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ON THE EVOLUTION OF HEAT AND MOISTURE IN BUILDING MATERIALS *

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Abstract. The paper discusses some possibilities of mathematical modelling of the problem of slow redistribution of heat, driven by transfer of moisture in various phases in building materials and constructions. The study of a structure of real building materials generates the system of at least two macroscopic equations of evolution, containing two unknown fields of temperature and pressure, with some initial and boundary conditions. Unfortunately, the standard mathematical analysis, based on the method of Rothe, is not available here, as the parabolic part of the system is not symmetric and cannot be easily converted to the symmetric one as in the classical case with time-independent material characteristics. Nevertheless, some existence and convergence results can be derived, applying other transformations, forcing certain symmetry in the elliptic part of the system.

Key words. Heat and moisture transfer, building materials, method of Rothe, problems of evolution with a non-symmetrical parabolic part.

AMS subject classifications. 35K05, 35K15.

1. Modelling of heat and moisture transfer. Both the durability and the comfortable exploitation of particular building elements and complete structures and engineering constructions are influenced by two basic physical processes – of the heat transfer and of the diffusion of moisture through a system of pores. Such pores can have various sizes (from micro- to macroscopic ones) and mutual positions, depending on the choice of materials, usually determined by the requirement of minimization of strain and stresses, caused by external static or dynamic loads, a posteriori supplied by special insulation layers to ensure an acceptable thermal stability of the whole structure (cf. [18]). The redistribution of moisture in materials is (related to the heat transfer) a very slow process, which complicates any practical validation of outputs from numerical solvers, based on some physical and mathematical simplifications. Nevertheless, to obtain results not far from the realistic ones, at least a coupled problem of evolution of two unknown fields, typically of the temperature T and the pressure p, with appropriate initial and boundary conditions should be analyzed, using a differential (classical) or an integral (weak, variational) form of the equations for heat and moisture balance.

Probably the simplest system of this type, proposed by [13] originally, is the system "for the non-stationary transfer of heat and mass" (in practice, mass is understood as water in various phases) on a domain Ω in R^2, presented in the textbook [10], p. 210:

$$\mathcal{A}\dot{\tau} = \nabla^2\tau + \mathcal{K}\mathcal{A}\dot{\phi}\,, \quad \mathcal{A}\dot{\phi} = \mathcal{L}\mathcal{P}\nabla^2\tau + \mathcal{L}\nabla^2\phi\,.$$

In its equations (where dots denote time derivatives) all multiplicative factors are considered as positive constants: $\mathcal{A}$ is the thermal diffusivity (as defined in [10], p. 203), $\mathcal{P}$ the Posnov number, $\mathcal{K}$ the Kossovich number and $\mathcal{L}$ the Luikov number (introduced in [10], pp. 132, 134, 138). Let us notice that certain so-called moisture potential ϕ, is

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used here instead of p; unfortunately, this ϕ (unlike p) has no transparent physical meaning and often (as in [8], namely for higher moisture concentrations) comes from strange empirical relations. Alternative forms of this linear system, whose solution is known, force the symmetry either in the parabolic part or in the elliptic one; their non-substantial modifications (preserving linearity) can be found in later publications: e. g. [4] refers to [12], presenting (in English) the same approach as [13] (in Russian).

For reasonable applications in civil engineering the assumption on constant material characteristics is too strict: it is well-known that the heat transfer factor depends both on T and p (or ϕ) and the nonlinear behaviour of other characteristics (as observed in laboratories) seems to be even stronger; this is partially reflected also in [10], p. 205. Therefore the simplest acceptable system is the quasilinear one

$$b(u)\dot{u} = \nabla(a(u)\nabla u) + f(u)\,, \tag{1.1}$$

where a and b are square matrices of material characteristics of order 2, f is a column vector of internal sources of order 2 (time-dependent in general) and $u = (T, p)^T$; for simplicity we shall consider (as in [10], p. 210) a plane problem on $\Omega \subset R^2$ only. The system of such type (with p replaced by ϕ), based on the extensive experimental work (but without deeper physical and mathematical analysis), was investigated in [8]; more historical information can be found in [1]. The system (1.1) was then proposed in [11] and later used e. g. in [16] and [9] (with neglected non-diagonal elements in $b(u)$). In addition, let us consider such column vector g of external sources of order 2 (time-dependent in general) that

$$g(u) = \nu \cdot a(u)\nabla u \quad \text{on } \Gamma\,,$$

where ν is the column unit vector ν of the local outside normal of order 2, defined on certain subset Γ of $\partial\Omega$, and that the standard Green-Ostrogradskiĭ theorem for a domain Ω is valid. Then (1.1) receives the integral form

$$\int_\Omega v \cdot b(u)\dot{u}\,\mathrm{d}\mu + \int_\Omega \nabla v \cdot a(u)\nabla u\,\mathrm{d}\mu = \int_\Omega v \cdot f(u)\,\mathrm{d}\mu + \int_\Gamma v \cdot g(u)\,\mathrm{d}\sigma \tag{1.2}$$

(the standard Lebesgue measure μ on Ω is used here, σ denotes the surface Hausdorff measure on $\partial\Omega$, the sign $\cdot$ is used for dot products both in R^2 and in $R^{2\times 2}$, the dependance of u, f, g on the time t is not emphasized explicitly) for any $v \in V$, where V is a subspace of the Sobolev space $W^{1,2}(\Omega, R^2)$ satisfying prescribed homogeneous Dirichlet boundary conditions on $\partial\Omega \setminus \Gamma$. To avoid technical difficulties, we shall suppose $a, b \in C(\Omega, R^{2\times 2})$ (if necessary, to substitute the continuity here e. g. by the piecewise continuity is not difficult), $f \in C_L(I, L^2(\Omega, R^2))$ and $g \in C_L(I, L^2(\Gamma, R^2))$; the lower index $_L$ forces the Lipschitz continuity.

The aim of the existence and convergence analysis for (1.2) is: (i) to find some $u \in L^\infty(I, V)$ with $u \in L^2(I, L^2(\Omega, R^2))$ satisfying (1.2) for certain time interval $I = \{t \in R : 0 \le t \le T\}$ of a finite positive length T such that its initial value $u(0)$ coincides with the prescribed $u_0 \in V$ and (ii) to receive u as a limit of solutions of a sequence of some elliptic problems (instead of the original parabolic one). The standard approach, based on the method of Rothe (of semi-discretization with respect to time), analyzed in [7], does not handle non-symmetrical matrices $b(u)$. Thus, the main difficulty is that no tricks like multiplying by $b(u)^{-1}$ or $b(u)^T$ in (1.1) from the left (compatible with the choice of v in (1.2)) are available, since all elements of the matrix $b(u)$ are far from constants in practice. The modified approach of [19] admits various non-symmetrical matrices $b(u)$, but needs the seemingly non-realistic symmetry in the elliptic part. In the following text we shall demonstrate that such symmetry can be preserved thanks to special transformations, whose design requires solving some non-trivial auxiliary problems.

2. Sequences of Rothe. Let us introduce the family M of all continuously differentiable mappings defined on V with values in $R^{2\times 2}$. If $\alpha \in M$ then the transformation $v = \alpha(w)w$ is available for any $w \in V$ and returns $v \in V$ again; moreover, such mapping $\widehat{\alpha}$ from V to $C(\Omega, R^{2\times 2})$ can be constructed that $\nabla v = \widehat{\alpha}(w)\nabla w$. More precisely: for $i, j, k, l \in \{1, 2\}$, using the Einstein summation rule for j, l, we have $v_i = \alpha_{ij}(w)w_j$ and

$$v_{i,k} = \alpha_{ij}(w)w_{j,k} + \alpha_{ij,l}(w)w_{l,k}w_j = (\alpha_{ij}(w) + \alpha_{il,j}(w)w_l)\, w_{j,k} = \widehat{\alpha}_{ij}(w)w_{j,k}$$

(in the whole paper we use Cartesian coordinates and corresponding derivatives). Let us notice that the inverse problem of practical calculation of $\alpha \in M$ to some given $\widehat{\alpha}$ is non-trivial. In particular cases: (i) if $\widehat{\alpha}$ is independent of w then $\alpha = \widehat{\alpha}$ evidently, (ii) if $\alpha_{ij} = \overline{\alpha}_{i,j}$ for some potentials $\overline{\alpha}_i$ and any $i, j \in \{1, 2\}$ then the whole system degenerates to separate equations $\alpha(w) + \alpha_{,1}(w)w_1 + \alpha_{,2}(w)w_2 = \widehat{\alpha}(w)$ (indices i, j may be omitted here), convertible (using the transformation to polar coordinates $x_1 = \rho\cos\omega$, $x_2 = \rho\sin\omega$, $\rho \geq 0$, $0 \leq \omega < 2\pi$) to the easily solvable form $\alpha(w) + \rho\alpha'(w) = \widehat{\alpha}(w)$ ($'$ is used for the partial derivative by ρ here), (iii) in some more complicated cases various analytical constructions of first integrals, described in [17], p. 44, are available, (iv) in more general cases no analytical solutions are known and the existence considerations similar to those from [15], based on the Leray-Schauder fixed point theorem, must be done. Let us assume that $b(v) = \widehat{\beta}(v)$ (derived in the same way as $\widehat{\alpha}$ from α) for some $\beta \in M$ and each $v \in V$; this implies e.g. $(\beta(u)u)^{\cdot} = \widehat{\beta}(u)\dot{u} = b(u)\dot{u}$. Choosing $v = \alpha(w)w$ with $w \in V$, from (1.2) we obtain

$$\int_\Omega \alpha(w)w\cdot[\beta(u)u]^{\cdot}\,\mathrm{d}\mu + \int_\Omega \widehat{\alpha}(w)\nabla v\cdot a(u)\nabla u\,\mathrm{d}\mu = \int_\Omega \alpha(w)w\cdot f(u)\,\mathrm{d}\mu + \int_\Gamma \alpha(w)w\cdot g(u)\,\mathrm{d}\sigma$$

and consequently

$$\begin{aligned}(2.1)\quad &\int_\Omega \alpha(w)w\cdot\beta(u)u\,\mathrm{d}\mu - \int_\Omega \alpha(w)w\cdot b(u_0)u_0\,\mathrm{d}\mu + \int_0^t\int_\Omega \widehat{\alpha}(w)\nabla w\cdot a(\widetilde{u})\nabla\widetilde{u}\,\mathrm{d}\mu\,\mathrm{d}\widetilde{t} \\ &= \int_0^t\int_\Omega \alpha(w)w\cdot f(\widetilde{u})\,\mathrm{d}\mu\,\mathrm{d}\widetilde{t} + \int_0^t\int_\Gamma \alpha(w)w\cdot g(\widetilde{u})\,\mathrm{d}\sigma\,\mathrm{d}\widetilde{t},\end{aligned}$$

where $\widetilde{\ }$ informs that corresponding values are taken in time $\widetilde{t}$ (instead of t, $0 \leq \widetilde{t} \leq t$).

Let us study a discrete analogue of (2.1)

$$\begin{aligned}(2.2)\quad & h^{-1}\int_\Omega \alpha(w)w\cdot[\beta(u_s)u_s - \beta(u_{s-1})u_{s-1}]\,\mathrm{d}\mu + \int_\Omega \widehat{\alpha}(w)\nabla w\cdot a(u_s)\nabla u_s\,\mathrm{d}\mu \\ &= \int_\Omega \alpha(w)w\cdot f_s(u_s)\,\mathrm{d}\mu + \int_\Gamma \alpha(w)w\cdot g_s(u_s)\,\mathrm{d}\sigma,\end{aligned}$$

where $u_s^m \in V$ for $s \in \{1, \dots, m\}$ (the upper index m is usually omitted for brevity) are unknown time-independent functions, m is an arbitrary positive integer, $h = T/m$ and the indices in f_s^m and g_s^m emphasize that corresponding values are taken in time sh (as f and g in (2.1) can depend on t directly, not only thanks to u). The sequence of Rothe, based on the piecewise linear approximation, is compound from elements $u^m = u_{s-1} + (t - t_{s-1})u_s$ for any $t \in I_s$ and $s \in \{1, 2, \dots, m\}$, where $I_s = \{t \in I : (s-1)h < t \leq sh\}$; for $t = 0$ naturally $u^m = u_0$. Consequently, the sequence of derivatives of u^m can be calculated directly from the formula $\dot{u}^m = (u_s - u_{s-1})/h$ for each $t \in I_s$. In particular, subtracting two equations (2.2) for $w = u_s$ and $w = u_{s-1}$, we have

$$\begin{aligned} &h^{-1}\int_\Omega [\alpha(u_s)u_s - \alpha(u_{s-1})u_{s-1}] \cdot [\beta(u_s)u_s - \beta(u_{s-1})u_{s-1}]\,\mathrm{d}\mu \\ &+\int_\Omega [\widehat{\alpha}(u_s)\nabla u_s - \widehat{\alpha}(u_{s-1})\nabla u_{s-1}] \cdot a(u_s)\nabla u_s\,\mathrm{d}\mu \\ &= \int_\Omega [\alpha(u_s)u_s - \alpha(u_{s-1})u_{s-1}] \cdot f_s(u_s)\,\mathrm{d}\mu + \int_\Gamma [\alpha(u_s)u_s - \alpha(u_{s-1})u_{s-1}] \cdot g_s(u_s)\,\mathrm{d}\sigma\,. \end{aligned}$$

Assuming the symmetry $\widehat{\alpha}(v)\nabla v \cdot a(w)\nabla w = \widehat{\alpha}(w)\nabla w \cdot a(v)\nabla v$ for every $v, w \in V$ (which is satisfied e. g. for $\widehat{\alpha}$ identical with a) and summing up with all indices $s \in \{1, \dots, r\}$ for an arbitrary $r \in \{1, \dots, m\}$, we receive

$$\begin{aligned} &h^{-1}\int_\Omega [\alpha(u_r)u_r - \alpha(u_{r-1})u_{r-1}] \cdot [\beta(u_r)u_r - \beta(u_{r-1})u_{r-1}]\,\mathrm{d}\mu \\ &+\frac{1}{2}\int_\Omega \widehat{\alpha}(u_r)\nabla u_r \cdot a(u_r)\nabla u_r\,\mathrm{d}\mu - \frac{1}{2}\int_\Omega \widehat{\alpha}(u_0)\nabla u_0 \cdot a(u_0)\nabla u_0\,\mathrm{d}\mu \\ &+\frac{1}{2}\sum_{s=1}^{r}\int_\Omega [\widehat{\alpha}(u_s)\nabla u_s - \widehat{\alpha}(u_{s-1})\nabla u_{s-1}] \cdot [a(u_s)\nabla u_s - a(u_{s-1})\nabla u_{s-1}]\,\mathrm{d}\mu \\ &= \sum_{s=1}^{r}\int_\Omega [\alpha(u_s)u_s - \alpha(u_{s-1})u_{s-1}] \cdot f_s(u_s)\,\mathrm{d}\mu \\ &+\sum_{s=1}^{r}\int_\Gamma [\alpha(u_s)u_s - \alpha(u_{s-1})u_{s-1}] \cdot g_s(u_s)\,\mathrm{d}\sigma\,. \end{aligned}$$

To be able to guarantee a priori estimates for u^m in $L^2(I, V)$ and for $\dot{u}^m$ in $L^2(I, L^2(\Omega, R^2))$ from this equation, we need some additional assumptions; in this paper we shall demonstrate simple sufficient ones:

1. There exists such positive constant c_b that

$$[\alpha(v)v - \alpha(w)w] \cdot [\beta(v)v - \beta(w)w] \geq c_b(v - w) \cdot (v - w) \quad \text{on } \Omega$$

   for every $v, w \in V$. This is always true if $\widehat{\alpha}(v)^T b(w)$ is a positive definite matrix, since the Taylor expansions $\alpha(v)v - \alpha(w)w = \widehat{\alpha}(\widetilde{v})(v - w)$, $\beta(v)v - \beta(w)w = b(\widetilde{w})(v - w)$ are valid with both $\widetilde{v}$ and $\widetilde{w}$ expressible in form $(1 - \zeta)w + \zeta v$ with some real factors ζ between 0 and 1. Let us notice that also $|\alpha(v)v - \alpha(w)w| \leq c|v - w|$ holds with some positive constant c, which is useful for the right-hand-side estimate (except the surface integral).
2. There exists such positive constant c_a that

$$\begin{aligned} &\widehat{\alpha}(v)\nabla v \cdot a(v)\nabla v \ \geq c_a \nabla v \cdot \nabla v\,, \\ &[\widehat{\alpha}(v)\nabla v - \widehat{\alpha}(w)\nabla w] \cdot [a(v)\nabla v - a(w)\nabla w] \geq 0 \quad \text{on } \Omega \end{aligned}$$

   for every $v, w \in V$. In particular, the choice of $\widehat{\alpha}$ identical with a makes these conditions trivial: $a(v)^T a(v)$ should be a positive definite matrix only, which is true for every regular $a(v)$.

3. There exist some positive constant c_g and for any time $t \in I$ such potential G (cf. [3], p. 96) that

$$(\alpha(v)v - \alpha(w)w) \cdot g(v) \geq G(v) - G(w)\,, \qquad G(v) \leq c_g |v|^2 \quad \text{on } \Gamma$$

for every $v, w \in V$. Moreover, the geometric configuration admits the estimate

$$\|v\|^2_{L^2(\Gamma,R^2)} \leq \theta \|\nabla v\|^2_{L^2(\Omega,R^{2\times 2})} + K\theta^{-1}\|\nabla v\|^2_{L^2(\Omega,R^2)}$$

with some positive constant K and any positive constant θ (this "trace theorem" is analyzed in [14], p. 220). Let us remark that the notation $\overline{v} = \alpha(v)v$, $\overline{w} = \alpha(w)w$ can be sometimes helpful to reformulate the first condition as $(\overline{v} - \overline{w}) \cdot \overline{g}(\overline{v}) \geq G(\overline{v}) - G(\overline{w})$ for a new function $\overline{g}(\overline{v}) = g(v)$, too.

Applying the discrete version of the Gronwall lemma (see [6], p. 29), we are able (after rather long calculations) to conclude that the sequence $u^m(t)$ is bounded in V for every $t \in V$ and the sequence $\dot{u}^m$ is bounded in $L^2(I, L^2(\Omega, R^2))$.

3. Illustrative example. Physically realistic matrices a, b usually do not admit transparent analytical results for α, β. Nevertheless, we shall illustrate the applicability of suggested transformations on one very simple example with $\widehat{\alpha} = a$. We shall assume that $g(v)$ does not depend on $v \in V$ (thus an argument v can be omitted); this yields $G(\overline{v}) = g\overline{v}$ evidently.

Let $\xi, \eta, \delta, \varepsilon$ be such real factors that $\xi\eta < 4$, $\delta\varepsilon < 4$, $\eta\varepsilon > -4$. For arbitrary $v, w \in V$ let us consider

$$a(v) = \begin{bmatrix} 1 + (1+v_1^2)^{-1} & \xi(1+v_2^2)^{-1} \\ \eta(1+v_1^2)^{-1} & 1 + (1+v_2^2)^{-1} \end{bmatrix},$$
$$b(w) = \begin{bmatrix} 1 + (1+w_1^2)^{-1} & \delta(1+w_2^2)^{-1} \\ \varepsilon(1+w_1^2)^{-1} & 1 + (1+w_2^2)^{-1} \end{bmatrix}.$$

Using the notation $\kappa(z) = (\arctan z)/z$ for all non-zero values of z and $\kappa(z) = 1$ for the opposite (singular) case, we can see that

$$\alpha(v) = \begin{bmatrix} 1 + \kappa(v_1) & \xi\kappa(v_2) \\ \eta\kappa(v_1) & 1 + \kappa(v_2) \end{bmatrix}, \qquad \beta(w) = \begin{bmatrix} 1 + \kappa(w_1) & \delta\kappa(w_2) \\ \varepsilon\kappa(w_1) & 1 + \kappa(w_2) \end{bmatrix}.$$

The positive definiteness of every matrix $\gamma(v, w) = a(v)^T b(w)$ is clear: from direct calculations we obtain

$$\gamma_{11}(v,w) = \frac{(2+v_1^2)(2+w_1^2) + \eta\varepsilon}{(1+v_1^2)(1+w_1^2)}, \qquad \gamma_{12}(v,w) = \frac{(2+v_1^2)\delta + (2+w_2^2)\eta}{(1+v_1^2)(1+w_2^2)},$$
$$\gamma_{21}(v,w) = \frac{(2+v_2^2)\varepsilon + (2+w_1^2)\xi}{(1+v_2^2)(1+w_1^2)}, \qquad \gamma_{22}(v,w) = \frac{(2+v_2^2)(2+w_2^2) + \xi\delta}{(1+v_2^2)(1+w_2^2)}$$

and consequently

$$\begin{aligned} \det\gamma(v,w) &= \gamma_{11}(v,w)\gamma_{22}(v,w) - \gamma_{12}(v,w)\gamma_{21}(v,w) \\ &= \frac{(2+v_1^2)(2+v_2^2) - \xi\eta}{(1+v_1^2)(1+v_2^2)} \cdot \frac{(2+w_1^2)(2+w_2^2) - \delta\varepsilon}{(1+w_1^2)(1+w_2^2)}, \end{aligned}$$

which gives (since principal minors of $\gamma(v, w)$ are positive) the expected result. The regularity of $a(v)$ can be verified similarly.

4. Existence and convergence results, conclusions and generalizations. To verify the solvability of (2.2) is relatively simple: it can be done in the same way as in [19], applying the properties of generalized (pseudo)monotone operators from [5]. The crucial point in the existence and convergence proof is just the verification of the boundedness of sequences of Rothe. Following [19], where much more general assumptions occur (a reflexive Banach space V, replacing our special subspace of $W^{1,2}(\Omega, R^2)$, whose mapping into an other Banach space H, substituted by $L^2(\Omega, R^2)$ here, is strongly continuos, operators $A : V \mapsto V^\star$, $B : H \mapsto H^\star$ with prescribed properties, etc.), making use of the reflexivity of V ($W^{1,2}(\Omega, R^2)$, $L^2(\Omega, R^2)$ are even Hilbert spaces) and certain modification of the Arzelà-Ascoli theorem (cf. [6], p. 24), we find that such mapping u of I into V exists that for $m \to \infty$, up to a subsequence, $\{u^m(t)\}_{m=1}^{\infty}$ has some weak limit $u(t)$ in V for every $t \in I$, while u is a strong limit of $\{u^m\}_{m=1}^{\infty}$ in $C(I, L^2(\Omega, R^2))$. The analogous analysis of behaviour of $\{u^m\}_{m=1}^{\infty}$ yields, thanks to the reflexivity of $L^2(\Omega, R^2)$, the stronger result $u \in L^\infty(I, V) \cap W^{1,2}(I, L^2(\Omega, R^2))$. Then it is not difficult to prove that such u satisfies (2.1) and (1.2); (1.1) may be violated (mappings u are allowed not to be smooth enough) in classical sense (if not understood in sense of distributions).

Presented results guarantee the existence of some solution and the convergence of (sub)sequences of Rothe, using the discretization in time. For practical calculations, the discretization in R^2 is needed, too; this can be done using standard variational methods as FEM, FDM, FVM, etc. It is possible to prove that, preserving some rules for interpolation and numerical integration, the convergence properties of the sequences of Rothe cannot be corrupted. Unfortunately, for the numerical modelling of problems of heat and moisture transfer in building materials no standard software seems to be available up to now. To justify theoretical results by numerical experiments, several special PC programs have been written by the authors of [2] in the Fortran and Pascal code; [2] includes also some recommendations, how to obtain reasonable values (depending on u) of material characteristics from experiments in laboratories (at the Faculty of Civil Engineering, University of Technology in Brno, and the Institute of Physics of Materials, Academy of Sciences of the Czech Republic in Brno); this is not easy due to the long-time redistribution of moisture in building materials of common use. The complete development of the original software package would be very expensive; this difficulty might be overcome with help of MATLAB (PDE toolbox) and FEMLAB mathematical software.

Another (and more sophisticated) access comes out from more advanced analysis of a material microstructure and generates a mathematical model, using an appropriate homogenization technique. Unfortunately, both the structure of building materials and all factors determining their insulation properties are typically complicated and their better understanding requires more knowledge not only from physics, but also from chemistry, biology, etc. (remember unintentional caves in concrete structures and hibernating bats in panel houses). Thus, the more-scale convergence approach with general measures, covering domains with holes and capillaries, discussed in [20], cannot be applied directly – the main reason is that it involves no reliable mechanism explaining, how pores of various shapes and sizes are filled in with liquid water, vapour and ice (regardless of some considerations of this type in [2]). However, such approach should contribute to better understanding and predicting of seemingly surprising behaviour of structures and constructions in civil engineering in future.

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