F^s can be derived using the derivatives of displacements of particular points with respect to Cartesian coordinate system $x = (x_1, x_2, x_3)$ in the 3-dimensional Euclidean space. If ω^ε is a source corresponding to certain scalar quantity ϕ^ε then the conservation of such quantity can be expressed by [4], p. 4, and [10], p. 9, as

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

this formula contains the dot notation for the derivative with respect to any positive time t, $(\dots)_{,i}$ means the derivative with respect to x_i where $i \in \{1, 2, 3\}$, $v_i^\varepsilon = \dot{u}_i^\varepsilon$, with u_i^ε referring to displacements related to the initial geometrical configuration $x_0 = (x_{01}, x_{02}, x_{03})$ (for $t = 0$) and later also $a_i^\varepsilon = \ddot{u}_i^\varepsilon$; the Einstein summation is applied to i and j from $\{1, 2, 3\}$ everywhere. For the brevity, ϕ_ε will be moreover used instead of $\phi^\varepsilon \eta^\varepsilon$ where $\eta^\varepsilon(n, S)$ is the volume fraction of the phase ε, a function of the material porosity n and the saturation S. Clearly $\det F^s = (1-n)/(1-n_0)$ with n_0 corresponding to x_0. The saturation S is an experimentally identified function of the absolute temperature T and of the capillary pressure p^c, needed later; the assumption of local thermal equilibrium yields the same values of T for all phases.

In addition to T, we have 4 a priori unknown material densities ρ^ε and 12 velocity components v_i^ε. Assuming that vapour and dry air are perfect gases, we are able to evaluate their pressures $p^v(\rho^v, T)$ and $p^a(\rho^a, T)$ from the Clapeyron law; the capillary pressure is then $p^c = p^v + p^a - p^w$, with the liquid water pressure p^w, or alternatively just with p^c, as an additional unknown variable.

In the deterioration of a composite structure 2 crucial quantities occur: the mass m^w of liquid water lost from the skeleton and the vapour mass m^v caused by evaporation and desorption. The time evolution of mass m^w can be determined from the formally simple formula $m^w = \Gamma m_0^w$, with m_0 related to $t = 0$. The vapour fraction ζ remains to be calculated from the system of balance equations of the type (1), supplied by appropriate constitutive relations.

The mass balance works with

$$\begin{aligned} &\phi^\varepsilon = \rho_\varepsilon \,, \\ &\omega^s = -\dot{m}^w \,,\ \omega^w = \dot{m}^w - \dot{m}^v \,, \\ &\omega^v = \dot{m}^v \,,\ \omega^a = 0 \end{aligned}$$

in (1). No additional algebraic relations are necessary.

Since all phases are considered as microscopically nonpolar, the angular momentum balance forces only the symmetry of the partial Cauchy stress tensor τ, i. e. $\tau_{ij} = \tau_{ji}$ for such stress components. The formulation of the linear momentum balance in 3 direction is more delicate. Introducing $w_i^\varepsilon = \rho_\varepsilon v_i^\varepsilon$ and choosing (for particular i)

$$\phi^\varepsilon = w_i^\varepsilon \,,$$

we can evaluate, using the Kronecker symbol δ, the total Cauchy stress σ in the form $\sigma_{ij} = \tau_{ij}\delta^{s\varepsilon}$ and finally set

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

in (1) where g_i denotes the gravity accelerations and t_i^ε the additional accelerations caused by interactions with other phases, whose evaluation is possible from the Darcy law, as explained lower. The constitutive relationships for the solid phase, e. g. those between τ and u^s, v^s, etc., need the multiplicative decomposition into a finite number m of matrix components $F^s = F^{s1} \dots F^{sm}$ (elasticity, creep, damage, etc. ones) to express $\tau(F^{s1} \dots F^{sm}, \dot{F}^{s1} \dots \dot{F}^{sm}, \dots)$. For $\varepsilon \neq s$, introducing the dynamical viscosity μ^ε and the permeability matrix K_{ij}^ε, depending on ρ_ε again, we can formulate the Darcy law as

$$\mu^\varepsilon \rho_\varepsilon (v_i^\varepsilon - v_i^s) = K_{ij}^\varepsilon (\rho_\varepsilon (g_j - a_j^\varepsilon + t_j^\varepsilon) - p_{\varepsilon,j}) \,. \tag{2}$$

The energy balance inserts

$$\phi^\varepsilon = \frac{1}{2} w_i^\varepsilon v_i^\varepsilon + \rho_\varepsilon \kappa^\varepsilon$$

with κ^ε usually defined as $c^\varepsilon T$, using the thermal capacities c^ε, in general functions of T and p^c again, and some internal heat fluxes q_i^ε, and also

$$\begin{aligned} &\omega^\varepsilon = (\sigma_{ij,j}^\varepsilon + q_i^\varepsilon)_{,j} + (g_i - a_i^\varepsilon + t_i^\varepsilon) + \varpi^\varepsilon \,, \\ &\varpi^s = -\dot{m}^w h^w \,,\ \varpi^w = \dot{m}^w h^w - \dot{m}^v h^v \,, \\ &\varpi^v = \dot{m}^v h^v \,,\ \varpi^a = 0 \end{aligned}$$

into (1); two new characteristics here are the specific enthalpies of cement dehydration h^w and evaporation h^v. The internal heat fluxes q_i^ε come from the constitutive relation

$$q_i^\varepsilon = -\lambda_{ij}^\varepsilon T_{,j} - \xi_{ij}^\varepsilon p_{,j}^c \,; \tag{3}$$

the first (typically dominant) additive term corresponds to the well-known Fourier law of thermal conduction, the second one to the Dufour effect, with some material characteristics $\lambda_{ij}^{\varepsilon}$ and ξ_{ij}^{ε} dependent on T and p^c.

Similarly to (3), it is possible derive the diffusive fluxes $r_i^{\varepsilon} = \rho_{\varepsilon}(v_i^{\varepsilon} - v_i^s)$ with $i \in \{v, w\}$ in the form

$$r_i^{\varepsilon} = -\varsigma_{ij}^{\varepsilon} T_{,j} - \gamma_{ij}^{\varepsilon} p_{,j}^c \,, \tag{4}$$

due to the Fick law (the second additive term), respecting the Soret effect (the first one), with some material characteristics $\varsigma_{ij}^{\varepsilon}$ and $\gamma_{ij}^{\varepsilon}$ dependent on T and p^c; for more detailed analysis of Dufour and Soret effects cf. [19].

Now we have 4 mass balance equations, 3×4=12 momentum ones and 4 energy ones, in total 20 partial differential equations of evolution for 3 groups of variables:

$$\mathcal{R} = (\rho^s, \rho^w, \rho^v, \rho^a)\,,$$
$$\mathcal{V} = (v_1^s, v_2^s, v_3^s, v_1^w, v_2^w, v_3^w, v_1^v, v_2^v, v_3^v, v_1^a, v_2^a, v_3^a),$$
$$\mathcal{T} = (T, p^c, m^v, \zeta)\,,$$

supplied by appropriate initial and boundary conditions, e. g. for a priori known values of all variables for $t = 0$ of the Dirichlet, Cauchy, Neumann, Robin, etc. types, for local unit boundary outward normals $n(x) = (n_1(x), n_2(x), n_3(x))$ in particular

- $\sigma_{ij} n_j = \bar{t}_i$ with imposed tractions t_i,
- $(\rho_a(v_i^a - v_i^s) + r_i^a)n_i = \overline{r}^a$ with imposed air fluxes $\overline{r}^a$,
- $(\rho_w(v_i^w - v_i^s) + r_i^w + \rho_v(v_i^v - v_i^s) + r_i^v)n_i = \overline{r}^w + \overline{r}^v + \beta(\rho_v)$ with imposed liquid water and vapour fluxes $\overline{r}^w$, $\overline{r}^v$ and some mass exchange function β,
- $(\rho_w(v_i^w - v_i^s)h_v - \lambda_{ij} T_{,j} - \xi_{ij}^{\varepsilon} p_{,j}^c)n_i = \bar{q} + \alpha(T)$ with imposed heat fluxes and some heat exchange function α, e. g. by the Stefan - Boltzmann law, proportional to T^4.

This seems to be a correct and complete formulation for the analysis of time development of $\mathcal{R}$, $\mathcal{V}$ and $\mathcal{T}$.

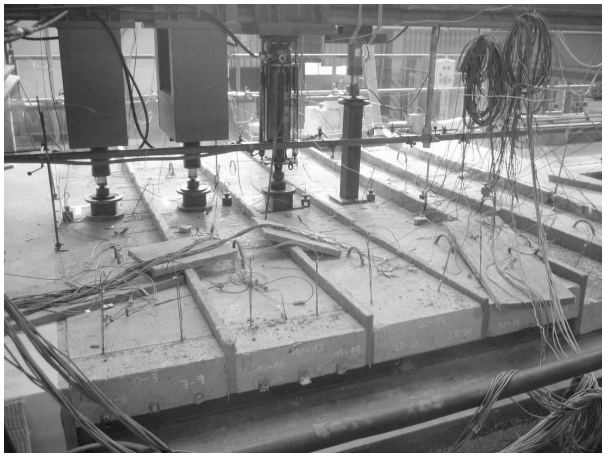

Figure 3: Fire simulation at Brno University of Technology: laboratory setting.

Figure 4: Fire simulation at Brno University of Technology: detail of real experiment.

4 Computational analysis

Unfortunately, a lot of serious difficulties is hidden in the above presented formulation, e. g. the still missing "Millenium Prize" existence result on the solvability of Navier - Stokes equations (cf. the "mysteriously difficult problem" of [23], p. 257), the physical and mathematical incompatibilities like [11], as well the absence of sufficiently robust, efficient and reliable numerical algorithms based on the intuitive time-discretized computational scheme:

1. set $\mathcal{R}$, $\mathcal{V}$ and $\mathcal{T}$ by the initial conditions for $t = 0$,
2. go to the next time step, preserving $\mathcal{R}$, $\mathcal{V}$ and $\mathcal{T}$,
3. solve some linearized version of (1) with the mass balance choice, evaluate and perform the correction $\epsilon_{\mathcal{R}}$,
4. solve some linearized version of (1) with the momentum balance choice, evaluate and perform the correction $\epsilon_{\mathcal{V}}$,
5. solve some linearized version of (1) with the energy balance choice, evaluate and perform the correction $\epsilon_{\mathcal{T}}$,

6. if $\epsilon_{\mathcal{R}}$, $\epsilon_{\mathcal{V}}$ and $\epsilon_{\mathcal{T}}$ are sufficiently small, return to 3,

7. stop the computation if the final time is reached, otherwise return to 2.

Consequently all practical computational tools make use of strong simplifications. The rather general approach of [12] introduces the additive linearized strain decomposition instead of the multiplicative finite strain one, ignores some less important terms, as the kinetic energy (the first additive term in ϕ^{ε}) in the energy balance interpretation of (1), as well as the Dufour and Soret effects in (3) and (4), and reduces the number of variables, comparing (2) with the differences $v_i^{\varepsilon} - v_i^s$ with $\varepsilon \in \{v, w, a\}$ from the momentum balance interpretation of (1), and presents a computational scheme of the above sketched type, applying the Galerkin formulation and the finite element technique. Nevertheless, most engineering approaches, as [3] or [18], endeavour to obtain a system of 2 equations of evolution for T and p^c (or some equivalent quantity) only, pre-eliminating or neglecting all remaining ones, using arguments of various levels: from micro-mechanically motivated physical considerations to formal simplification tricks.

The reliability of computational results depends on the quality and precision of input data, including the design and identification of all material characteristics. Even the reasonable setting of basic material characteristics, just at elevated and high temperatures, for separate non-stationary heat transfer is not trivial; the relevant least-squares approach is discussed in [25]. Probably all authors take some of them from the literature, not from their extensive original experimental work; the variability of forms of such characteristics and generated values, accenting those from (2), including the formulae from [12], has been discussed in [7]. Nevertheless, the proper analysis of uncertainty and significance of particular physical processes lead to even more complicated formulations, analyzed (for much easier direct model problems) in [26] using the spectral stochastic finite element technique, or in [14] the Sobol sensitivity indices, in both cases together with the Monte Carlo simulations.

Unlike most experiments in civil and material engineering in laboratories and in situ, nearly no relevant results for advanced numerical simulations are available from real unexpected fires, as the most dangerous conditions for building structures, crucial for the reliable prediction of behaviour of concrete and similar structures. Since also laboratory experiments with cementitious composites under the conditions close to a real fire, as that documented on Fig. 1 and Fig. 2, performed at the Brno University of Technology, similar to the building structure considered in [22], are expensive, producing incomplete and uncertain quantitative data anyway, the reasonable goal of numerical simulation is to test simple numerical models with acceptable correlation with real data, as the first step for the development of more advanced multi-physical models.

5 Example

Let us present rather simple mathematical model based on previous considerations. The model is compatible with the slightly modified and revisited approach of [3].

Let us consider $x \in \Omega$, where Ω is a simple domain and represents the part of space occupied by concrete. Further, let Γ be its boundary, which consist of two non-intersecting parts: Γ_N and Γ_R and it holds $\Gamma_N \cup \Gamma_R = \Gamma$. The part Γ_R represents piece of the boundary, which is exposed to the fire and Γ_N denotes the part exposed to the atmosphere.

Model is two-dimensional, i.e. $x = (x_1, x_2)$, and it neglects mechanical loads, strains and stresses, i.e.

$$u_i^s = 0, \quad v_i^s = 0, \quad a_i^s = 0, \tag{5}$$

and

$$\tau = 0, \quad \sigma = 0, \quad F^s = 0.$$

We consider only two phase - solid phase and free evaporable water. Let us denote by $\rho = \rho(x, t)$ density of the free water, i.e.

$$\rho = \rho_w + \rho_v,$$

and its velocity by $v = (v_1, v_2)$.

The mass balance equation for free water reads:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\, v) = \frac{\partial m^w}{\partial t} \quad \text{in } \Omega \times (0, \infty), \tag{6}$$

where $m^w = \Gamma\, m_0^w$. Hydration degree Γ is empirical function specified for example in [8].

In the model, we suppose the concrete be an isotropic material, therefore all material characteristic are not represent by the matrix but by a function. For that reason let us denote by $K = K(T, p^c)$ the permeability of concrete and by $\lambda = \lambda(T)$ thermal conductivity of concrete.

Diffusive flux $r = \rho\, v$ we approximate only by Fick law since Soret effect is appeared to be rather small [2], i.e.

$$r = -\frac{K}{g}\, \nabla p^c,$$

in which g is gravity acceleration (included for the reasons of dimensionality).

Since (5) is assumed, the mass balance for solid phase is trivial.

Summing up the enthalpy balances for free water and solid phase, we obtain

$$\rho_s C^s \frac{\partial T}{\partial t} + \nabla \cdot q = \tag{7}$$
$$C^w \rho\, v \cdot \nabla T + h^w \frac{\partial m^w}{\partial t} - h^v \frac{\partial \rho}{\partial t} \quad \text{in } \Omega \times (0,\infty)\,.$$

The last term on right-hand side approximates $h^v \dot{m^v}$. Heat flux q is considered only in form of Fourier law

$$q = -\lambda \nabla T,$$

since Dufour effect is negligible [2].

To keep the model simple we do not consider momentum balance equations at all.

Now, we have three variables ρ, p^c, T and only two equations (6), (7). For that reason we add empirical state equation

$$\rho = \Phi(p^c, T).$$

Function Φ can be found in [6], p. 530.

The model is completed by boundary and initial conditions. The boundary conditions are:

$$-r \cdot n = \beta(p^c - p_\infty) \qquad \text{on } \Gamma \times (0,\infty)\,,$$
$$-q \cdot n = \alpha(T - T_\infty) \qquad \text{on } \Gamma_N \times (0,\infty)\,,$$
$$-q \cdot n = \alpha(T - T_{\text{en}}) + e\sigma(T^4 - T_{\text{en}}^4) \quad \text{on } \Gamma_R \times (0,\infty)\,.$$

By $n = (n_1, n_2)$ we denote an outer unit normal, p_∞ and T_∞ is pressure and temperature of the outer environment. T_{en} represents temperature caused by fire. We used T_{en} given by ISO curve [9]. e denotes emissivity of concrete and σ is Stefan- Boltzmann constant.

Initial conditions are

$$p^c(x,0) = p_0 \qquad \text{for } x \in \Omega,$$
$$T(x,0) = T_0 \qquad \text{for } x \in \Omega,$$

where p_0 and T_0 are pressure and temperature for $t = 0$.

Fig. 5, Fig. 6 and Fig. 7 are the outputs from the model described above. Solver combines the finite element techniques together with the iterated time discretization scheme (the numerical construction of Rothe sequences), implemented in the MATLAB environment. Fig. 6 demonstrates the time development of temperature, Fig. 5 that of pressure and Fig. 7 that of moisture content. The fire is considered as the boundary thermal radiation on the left and upper edges of the rectangle. Surprisingly some phenomena observed in situ can be explained from the deeper analysis of results of such seemingly simple calculations; the deeper analysis of this preliminary results, directed just to the practical application to fire protection in civil engineering, is in preparation.

6 Conclusion

Development of reasonable models and computational algorithms for the prediction of thermal, mechanical, etc. behaviour of cementitious composites and whole building structures, is strongly required by the applied research in civil engineering, which cannot be ignored, although the formal mathematical verification of such models is not available and the practical validation suffers from the lack of data from observations in situ, as well as of large databases from relevant (very expensive) experiments. The first steps, both in the sufficiently general formulation of the problem, containing most practical computational approaches as special ones, as well as the methodology of computational and experimental work, sketched in this paper, should be a motivation for further extensive research.

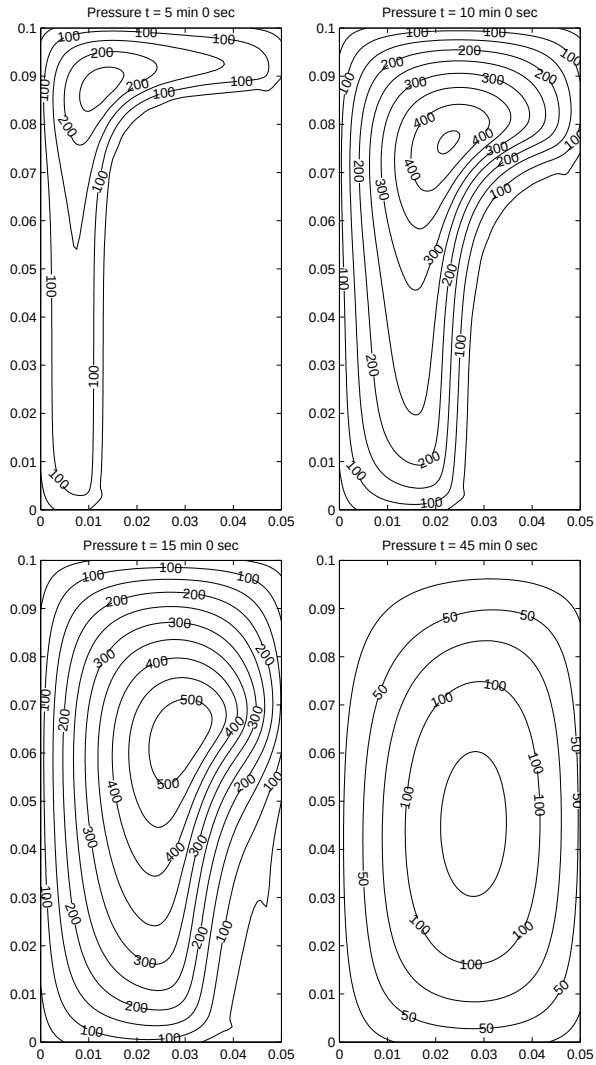

Figure 5: Time development of pressure p^c [kPa].

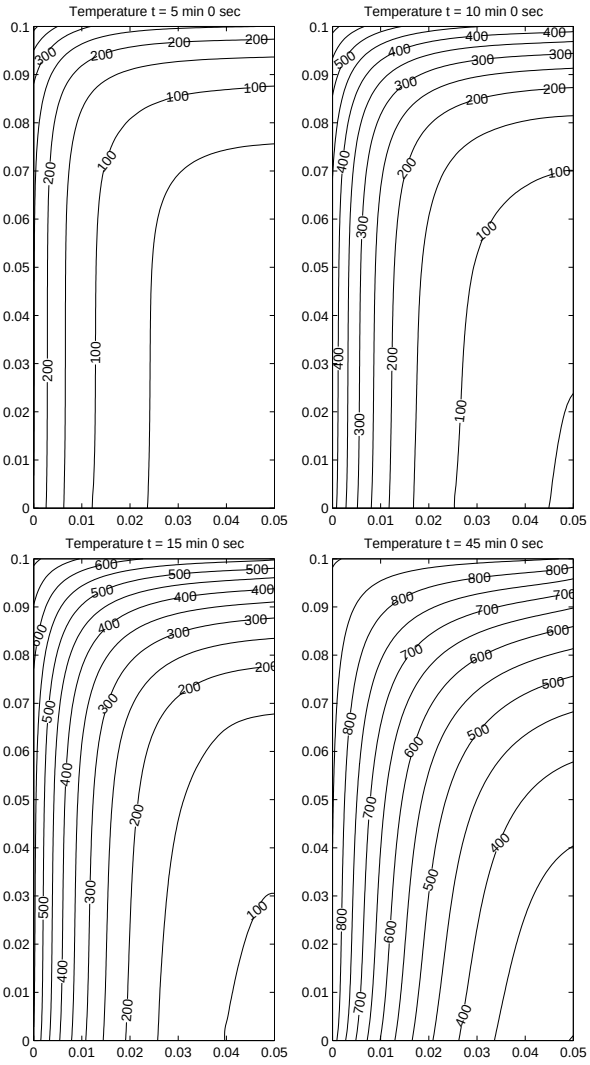

Figure 6: Time development of temperature T [°C].

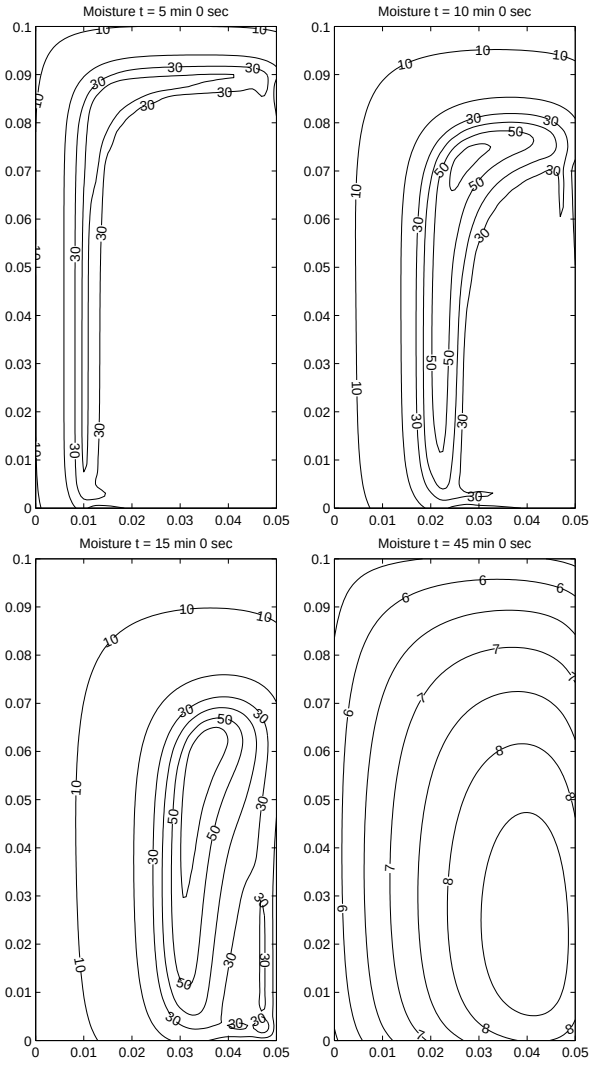

Figure 7: Time development of moisture content $\rho_w + \rho_v$ [kg m^{-3}].

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