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MODELLING OF HEAT AND MOISTURE TRANFER IN POROUS MATERIALS

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Abstract. The aim of this paper is to demonstrate the mathematical problems of modelling the physical process of heat and moisture transfer in porous materials. The method of discretization in time is applied to derive a discretized (generally non–potential) system of PDEs of elliptic type from the original variational problem of evolution. The convergence of corresponding Rothe sequences is studied.

Key words. heat and moisture transfer, porous materials, PDEs of evolution, Rothe sequences

AMS subject classifications. 35K22, 35K55

1. Introduction. Porous structure is typical for all ceramic materials and for the most building materials. The amount of moisture (including the solid, liquid and gas phases of water) in the porous structure of building materials is one of the essential factors influencing the durability of building constructions. As there exists a strong relation between moisture and heat in porous materials, every reasonable model of moisture transfer has to take into account the heat transfer, too. From the known models, especially [14], [15], [17], we have devoted most attention to the generally acknowledged Kiessl model [14], see [21] and others, in the papers [2], [3].

On the basis of a critical assessment of the above-mentioned models, J. Svoboda [4] proposed an original, physically well–founded model of the moisture and heat transfer in porous media. In this paper we present mathematical tools for the proof of existence of a weak solution of this model.

2. Physical background. State variables of the model are the *effective stress* $P(x,t) = h(x)g - \sigma/\varrho(x,t)$ $[\mathrm{m^2\,s^{-2}}]$ and *(absolute) temperature* $T(x,t)$ [K]. Here $x \in \Omega \subseteq R^2$, $t \in (0, t_{\max}) = I$ for some fixed positive number $t_{\max}$ and h [m] is the *relative height*, g $[\mathrm{m\,s^{-2}}]$ is the *gravitational constant*, ϱ $[\mathrm{kg\,m^{-3}}]$ is the *density of condensed water* (liquid and ice) in the porous structure and σ $[\mathrm{N\,m^{-2}}]$ is the *hydrostatic stress* in the condensed water.

The differential equations express the laws of conservation of moisture $\mathcal{M}$ and of heat $\mathcal{H}$

$$\frac{d\mathcal{M}}{dt} - \nabla\left(a_{11}\nabla P + a_{12}\nabla T\right) = 0\,, \quad \frac{d\mathcal{H}}{dt} - \nabla\left(a_{21}\nabla P + a_{22}\nabla T\right) = 0$$

for $x \in \Omega$, $t \in I$. If we denote by $u = u(P,T)$ $[\mathrm{kg\,m^{-3}}]$ the *sorption isotherme* expressing the amount of condensed water in 1 $\mathrm{m^3}$ of the porous material, ε [-] the *open porosity*, $V(u) = u/\varrho$ [-] the part of 1 $\mathrm{m^3}$ of the porous material occupied by condensed water and $\varphi\, c_0$ $[\mathrm{kg\,m^{-3}}]$ the amount of vapour in 1 $\mathrm{m^3}$ of air with relative humidity φ, then the amount of moisture in 1 $\mathrm{m^3}$ of the porous structure is

$$\mathcal{M} = u + (\varepsilon - V(u))\,\varphi c_0 \qquad [\mathrm{kg\,m^{-3}}].$$

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Further, if there are $\tau = T - 273.15$ [^{0}C], χ [-] the relative amount of liquid in condensed water ($\chi(\tau)$ is a smooth function increasing between -5^0C and 0^0C), ϱ_m [kg m^{-3}] the *density* of dry porous material, c_m, c_s, c_l, c_v [J kg^{-1} K^{-1}] the *heat capacity* of porous material, ice, liquid, vapour, respectively, τ_b [^0C] the *temperature of boiling water* and L_{sl}, L_{lv} [J kg^{-1}] the *latent heat of melting* of ice at $\tau = 0\,^0C$, of *evaporation* at $\tau = \tau_b\,^0C$, respectively and if we put

$$h_m = c_m\tau\,,\quad h_s = c_s\tau\,,\quad h_l = L_{sl} + c_l\tau\,,\quad h_v = L_{sl} + c_l\tau_b + L_{lv} + c_v(\tau - \tau_b)\,,$$

then

$$\mathcal{H} = h_m\varrho_m + h_s u(1-\chi) + h_l u\chi + h_v\,(\varepsilon - V(u))\,\varphi c_0 \qquad [\mathrm{J\,m^{-3}}]$$

is the amount of heat in 1 m^3 of the porous material. Finally, if we denote by ξ [kg m^{-3}s] the *convectivity of liquid*, D [kg m^{-3}s] the *diffusivity of vapour* and λ [J m^{-3}K^{-1}s^{-1}] the *heat conductivity*, then

$$a_{11} = \xi + D\,,\quad a_{12} = \frac{DL_{lv}}{T}\,,\quad a_{21} = h_l\xi + h_v D\,,\quad a_{22} = \lambda + h_v a_{12}\,.$$

Initial conditions

$$P(x,0) = P_0(x) \;\text{ and }\; T(x,0) = T_0(x) \;\text{ for any } x \in \Omega$$

and *boundary conditions*

$$a_{i1}\frac{\partial P}{\partial \vec{n}} + a_{i2}\frac{\partial T}{\partial \vec{n}} = g^i(x,t,P,T) \;\text{ for any } x \in \partial\Omega,\; t \in I \text{ and } i \in \{1,2\}$$

make the model complete.

3. General formulation of the problem. In the whole paper we shall apply the standard notation. All classes of special mappings applied here are introduced in [8] or [5], the notation of Lebesgue and Sobolev spaces is compatible with [18], the symbol * is reserved for adjoint spaces, the dot symbol (rarely) for time derivatives and R_0 is used instead of $R_+ \cup \{0\}$, too.

Following [23], we shall formulate the abstract problem in a reflexive and separable Banach space V (u will be considered in general as an abstract function mapping every time from I into V, although V can be identified with some Sobolev or similar space of functions in most available applications). Using the method of discretization in time, we shall then consider linear splines u^n instead of u. This enables us to decompose the problem of evolution into particular problems for discrete times. Finally, the limit passage for $n \to \infty$, making use of certain a priori estimates, will verify the existence of a variational solution. Unfortunately, the arguments from [23] cannot be applied directly to realistic problems with more than one unknown fields (unlike simple examples with one field in [23], pp. 490, 495) that are not generated by the weak differentiation of certain potentials (no other case is studied in [11], [12] [13], [9] or [10]) which is generally not true in our model, derived in [4].

In addition to a reflexive and separable Banach space V (especially for $\rho \in R_+$ symbol V_ρ is reserved for the set of all $v \in V$ such that $\|v\|_V \le \rho$ and symbol V'_ρ for the set of all $v \in V$ such that $\|v\|_V \ge \rho$), let us consider an other Banach space H and some mappings $A : I \to V$ and $B : I \to H$. The symbol $\langle .\,,.\rangle$ will be used for the duality between V and $V^\star$ and the symbol $(.\,,.)$ for the duality between H and $H^\star$. Let these spaces and mappings preserve the following properties:

(a) There exists a strongly continuous imbedding of V into H.
(b) A is weakly continuous.
(c) B is demicontinuous.
(d) The estimate

$$\sup_{v\in V'_\rho} (\varphi(\|v\|_V)\|v\|_V)^{-1} \int_0^1 \langle A(w+\xi(v-w)) - Aw, w\rangle \, \mathrm{d}\xi < \infty$$

is true for some $\rho \in R_+$ and arbitrary fixed $w \in V$; the function $\varphi(\|v\|_V)$ comes from (i).
(e) The estimate

$$\sup_{v\in V'_\rho} (\varphi(\|v\|_V)\|v\|_V)^{-1} (Bv, w) < \infty$$

is true for some $\rho \in R_+$ and arbitrary fixed $w \in V$; the function $\varphi(\|v\|_V)$ comes from (i).
(f) There exists an increasing continuous function $\psi : R_0 \to R_0$ such that

$$(Bv - Bw, v-w) \ge \psi(\|v-w\|_H)$$

for any $v, w \in V$.
(g) For the function ψ from (f) the estimate

$$\psi\left(\sum_{i=1}^{j} c_i\right) \le \mu(j)\sum_{i=1}^{j}\psi(c_i)$$

is valid for every positive integer j, $c_i \in R_+$ with $i \in \{1,\dots,j\}$ and certain increasing function μ mapping all positive integer into R_+.
(h) The function μ from (g) has the limit behaviour

$$\lim_{j\to\infty} \frac{\mu(j)}{j} < \infty\,.$$

(i) There exist an increasing continuous function $\varphi : R_0 \to R$ and a $\nu \in R_+$ such that

$$\int_0^1 \langle A(\xi v), v\rangle \, \mathrm{d}\xi + \nu\,(Bv, v) \ge \varphi(\|v\|_V)\|v\|_V$$

for any $v \in V$.
(j) There exists a $\gamma \in R_+$ such that

$$0 \le (Bv, v) \le \gamma\psi(\|v\|_H)$$

for any $v \in V$.
(k) There exist $\omega, \kappa \in R_+$ such that

$$\int_0^1 \langle A(w+\xi(v-w)), v-w\rangle \, \mathrm{d}\xi \ge \int_0^1 \langle A(\xi v, v\rangle \, \mathrm{d}\xi - \int_0^1 \langle A(\xi w), w\rangle \, \mathrm{d}\xi$$
$$-\kappa\sqrt{\varphi(\|v\|_V)\|v\|_V + \varphi(\|w\|_V)\|w\|_V + \omega}\,\sqrt{\psi(\|v-w\|_H)}$$

for any $v, w \in V$.

Let us study the existence of $u : I \to V$ satisfying the equation of evolution

$$(Bu(t) - Bu_0, v) + \int_0^t \langle Au(t'), v\rangle \,\mathrm{d}t' = 0 \tag{1}$$

for all $v \in V$ and arbitrary $t \in I$ where the initial value $u(0) = u_0 \in V$ is prescribed. Let us choose an integer n and a $h_i \in R_+$ for $i \in \{1, \dots, n\}$ such that $h_1 + h_2 + \dots + h_n = T$. Later we will write only h instead of the largest and h_0 instead of the smallest h_i and apply the notation $\vartheta = h/h_0$. For $i \in \{1, \dots, n\}$ let us also consider the partial time intervals $I_i = \{t \in I : t_{i-1} < t \le t_i\}$ where $t_0 = 0$ and $t_i = h_1 + \dots + h_i$; for the sake of brevity let us define $J = \{t \in R_0 : t \le 1\}$, too. Instead of $u(t)$ let us consider a linear spline

$$u^n(t) = u_{i-1} + \frac{t - t_{i-1}}{h_i}(u_i - u_{i-1})$$

for each I_i with $i \in \{1, \dots, n\}$ (evidently, $u_1, \dots, u_n$ as well as $h_1, \dots, h_n$ depend on the choice of n, but we will not emphasize this fact explicitly) Thi simplifies (1) to the form

$$(Bu_j - Bu_0, v) + \sum_{i=1}^{j} \int_{t_{i-1}}^{t_i} \left\langle A\left(u_{i-1} + \frac{t' - t_{i-1}}{h_i}(u_i - u_{i-1})\right), v\right\rangle \mathrm{d}t' \tag{2}$$

for arbitrary $t = t_j$ with $j \in \{1, \dots, n\}$ and for any $v \in V$. We set $u^n(0) = u_0$ formally.

In the following lemmas, theorems and sketches of proofs we verify the existence of u_i satisfying (2) with $i \in \{1, \dots, n\}$ in the first place; then we shall prove that some subsequence of $\{u^n\}_{n=1}^{\infty}$ has a limit u which is identical with a solution of (1). In the more exact form the first result will be presented in Theorem 1, the second one in Theorem 2. Later we will study more regular solutions.

Lemma 1. For every integer n and $i \in \{1, \dots, n\}$, (2) can be converted into the discretized form

$$(Bu_i - Bu_{i-1}, v) + h_i \int_0^1 \langle A(u_{i-1} + \xi(u_i - u_{i-1})), v\rangle \,\mathrm{d}\xi = 0 \tag{3}$$

with arbitrary $v \in V$.

P r o o f is based only on simple algebraic manipulations and on the linear transformation $\xi = (t' - t_{i-1})/h_i$.

Lemma 2. For some $i \in \{1, \dots, n\}$, let T_i be the operator mapping each $w \in V$ into $V^\star$ using the definition

$$\langle T_i w, v\rangle = (Bw - Bu_{i-1}, v) + h_i \int_0^1 \langle A(u_{i-1} + \xi(w - u_{i-1})), v\rangle \,\mathrm{d}\xi$$

for all $v \in V$. Then, for a fixed $u_{i-1} \in V$, the operator T_i is weakly continuous.

P r o o f follows by the properties (a), (b), (c), (d), by the boundedness of any weakly continuous sequence (cf. [7], p. 193) and by the Lebesgue dominated convergence theorem (see [19], p. 110).

Lemma 3. For every $i \in \{1, \dots, n\}$, h_i small enough and a fixed u_{i-1} the operator T_i from Lemma 2 is coercive.

Proof starts by putting $v = w$ in the definition of T_i in Lemma 2. Estimates based on the properties (d), (e), (f), (i) and (k) guarantee the coerciveness of V for h_i small enough.

Theorem 1. For every $i \in \{1, \dots, n\}$, h_i small enough and for a fixed u_{i-1} there exists some u_i satisfying (3).

Proof applies the result from [6], p. 46, saying that every weakly continuous and coercive mapping of V into $V^\star$ maps V onto $V^\star$, Lemma 2 and Lemma 3.

Lemma 4. The sequence of piecewise linear abstract functions $\{u^n\}_{n=1}^\infty$ mapping I into V is equibounded.

Proof uses more precise a priori estimates than the Proof of Lemma 3. The choice $v = (u_i - u_{i-1})/h_i$ in (3) and the application of the properties (f), (g), (h), (i), (j) and (k) together with the discrete version of the Gronwall lemma (see [11], p. 29, and [24], p. 370) yield the required equiboundedness after long computations.

Lemma 5. The sequence $\{u^n\}_{n=1}^\infty$ from Lemma 4 is equicontinuous as a sequence of abstract functions mapping I into H.

Proof is based on the estimates making use of Lemma 4 and (3) again.

Lemma 6. There exists an $u : I \to V$ such that, up to a subsequence, $u(t)$ is a weak limit of $\{u^n(t)\}_{n=1}^\infty$ for every $t \in I$ and u is a strong limit of $\{u^n\}_{n=1}^\infty$ in $C(I, H)$.

Proof . The statement is a consequence of certain version of the Arzelà-Ascoli theorem (see [16], p. 36 and [11], p. 24) whose assumptions are satisfied thanks to Lemma 4 and Lemma 5.

Theorem 2. There exists an abstract function $u : I \to V$ satisfying (1) such that $u \in C(I, H)$.

Proof verifies the correctness of the limit passage from (2) to (1) (the relation between (3) and (2) is evident from Lemma 1), making use of Lemma 4, Lemma 5 and Lemma 6.

Lemma 7. Let the following assumption be added to the property (f):

(f') There exists a $\psi_0 \in R_+$ such that $\psi(c) \geq \psi_0 c^2$ for any $c \in R_0$.

Then there exists also a $\theta \in R_+$ such that the estimate for the sequence $\{\dot{u}^n\}_{n=1}^\infty$ (of time derivatives of the sequence $\{u^n\}_{n=1}^\infty$) from Lemma 4

$$\int_I \|\dot{u}^n(t)\|_H^2 \, \mathrm{d}t \leq \theta \tag{4}$$

is valid independently of the choice of an integer n.

Proof repeats the approach from Lemma 4 in a slightly modified form, using the property (f').

Theorem 3. Let H be reflexive and the property (f') from Lemma 7 be satisfied. Then every solution u of (1) in the sense of Theorem 2 belongs to $L^\infty(I, V) \cap W^{1,2}(I, H)$.

Proof comes from the general convergence theorem for Rothe sequences from [11], p. 25.

Now let us introduce a mapping $P : I \to V$ with the properties analogous to A:

(b') P is weakly continuous.

(d') The estimate

$$\sup_{v\in V'_\rho} \|v\|_V^{-2} \int_0^1 \langle Pv, w\rangle < \infty$$

is true for some $\rho \in R_+$ and arbitrary fixed $w \in V$.

(i') There exist an $\varepsilon \in R_+$ and $\lambda \in R_0$ such that

$$\langle Pv, v\rangle \,\mathrm{d}\xi \geq \epsilon \|v\|_V^2 - \lambda$$

for any $v \in V$.

(k') In the original property (k) the square root of $\psi(\|v-w\|_H)$ is allowed to be substituted by the square root of the sum of $\psi(\|v-w\|_H) + \|v-w\|_V^2$ only (this makes (k) less strict).

In the following lemmas and theorems we will study the analogue of (2)

$$(Bu_j - Bu_0, v) + \sum_{i=1}^{j} h_i \left\langle P\left(\frac{u_i - u_{i-1}}{h_i}\right), v\right\rangle + \sum_{i=1}^{j} \int_{t_{i-1}}^{t_i} \left\langle A\left(u_{i-1} + \frac{t' - t_{i-1}}{h_i}(u_i - u_{i-1})\right), v\right\rangle \mathrm{d}t' = 0\,,$$

for any $v \in V$ (clearly the argument of P is equal to $\dot{u}^n$ everywhere)

Lemma 8. For every integer n and $i \in \{1, \ldots, n\}$, the analogue of (2) can be converted into the form similar to (3)

$$(Bu_i - Bu_{i-1}, v) + h_i \left\langle P\left(\frac{u_i - u_{i-1}}{h_i}\right), v\right\rangle + h_i \int_0^1 \langle A(u_{i-1} + \xi(u_i - u_{i-1})), v\rangle \,\mathrm{d}\xi = 0 \tag{5}$$

with arbitrary $v \in V$. Moreover, the operator T_i' mapping each $w \in V$ into $V^\star$ and defined by means of the operator T_i from Lemma 3 by the formula

$$\langle T_i' w, v\rangle = \langle T_i w, v\rangle + h_i \left\langle P\left(\frac{u_i - w}{h_i}\right), v\right\rangle$$

for all $v \in V$ is weakly continuous and coercive.

P r o o f repeats the arguments of the proofs of Lemma 1, Lemma 2 and Lemma 3, taking into account the new operator P and the properties (b'), (d') and (k').

Theorem 4. Theorem 1 holds with (5) instead of (3), too.

P r o o f is the same as the proof of Theorem 1; Lemma 8 instead of Lemma 2 and Lemma 3 is applied.

Lemma 9. Under the assumptions of Lemma 8 the inequality (4) from Lemma 7 holds even with the norm of V instead of the norm of H.

P r o o f of Lemma 4 can be repeated; the property (i') is substantial here.

Lemma 10. There exists an abstract function $u : I \to V$ such that Lemma 6 is valid and (up to a subsequence) also $\dot{u}$ is a weak limit of $\{\dot{u}^n\}_{n=1}^{\infty}$ in $L^2(I, V)$.

P r o o f can apply Lemma 9 (similar to Lemma 7), and the Eberlein - Shmul'yan theorem (see [25], p. 201); this implies the existence of some weak limit $\dot{u}$ of $\{\dot{u}^n\}_{n=1}^{\infty}$ in $L^2(I,V)$ and consequently the weak convergence of $\{u^n(t)\}_{n=1}^{\infty}$ to $\int_0^t \dot{u}(t')\,\mathrm{d}t'$ in V which can be identified with $u(t)$ for arbitrary $t \in I$.

Theorem 5. Theorem 2 holds with

$$(6) \qquad (Bu(t) - Bu_0, v) + \int_0^t \langle P\dot{u}(t'), v\rangle \,\mathrm{d}t' + \int_0^t \langle Au(t'), v\rangle \,\mathrm{d}t' = 0$$

instead of (1), too. Moreover, let the mapping P have the property (additional to (i')):

(i") If $w \in V_\rho$ for some $\rho \in R_+$ then $\langle Pw, v\rangle = 0$ for every $v \in V$.

Then Theorem 2 holds with (1) directly provided that $\dot{u}(t) \in V_\rho$ ($\rho \in R_+$ comes from the property (i")) for arbitrary $t \in I$.

P r o o f makes use of the compactness of the imbedding of $W^{1,2}$ into $L^2(I,H)$ and studies the limit passage from (5) to (6) in the same way as the proof of Theorem 2 (the relation between (5) and (5) is evident from Lemma 8). The last assertion follows from the property (i") applied to (6) directly.

Theorem 6. Let the assumptions of Theorem 5 (except the property (i")) be satisfied and, moreover, let H be reflexive and the property (f') from Lemma 7 and Theorem 3 be valid. Then (6) can be differentiated with the result

$$(7) \qquad ((Bu(t))^{\cdot}, v) + \langle P\dot{u}(t), v\rangle + \langle Au(t), v\rangle = 0$$

for every $v \in V$ and arbitrary $t \in I$.

P r o o f applies the Eberlein - Shmul'yan theorem which yields the existence of a strong limit $\dot{u}$ of $\{\dot{u}^n\}_{n=1}^{\infty}$ (up to a subsequence). The limit passage is similar to that from Theorem 2 and Theorem 5; moreover, the differentiation of (5) is well-defined and its result is (7).

We have demonstrated that for a rather large class of problems of evolution, including the problem of moisture and heat transfer in porous media in the formulation of [4] (which initiated this study), some reasonable existence and convergence results can be derived using the properties of Rothe sequences. The formulation in spaces of abstract functions avoids the discretization in R^N; in practical computation this can be done using the finite element or similar techniques. We have not discussed the case of weakly continuous operators B because this seems to be very strong assumption which may be physically non-realistic. From [1], pp. 63, 103, and [23], p. 360, we know that in the Lebesgue space $H = L^2(\Omega, R^N)$, where Ω is an open set in R^N, every weakly continuous mapping is linear. This is not true for weakly continuous operators A (and P, if necessary) in the Sobolev spaces: e. g. if V is some subspace of $W^{1,2}(\Omega, R^N)$ involving $W_0^{1,2}(\Omega, R^N)$ (to include prescribed boundary conditions of Dirichlet type) then many nonlinear weakly continuous mappings (as in examples from [6], pp. 52, 53) exist and the weak continuity can be tested efficiently using the theorem on Nemytskiĭ operators (cf. [7], p. 75, [5], p. 288, and [22], p. 36). The demicontinuity of B is easy to be verified in practice because the property (f) forces the monotony of B and (by [8], p. 66) for monotone operators demicontinuity and radial continuity coincide. One possible easy choice of φ, ψ and μ is $\varphi(c) = c - c_0$, $\psi(c) = c^2$, $\mu(j) = j$ for every $c \in R_0$, each positive integer j and some fixed $c_0 \in R$. Function spaces different from the Sobolev spaces can be also applied; e. g. in [2] the regularity questions are analyzed in the Morrey - Campanato spaces (cf. [20], p. 35).

For the concrete choice of spaces V and H (as the spaces of integrable functions defined on Ω) some additional assumptions on Ω must be accepted to ensure the validity of usual imbedding and trace theorems;. their geometrical interpretation is discussed in great details in [18], pp. 62, 220. From this point of view, the generalization of the access of [23], p. 490, brings no substantial difficulties. Let us notice that in our assumed properties no potentiality of A or B is required; nevertheless, by [8], p. 90, the demicontinuity of A implies that A is a potential operator iff the property (k) with $\kappa = 0$ is satisfied. In practical problems the property (k') is often more realistic than (k).

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