Jiří Vala

Modelling of heat and moisture propagation in building structures

In: Jan Chleboun and Petr Přikryl and Karel Segeth (eds.): Programs and Algorithms of Numerical Mathematics, Proceedings of Seminar. Dolní Maxov, June 6-11, 2004. Institute of Mathematics AS CR, Prague, 2004. pp. 248–256.

Persistent URL: http://dml.cz/dmlcz/702802

MODELLING OF HEAT AND MOISTURE PROPAGATION IN BUILDING STRUCTURES*

Jiří Vala

Abstract

The thermal technical analysis is an important part of the design of building constructions. Especially for dwelling structures valid Czech(oslovak) and European standards formulate criteria of maximal thermal stability and minimal energy consumption that have to be verified by credible calculations. The propagation of heat through a building construction, consisting typically of several porous layers, is conditioned by the amount of moisture in such construction; simultaneously it is affected by the heat propagation in living rooms, determined by the dynamics of air flow. This contribution presents an overview of various approaches to mathematical modelling and algorithms of technical calculations, known as HAM ("heat, air and moisture") modelling; it contains also references to corresponding software packages.

1. Introduction

The design and judgement of modern building structures from the point of view of required calculations is a rather complicated work, consisting of much more items than only from the usual stress and strain analysis of constructions as their response to external mechanical (static or dynamic) loads. Both Czech(oslovak) and European technical standards force to verify how the quasiperiodic changes of temperature in outer environment in day and year cycles contribute to the deformation of a structure (and consequently to the reduction of its durability), but also which level of comfort is guaranteed for human activities, proposed for such structure.

Various paragraphs of such standards as ČSN 730540, DIN 4108 and of CIB recommendations include two types of criteria: i) preserving of thermal stability – this means that some lower and upper bounds for a temperature are prescribed, alternatively also its change rate is bounded (nearly independent of similar changes in outer environment), ii) reduction of energy consumption (by heating and air-conditioning). In this paper we intend to demonstrate how these criteria are circumvented by some (rather tricky) simplified approaches. From the conservation principles we shall later come to physically correct formulations of separate elements of HAM. Finally we shall mention some important generalizations, useful for the study of selected practical interdisciplinary problems.

*This work was supported by the research project of the Ministry of Education, Youth and Sports of the Czech Republic CEZ : J22 : 261100007.

2. Elementary calculations

The most simple calculations come from the idea of one-dimensional heat conduction through a massive wall with a thickness l and heat convection between a wall and inner or outer environment. In the following text a dot symbol will be reserved for a partial derivative with respect to the time t, a prime symbol similarly for a partial derivative with respect to our unique "space" variable x. The heat conduction is described by a partial differential equation for some unknown temperature T

$$c\rho\dot{T} - (\lambda T')' = 0 \quad \text{on } (0,l)\,,$$

the heat convection is driven by a couple of boundary temperatures T_1 and T_2 (different in general, e. g. $T_1 < T_2$)

$$\lambda T'(l) = \alpha(T_2 - T(l)), \quad -\lambda T'(0) = \alpha(T_1 - T(0))\,;$$

material characteristics c, ρ, λ a α (for the details see lower) are allowed to be taken as constants.

Believing that the whole process is stationary, we may set $\dot{T} = 0$. Separating the variables (as in the elementary course of ordinary differential equations), we obtain the linear distribution of temperature in a wall

$$T = T_1 + \frac{\alpha x + \lambda}{\alpha l + 2\lambda}(T_2 - T_1)\,;$$

especially for $\alpha \ll \lambda$

$$T \approx (T_1 + T_2)/2$$

and for $\alpha \gg \lambda$

$$T \approx T_1 + \frac{x}{l}(T_2 - T_1)\,.$$

The main drawback of this approach is the fact that such stationary distributions of a temperature T are rarely observed in practice. The real building constructions consist of more layers with different properties – e. g. from bricks or from concrete panels, supplied by plasters and special insulation layers; thus the preceding equation should be solved separately for each layer with different material characteristics. Such characteristics can be variable also in one layer. However, we could expect (for nearly constant material characteristics) that the distribution of a temperature will be piecewise quasilinear, always monotone. In contradiction with this hypothesis the observed nonlinearities are very significant and the monotonicity cannot be guaranteed. To explain such phenomena at a qualitative level is rather simple – the heat conduction factor λ for water is (approximately) 20-times higher than the same factor for air and most building materials have porous structures. . . . The quantitative evaluation of the same phenomena without a non-elementary mathematical and physical theory is impossible.

3. The simplified model of heat transfer in a construction and in air in rooms

The most part of a volume in dwelling structures consists of rooms, occupied by air. The correct description of the air transfer through such rooms is rather complicated. Therefore in the first rough approximation it is useful to assume that a temperature in each point of the same room will be also the same, variable only in time. If some one-dimensional domain Ω represents the whole building object including inner rooms and if Ω^J $(J \in \{0,\dots,M\})$ describe separate constructive parts and rooms (whose number is M), the resulting variational formulation (derived formally from the Green - Ostrogradskiĭ theorem) obtains the form

$$\int_{\Omega^J} \varphi^J \rho^J (c^J T^J)^{\cdot}\,\mathrm{d}x + \int_{\Omega^J} \varphi^J_{,1} \lambda^J T^J_{,1}\,\mathrm{d}x + \Big[\varphi^J \alpha^J (T^J - T^J_*)\Big]^{x^J}_{x^{J-1}} = 0$$

for given lengths $0 = x^0 < x^1 < \ldots < x^M = l$; a comma followed by a lower index 1 here (to be compatible with a more general formulation later) means a derivative by our "spacial" variable $x = x_1$. On all contacts of material layers we must distinguish between "left" temperatures T^J and "right" temperatures T^J_*; we know that $T^0_*(x^0) = T_1$ a $T^M(x^M) = T_2$. The test variables φ^J must be chosen carefully to force the original (clearly non-physical) assumption on the non-variability of a temperature inside rooms. The Einstein summation rule for all indices will be assumed everywhere.

This approach can be generalized for the case of a three-dimensional domain Ω. Evidently we have $x = (x_1, x_2, x_3)$ in Cartesian coordinates here; in addition to $\mathrm{d}x$ we need also $\mathrm{d}\sigma(x)$ where σ is a measure on two-dimensional surfaces. The details (even for a slightly more general case) can be found in [5], whose final system (in our notation) is

$$\int_{\Omega^J} \varphi^J \rho^J (c^J T^J)^{\cdot}\,\mathrm{d}x + \int_{\Omega^J} \varphi^J_{,j} \lambda^J T^J_{,j}\,\mathrm{d}x$$

$$+ \sum_{K=1}^{M} \int_{\partial\Omega^J \cap \partial\Omega^K} \varphi^J \alpha^{JK} (T^J - T^K)\,\mathrm{d}\sigma + \int_{\partial\Omega^J \cap \partial\Omega} \varphi^J \alpha^J_* (T^J - T^J_*)\,\mathrm{d}\sigma = 0\,;$$

a comma followed by a lower index j here means always a derivative with respect to a variable x_j, a lower index in α^J_* refers to an outer boundary Ω only (in contrast to an inner contact in α^{JK}).

To study the pure thermal transfer, usual software means for the analysis of coupled problems in engineering (as ANSYS, SYSTUS, ADINA, ABAQUS, COSMOS or I-DEAS) can be applied, but for practical thermal technical calculations this approach is not user-friendly. In the USA the freeware programs FRAME and THERM (`www.enermodal.com`, `http://windows.lbl.gov/software/therm`) are much-favoured, in the Europe the Swedish (rather cheap) programs HEAT2, HEAT3 and their extensions (`www.blocon.se`) are frequently applied.

4. The model of heat transfer in a construction incorporating the process of air flow in rooms

To remove all non-physical assumptions on temperature distributions is not easy. To make necessary considerations well-arranged, let us start with the notation of needed physical quantities:

- T temperature [K],
- q thermal flux [J/(m^2 s)], $q = (q_1, q_2, q_3)$,
- v air flow rate [m/s], $v = (v_1, v_2, v_3)$,
- $\varepsilon(v)$ strain rate tensor for air flow [1/s] with components $\varepsilon_{ij}(v) = (v_{i,j} + v_{j,i})/2$ where $i, j \in \{1, 2, 3\}$,
- ρ building material density or air density [kg/m^3],
- w air momentum [kg/(m^2 s)]: $w = \rho v$,
- p air pressure [Pa],
- τ additional air stress tensor [Pa] (τ_{ij} s $i, j \in \{1, 2, 3\}$), caused by $\varepsilon(v)$ by the Newton pure viscous constitutive law,
- g acceleration of gravity [m/s^2],
- e total inner energy [J/m^3],
- f volumetric energy supply [J/(kg s)].

We can see that we shall have to work with four time-dependent fields T, p, ρ and v (whose initial status must be given). Their development is driven by material characteristics:

- λ thermal conductivity [W/(m K)] on Ω,
- α thermal convectivity [W/(m^2 K)] on $\partial\Omega$,
- c thermal capacity (specific heat) [J/(kg K)] on Ω,
- η_1 first viscosity [Pa s] on Ω,
- η_2 second viscosity [Pa s] on Ω.

From the physical point of view we need: a) 1 continuity equation for (non-stationary, in general) air flow on Ω, b) 3 Cauchy equilibrium equations for small deformations on Ω, c) 1 heat conduction equation (the Fourier - Kirchhoff law) on Ω, d) 1 heat convection equations on $\partial\Omega$ (as a boundary condition for c)), e) 6 purely viscous constitutive relations (by Newton) between components of symmetrical tensors of strains and stresses on Ω, f) 1 algebraic relation between T, p and ρ (the Gay-Lussac law) on Ω. Let us notice that b), combined with e) and f), generates 3 equations of the Navier-Stokes type with internal friction.

Let us start with a conservative principle for a general quantity ψ with some source ω

$$\dot{\psi} + (\psi v_j)_{,j} = \omega \qquad \text{on } \Omega\,.$$

In special cases we get: i) the mass conservation principle

$$\dot{\rho} + (\rho v_j)_{,j} = 0\,,$$

ii) the inertia conservation principle

$$\dot{w}_i + (w_i v_j)_{,j} = (\tau_{ij} - \delta_{ij} p)_{,j} + \rho g_i$$

and iii) the energy conservation principle

$$\dot{e} + (e v_j)_{,j} = ((\tau_{ij} - \delta_{ij} p) v_i + q_j)_{,j} + \rho(g_i v_i + f)\,.$$

Rather long formal calculations, whose details can be found in [7], verify that i), ii) and iii) give the resulting system of equations

$$w_i = \rho v_i\,, \quad \dot{\rho} = -w_{j,j} \quad \text{on } \Omega\,,$$

$$\int_\Omega \tilde{v}_i \rho v_i' \,\mathrm{d}x + 2\int_\Omega \varepsilon_{ij}(\tilde{v}) \eta_1 \varepsilon_{ij}(v) \,\mathrm{d}x - \int_\Omega \tilde{v}_{i,i} \eta_2 v_{j,j} \,\mathrm{d}x = \int_\Omega \tilde{v}_i \rho g_{,i} \,\mathrm{d}x - \vartheta \int_\Omega \tilde{v}_i (\rho T)_{,i} \,\mathrm{d}x\,,$$

$$\int_\Omega \varphi \rho (cT)' \,\mathrm{d}x + \int_\Omega \varphi_{,j} \lambda T_{,j} \,\mathrm{d}x = \int_\Omega \varphi \rho (f - \vartheta T v_{j,j}) \,\mathrm{d}x$$

$$-2\int_\Omega \varphi \eta_1 \varepsilon_{ij}(v) \varepsilon_{ij}(v) \,\mathrm{d}x + \int_\Omega \varphi \eta_2 (v_{j,j})^2 \,\mathrm{d}x - \int_{\partial\Omega} \varphi \alpha (T - T_*) \,\mathrm{d}\sigma$$

with appropriate test functions $\tilde{v}$ and φ and with initial conditions for ρ, v and T (p can be completed easily from f)); T_* is our prescribed temperature of outer environment again.

The numerical solution of this system, analysed in [7], includes: i) the approximation of material characteristics, dependent on ρ, v, T, using the least squares method, ii) the discretization of an evolution problem in time, applying the construction of Rothe sequences – for the prediction of ρ, v, T in each time step (with material characteristics from the previous one) the aim is to obtain a linear elliptic system where some corrections inside such time step are available, iii) the discretization in the three-dimensional (in the simplified case in the two-dimensional) Euclidean space, using the method of finite elements. Let us mention that the discretization iii) (where the greatest difficulties come from the strong nonlinearity of all equations of the Navier-Stokes type) is possible to be done using the methods of finite volumes, of finite differences or of their various combinations, too – see [3], p. 157. In practice we often meet the simplification where the first equation is removed (with the risk of some significant system error), applying an algebraic Boussinesq approximation; the theory is explained in [3], p. 15, some numerical experiments with the simulation of air flow through a two-dimensional vertical cut of a room with realistic (temperature-dependent) air characteristics will be presented in [6]. However, no reasonable reduction to an one-dimensional problem is known.

The above mentioned and other simulations show that the temperature redistribution caused by air flow is usually much more important than that caused by classical heat conduction. Thus, sufficiently general software systems for the analysis of flow of fluids can be useful for practical calculations. The development of a specialized software is possible using some functions of MATLAB (toolbox PDE) or FEMLAB. At various levels such problems are covered by some HAM programs (referenced later).

5. The influence of moisture propagation

Modelling of moisture propagation through porous materials, modifying their thermal technical properties very substantially, is nowadays a separate (not easy) research branch. Two autonomous (but collaborating) processes are active here – the heat propagation (which is relatively quick) and the very slow moisture redistribution in three phases (ice, liquid water and vapour) in macro- and microscopic pores in materials in separate constructive layers. Just the phase transformations are the most dangerous: e. g. the condensation of vapour from air can result (in the final effect) in the total degradation of a construction, not only of its thermal technical properties, but even of its primal bearing function (thanks to concrete crush, corrosion of reinforcement, etc.). A lot of complication is induced by the fact that the process of filling of pores by water (even without any visible material damage) is not fully reversible. Here we shall present only a simplified overview of corresponding problems, coming from the original analysis of [2]; more references to the practical assessment of its approach to the development of new insulation materials in civil engineering can be found in [7].

For the analysis of moisture propagation some additional physical quantities have to be introduced:

- $c^{\cdot}$ thermal capacities (specific heats) c^L, c^V, c^S [J/(kg K)] for corresponding phases of water (upper indices L, V and S refer to a “liquid”, “vapour” or “solid” phase),
- $\Lambda^{\cdot\cdot}$ latent heats $\Lambda^{SL}, \Lambda^{LV}$ [J/kg] for corresponding phase changes,
- χ a “quasi-characteristic function” of a temperature T: $\chi(T) = 0$ for $T \ll T^{SL}$, $\chi(T) = 1$ for $T \gg T^{SL}$,
- Υ a microstructurally motivated ratio [−] of a partial pressure of vapour over a curved water surface (with certain characteristic curvature) and of a partial pressure of vapour over a flat water surface, in general a function of p and T,

$\rho^{\cdot}$ densities for various phases of water

$$\rho^S = (1-\chi)u\,, \qquad \rho^L = \chi u\,, \qquad \rho^V = \left(P - \frac{(1-\chi)u}{\tilde{\rho}^S} - \frac{\chi u}{\tilde{\rho}^L}\right)\tilde{\rho}^V \Upsilon\,,$$

β a prescribed driving function [kg/(m^2 s)] for interface heat convection,

γ a prescribed driving function [J/(m^2 s)] for interface moisture convection.

Our conservation principles are: the principle of mass conservation i)

$$\int_\Omega \tilde{\varphi}(\rho^S+\rho^L+\rho^V)^{\cdot}\,\mathrm{d}x + \int_\Omega \tilde{\varphi}_{,j}\xi^L(p_{,j}-\rho^L g_j)\,\mathrm{d}x + \int_\Omega \tilde{\varphi}_{,j}\xi^V(p_{,j}-\rho^V g_j)\,\mathrm{d}x = \int_{\partial\Omega} \tilde{\varphi}\beta\,\mathrm{d}\sigma\,,$$

and the principle of energy (heat) conservation ii)

$$\int_\Omega \varphi(\rho\dot{\kappa} + (\rho^S\kappa^S + \rho^L\kappa^L + \rho^V\kappa^V)^{\cdot})\,\mathrm{d}x + \int_\Omega \varphi_{,j}\lambda T_{,j}\,\mathrm{d}x + \int_\Omega \varphi_{,j}\kappa^L\xi^L(p_{,j}-\rho^L g_j)\,\mathrm{d}x$$
$$+ \int_\Omega \varphi_{,j}\kappa^V\xi^V(p_{,j}-\rho^V g_j)\,\mathrm{d}x = \int_{\partial\Omega}\varphi\gamma\,\mathrm{d}\sigma$$

where

$$\kappa = cT\,, \qquad \kappa^S = c^S T\,, \qquad \kappa^L = c^S T^{SL} + \Lambda^{SL} + c^L(T - T^{SL})\,.$$

The choice of test functions φ and $\tilde{\varphi}$ must correspond to boundary conditions again; an initial status of T and p has to be known in advance.

The equations of a similar type (often without some terms, at least seemingly negligible for special applications) are handled by various software systems for thermal technical calculations as a part of design and judgement of building objects. The relatively simple analysis of thermally conditioned moisture propagation with prohibited phase changes, based on the classical works of H. Glasser (1958-59), is implemented frequently: this category includes e. g. the software EMPTIED ("Envelope Moisture Performance Through Infiltration, Exfiltration and Diffusion", G. O. Handegord 1985), SHAM ("Simplified Hygrothermal Analysis Methods", J. P. de Graauw 1997) and SMAHT ("Structural Moisture and Heat Transfer", M. J. Cunningham 1990). The attempts to simulate heat and moisture transfer together with air flow are reflected e. g. in TRATMO ("TRansient Analysis of Thermal and MOisture behavior", R. Kohonen 1984), WALLDRY ("WALL DRYing", G. D. Schuyler 1989), MATCH ("Combined Heat ANd Moisture TRansfer", C. R. Pedersen 1989), MOIST ("MOISTure transfer", D. M. Burch 1989), TCCD2 ("Transient Coupled Convection and Diffusion in 2D", R. Kohonen and T. Ojanen 1989) and FSEC ("Florida Solar Energy Center: heat, moisture and contaminant transport", A. Kerestecioglu 1989). The large HAM (which means the "Heat, Air and Moisture" transfer) program systems from the last years are namely WUFI ("Wärme Und Feuchte

Instationär", K. Kiessl, H. Künzel a M. Krus 1997, Frauenhofer Institut für Bauphysik, download of the freeware version `www.ornl.gov/ORNL/BTC/moisture`, commerce products and applications `www.hoki.ibp.fhg.de/wufi/wufi_frame_e.html`), DELPHIN (TU Dresden, A. Häupl and J. Grunnenwald 1999), TRNSYS ("TRaNsient SYstem Simulation", J. Duffie a S. Klein 1988, the system approach, applying the zonal model) and LATENITE (National Research Council Otawa, H. Hens, A. Karagiozis and M. Solonvaara 1993, the extended version LATENITE-VTT, 2001, offers also certain kind of stochastic modelling). For more detailed information it is useful to read research reports of the International Energy Agency; an extensive overview of programs of programs can be found in [4] (where North-American and Canadian software codes are preferred, but, e. g., some widely-used German ones are ignored totally); more references to software means of various categories are involved in [7], too.

6. Some practical generalizations

Up to now, we have discussed (to avoid too complicated notations and formulae) only particular elements of HAM models. The complex HAM models are able to combine such elements at various levels; such coupling can results in transfer models for air, moisture and heat in building structures. However, all available models apply some simplifications (both theoretical and numerical, rarely with the complete documentation), necessary for sufficiently cheap and effective computations – let us remind that one expected part of such complex model should be the analysis of air flow in every 3-dimensional room located in a building.

Open questions are still hidden in perhaps every model – from existence problems in mathematical formulations to constructions of optimal algorithms and their practical implementations. Nevertheless, the engineering applications provoke further important generalizations, namely with the aim to include: i) the heat radiation (especially in the vicinity of artificial heat sources – power-law relations lead to "rapid nonlinearities"), ii) the mechanical strains and stresses (to couple static and dynamic calculations with the thermal technical ones), iii) the chemical reactions (like carbonation in elements of concrete structures), iv) the biocorrosion (using the "biological damage" function together with the evaluation of liquid moisture) v) the microstructural and stochastic analysis (the homogenization, the (more-)scale convergence, etc., applying the deep mathematical results, analysed in [1]).

We can conclude: one of principal tendencies of the computer-supported technical design in civil engineering is to construct more user-friendly and less energy-consuming buildings. The absence of long-time observations and extensive experimental results can be overcome just using new achievements of the HAM modelling.

References

[1] Cioranescu D., Donato P.: *An introduction to homogenization.* New York, Oxford University Press 2000.

[2] Dalík J., Svoboda J., Šťastník S.: *A model of moisture and temperature propagation.* Research report, Faculty of Civil Engineering, Brno University of Technology 1998.

[3] Ferziger J.H., Perić .: *Computational methods for fluid dynamics.* Berlin, Springer-Verlag 2002.

[4] Straube J., Burnett E.: *Review of modelling methods for building enclosure design.* University of Waterloo 1999.

[5] Vala J.: *Building as a thermal system.* (In Czech.) In: Proceedings of the PRASTAN Conference in Kočovce, Slovak Technical University Bratislava 2000, 105–120.

[6] Vala J.: *Heat transfer and air flow in buildings.* In: Proceedings of the Mathematical Workshop in Brno, Brno University of Technology 2004, in print.

[7] Vala J., Šťastník S.: *On the modelling of heat propagation in buildings.* Building Research Journal **52**, 1, 2004, 31–56.