

Modeling of Annual Heat and Moisture Diffusion in a Multilayer Wall

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Abstract. We present a 1D numerical model of heat, steam, and water transfer across a wall consisting of several layers of different materials. The model is the system of coupled diffusion equations for wall temperature; vapor pressure, and water concentration in material pores, with account of vapor condensation and water evaporation. The system of nonlinear PDEs is solved numerically using the finite difference method. The main objective of modeling is simulation of long-term behavior of building wall moisture distribution under influence of seasonal variations in atmospheric air temperature and humidity.

1 Introduction

Simultaneous heat, steam, and moisture transfer with condensation and evaporation in porous materials is of practical importance in applications in civil engineering. The transport of water vapor across building walls and its possible condensation increases the thermal conductivity of the porous materials and may cause structural damage. Complexity of the phenomenon and the large variety of conditions under which it can proceed cause the development of new models and approaches to the problem in a lot of research works. In particular, we can refer the works [1–9].

The main goal of this paper is not the development of original model of the phenomenon, but the presentation of a sufficiently precious and stable numerical algorithm for solution of the model of coupled heat, steam, and moisture diffusion, invented by Fokin K.F. in his book [10]. The Fokin model is widely used in civil engineering practice in Russia for estimation of long term thermal and moisture behavior in building envelopes [11]. The model is phenomenological model based on simple, intuitive physical principles. The diffusion flux of each component is proportional to gradient of corresponding variable: temperature, partial pressure of steam, and water concentration. All parameters of the model can be measured experimentally. Evolution equation for each component is the diffusion equation. Mutual coupling between equations is performed by the dependence of diffusion coefficients on moisture, and through the source terms related to the phase transitions. Main difficulty in numerical solution of the model is connected with variability in time of regions of vapor condensation.

2 Mathematical Formulation of the Model

Model parameters. For definiteness, in this paper we will consider three-ply wall. The thickness of wall layers is denoted as d_1 , d_2 , and d_3 [m] respectively. Let the first layer is the external (outward building) and the third layer is the internal (inward building) layer of the wall. We will consider the fluxes of heat and moisture in the direction traversal to wall only, $-$ the direction along x axis. The point $L_0 = 0$ is the outer edge of external layer, the points $L_1 = d_1$ and $L_2 = L_1 + d_2$ are the interface points between layers, and the point $L_3 = L_2 + d_3$ is the outer edge of internal layer.

The material of each layer is characterized by following parameters: density $-\rho$ [kg/m³]; heat capacity $-c$ [kJ/(kg·K)]; coefficients of thermal $-\lambda$ [kJ/(h·m·K)]; vapor $-\mu$ [g/(h·m·Pa)]; and hydraulic $-\beta$ [g/(h·m·%)], conductivity. The parameters ρ , c , and μ are supposed to be constant in considered range of temperature T [K] and moisture volumetric concentration ω [%], while other parameters can depend on ω . For given material the dependencies $\lambda(\omega)$ and $\beta(\omega)$ used in calculations are polynomial interpolations of experimental measurements. Under equilibrium conditions at constant temperature the relation between air humidity φ and moisture ω is determined from experimentally measured sorption isotherm $\omega = o(\varphi)$.

The external layer of the wall contacts with atmospheric air, and the internal layer contacts with building interior air. The air temperature $T_{\text{ex}}(t)$, $T_{\text{in}}(t)$, and humidity $\varphi_{\text{ex}}(t)$, $\varphi_{\text{in}}(t)$ are given function of time t [h]. Heat exchange between wall and air is determined by coefficients α_{ex} and α_{in} [kJ/(h·m²·K)]. Steam exchange at the wall borders is determined by coefficients γ_{ex} and γ_{in} [g/(h·m²·Pa)].

Heat conductivity. The transversely heat transfer in each wall layer is described by the heat conduction equation for the material temperature $T(t, x)$:

$$c\rho \frac{\partial T(t, x)}{\partial t} = \frac{\partial}{\partial x} \left(\lambda(\omega) \frac{\partial T(t, x)}{\partial x} \right) + Q(T, \omega). \quad (1)$$

The source term Q takes into consideration the latent heat of vapor condensation and water evaporation (the water-ice transitions are not included in the model).

At the wall borders and layer interfaces there are imposed boundary and conjugation conditions:

$$-\lambda(\omega) \frac{\partial T(t, x)}{\partial x} \Big|_{x=L_0} = \alpha_{\text{ex}} (T_{\text{ex}}(t) - T(t, x)) \Big|_{x=L_0}; \quad (2)$$

$$T(t, L_i - 0) = T(t, L_i + 0),$$

$$\lambda(\omega) \frac{\partial T(t, x)}{\partial x} \Big|_{x=L_i-0} = \lambda(\omega) \frac{\partial T(t, x)}{\partial x} \Big|_{x=L_i+0}, \quad i = 1, 2; \quad (3)$$

$$-\lambda(\omega) \frac{\partial T(t, x)}{\partial x} \Big|_{x=L_3} = \alpha_{in} (T(t, x) - T_{in}(t)) \Big|_{x=L_3}. \tag{4}$$

Vapor and liquid water conductivity. It is supposed that the water in wall material can be in three forms: water vapor (steam), and mobile liquid water in material pores, and immobile absorbed water rigidly connected with material skeleton. The concentration of absorbed water ω depends upon local air humidity in pores $\varphi(t, x)$ and assumed to be equal to equilibrium concentration $o(\varphi)$. If $\varphi < 1$, the material contains only steam and absorbed water, the mass of absorbed water in unit volume of material is equal to $0.01\omega\rho$.

The air humidity φ is defined as ratio $\varphi = e/E(T)$, where e [Pa] is partial pressure of water vapor, and $E(T)$ is pressure of saturated vapor at air temperature T . For calculation of E we use the approximation formula:

$$E(T) = \begin{cases} 4.688(1.486 + T/100)^{12.3}, & T < 0, \\ 288.58(1.098 + T/100)^{8.02}, & T \geq 0. \end{cases} \tag{5}$$

The function $\varphi(t, x)$ is supposed to be continuous function of both variables. So, at every t one can define the subset $V_t \subseteq (L_0, L_3)$, $V_t = \{x : \varphi(t, x) < 1\}$, and the complementary subset $W_t = (L_0, L_1) \setminus V_t$.

In subset V_t the moisture moves in the form of steam only, and its motion is governed by the vapor conduction equation

$$\xi(\omega)\rho \frac{\partial e(t, x)}{\partial t} = \mu \frac{\partial^2 e(t, x)}{\partial x^2}. \tag{6}$$

(Thermo-diffusion of steam, that is the diffusion induced by temperature gradient, does not included in the model.) Here the parameter ξ defines the ‘vapor capacity’ of material and can be estimated by the equation

$$\xi(\omega) = \frac{do(\varphi)}{d\varphi}. \tag{7}$$

As noted above, Eq. (6) is defined in the subset V_t . If the point L_0 and/or L_3 are the boundary points of V_t , then the boundary conditions of convective exchange of steam between air in material pores and surrounding air are imposed similar to (2), (4) with replaced T by e , λ by μ , and α by γ . If any of interface points L_1, L_2 belongs to V_t , then the conjugation condition assuming continuity of vapor pressure and flux is imposed similar to (3).

In subset W_t the material pores contain liquid water together with water vapor, and it is supposed that between water and vapor there keeps up the dynamic equilibrium. That is the partial pressure of vapor in W_t equals to pressure of saturated vapor, $e(t, x) \equiv E(T(t, x))$ for all $x \in W_t$. To estimate the volumetric concentration of liquid water w [%] we propose the following formula

$$w(t, x) = \omega(t, x) - o(1), \tag{8}$$

where $o(1)$ is maximal concentration of absorbed water, corresponding to $\varphi = 1$.

Diffusive motion of liquid water is described by equation

$$10\rho \frac{\partial w(t, x)}{\partial t} = \frac{\partial}{\partial x} \left(\beta(w) \frac{\partial w(t, x)}{\partial x} \right) + \mu \frac{\partial^2 E(T)}{\partial x^2}. \tag{9}$$

Here numerical coefficient ‘10’ appears due to different dimensions of parameters (kg in ρ , g in μ and β , and % in w). Second term in the right hand side corresponds to vapor condensation or water evaporation depending on its sign. To avoid extra model complication the condition of water impermeability at border points of W_t is accepted

$$\left. \frac{\partial w}{\partial x} \right|_{\partial W_t} = 0. \tag{10}$$

If any of points L_1, L_2 is inner point of W_t , then there is imposed the condition of continuity of water concentration and water flux, similar to (3). In the points, separating subsets V_t and W_t , we suppose continuity of pressure $e(t, x)$.

Latent heat of phase transition. The term $\nu = \mu(\partial^2 E(T)/\partial x^2)$ [g/(h·m³)] in Eq. (9) represents the rate of change of water concentration due to water evaporation or vapor condensation, that is in result of phase transition. The phase transitions are accompanied by release or absorption of latent heat, depending on the sign of ν . The latent heat of phase transition is accounted in Eq. (1) via the source term Q , numerical value of which is calculated with the formula

$$Q = \begin{cases} q_L \nu, & x \in W_t, \\ 0, & x \in V_t, \end{cases} \tag{11}$$

where q_L is the specific heat of water vaporization (= 2.26 kJ/g).

3 Numerical Scheme

The system of Eqs. (1), (6), and (9), with all additional conditions listed above is solved numerically with the help of the finite differences method. To approximate the space derivatives with finite differences we define the uniform grid of N nodes x_k on the interval (L_0, L_3) : $x_k = L_0 + (k - 0.5)h$, $k = 1, 2, \dots, N$, $h = (L_3 - L_0)/N$. The time derivative is approximated on the time grid $t_0 = 0, t_1, t_2, \dots, t_n, \dots$, with variable time step $\tau_n = t_{n+1} - t_n$, $n \geq 0$. Each function $f(t, x)$ is replaced its grid approximation $f_k^n = f(t_n, x_k)$. Below, for brevity, we will drop the upper index denoting f_k^n as f_k , and f_k^{n+1} as \hat{f}_k .

Finite difference equations. To derive the finite difference equations we use implicit scheme and heat and mass balance method. The finite-difference counterparts of Eqs. (1), (6), and (9) are the following

$$hc_k \rho_k \frac{\hat{T}_k - T_k}{\tau} = \hat{A}_k^- (\hat{T}_{k-1} - \hat{T}_k) - \hat{A}_k^+ (\hat{T}_k - \hat{T}_{k+1}) + \hat{Q}_k, \quad k = 1, \dots, N. \tag{12}$$

$$h\hat{\xi}_k\rho_k\frac{\hat{e}_k - e_k}{\tau} = M_k^-(\hat{e}_{k-1} - \hat{e}_k) - M_k^+(\hat{e}_k - \hat{e}_{k+1}), \quad x_k \in V_n. \quad (13)$$

$$10h\rho_k\frac{\hat{w}_k - w_k}{\tau} = \hat{B}_k^-(\hat{w}_{k-1} - \hat{w}_k) - \hat{B}_k^+(\hat{w}_k - \hat{w}_{k+1}) + \hat{\nu}_k, \quad x_k \in W_n. \quad (14)$$

The coefficients Λ are calculated as follows

$$\begin{aligned} \Lambda_1^- &= \frac{2\alpha_{\text{ex}}\lambda_1}{\alpha_{\text{ex}}h + 2\lambda_1}, \quad \Lambda_k^- = \frac{2\lambda_{k-1}\lambda_k}{h(\lambda_{k-1} + \lambda_k)}, \quad k = 2, \dots, N; \\ \Lambda_k^+ &= \frac{2\lambda_k\lambda_{k+1}}{h(\lambda_k + \lambda_{k+1})}, \quad k = 1, \dots, N - 1, \quad \Lambda_N^+ = \frac{2\lambda_N\alpha_{\text{in}}}{2\lambda_N + \alpha_{\text{in}}h}. \end{aligned} \quad (15)$$

The coefficients M and B are calculated similar to Λ . The term ν is approximated by second difference

$$\nu_k = M_k^-(E_{k-1} - E_k) - M_k^+(E_k - E_{k+1}), \quad (16)$$

where $E_k = E(T_k)$, if $x \in W_n$; $E_k = e_k$, if $x \in V_n$; $E_0 = e_{\text{ex}}(t_n)$, $E_{N+1} = e_{\text{in}}(t_n)$.

Assuming that $T_0 = T_{\text{ex}}(t_n)$, $T_{N+1} = T_{\text{in}}(t_n)$; $e_0 = e_{\text{ex}}(t_n)$, $e_{N+1} = e_{\text{in}}(t_n)$, one obtains the closed system of $2N$ algebraic equations with $2N$ unknowns. First N unknowns are the values of temperature \hat{T}_k at grid nodes x_k in time moment t_{n+1} . Other N unknowns are the values of steam partial pressure \hat{e}_k at nodes $x_k \in V_n$ or the values of water concentration \hat{w}_k at nodes $x_k \in W_n$.

Iterative solution. The system of finite-difference Eqs.(12), (13), (14) is the non-linear system because of the scheme is implicit and the coefficients λ and β depend on the system solution. To solve the non-linear system we use an iterative procedure.

Using known solution at time t_n we calculate the coefficients Λ and B (coefficients M are constant) and substitute them in system (12), (13), (14). Solving the resulting linear system we obtain first approximation to solution at moment t_{n+1} , $\{T_k^{(1)}, e_k^{(1)}, w_k^{(1)}\}$. Then the first approximation is used in the same way to obtain second approximation $\{T_k^{(2)}, e_k^{(2)}, w_k^{(2)}\}$, and so on. The iterations are ended when the relative difference between two successive approximations becomes sufficiently small.

Designation of subset W_t . At initial time moment t_0 all nodes x_k , where initial moisture concentration ω_k is not less than maximal adsorption concentration, $\omega_k \geq o(1)$, are included in subset W_0 . Further, the domain W is re-designated after each successful time step. The nodes x_k from V_n , where the vapor pressure $e_k \geq E_k$ pass from V_n in W_{n+1} , while the nodes x_k from W_n , where $w_k < 0$, pass from W_n in V_{n+1} . There are no restrictions on shape and size of subset V (and, therefore, of W).

Choice the value of time step τ . To avoid possible numerical instability time step τ is limited by some empirical maximal value τ_{max} . Initial time step is assigned less than τ_{max} in several orders of magnitude. Time step with assigned

value of τ is considered as successful, if (i) the number of iterations in solution of system (12), (13), (14) is not exceed assigned maximal number of iterations, and (ii) relative difference between solution at current time step and solution at previous time step is sufficiently small. If current time step is not successful, the value of τ is diminished by definite factor, and step is repeated until the time step becomes successful. If the number of successive successful steps exceeds assigned number, the value of τ increases by definite factor.

4 Numerical Example

As an example we consider a three-ply wall. The external layer of wall is a thin stucco, and other two layers of equal thickness are concrete and mineral wool as heat insulator. The main goal of our example is to demonstrate the difference (well-known in construction practice) in heat and moisture behavior in two walls consisting of these layers. First wall is ‘correct’ wall with layers order: stucco - heat insulator - concrete; and second wall is ‘incorrect’ with layers order: stucco - concrete - heat insulator.

In this paper we use some ‘typical’ values of material parameters, which can be found in numerous literature. The accepted values of constant material parameters are presented in Table 1 (dimensions were specified in text above). Two additional parameters k and λ_0 are used for calculation of material coefficient of thermal conductivity λ , $\lambda = \lambda_0 + k\omega$.

Table 1. Material parameters.

Material	d	ρ	c	μ	k	λ_0	$o(1)$
Concrete	0.2	2500	0.84	3×10^{-5}	0.1	1.45	3.997
Mineral wool	0.2	125	0.84	3×10^{-4}	0.001	0.06	1.875
Stucco	0.02	1800	0.84	9×10^{-5}	0.07	0.7	1.184

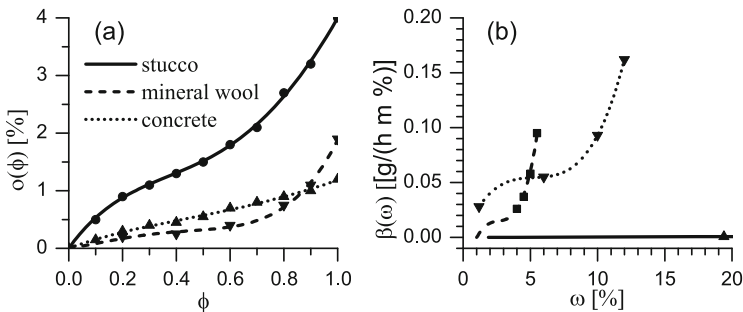


Fig. 1. (a) – sorption isotherm $o(\varphi)$, (b) – coefficient of water conductivity $\beta(\omega)$.

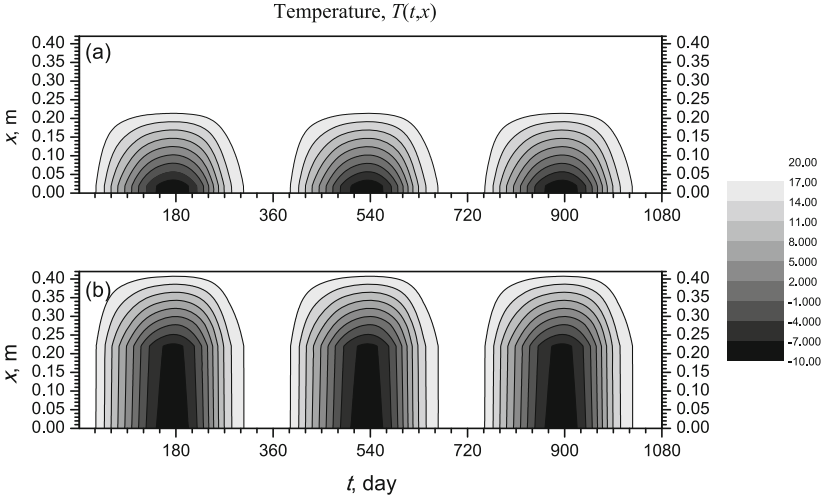


Fig. 2. Space-time plot of temperature in ‘correct’ (a), and ‘incorrect’ (b) wall.

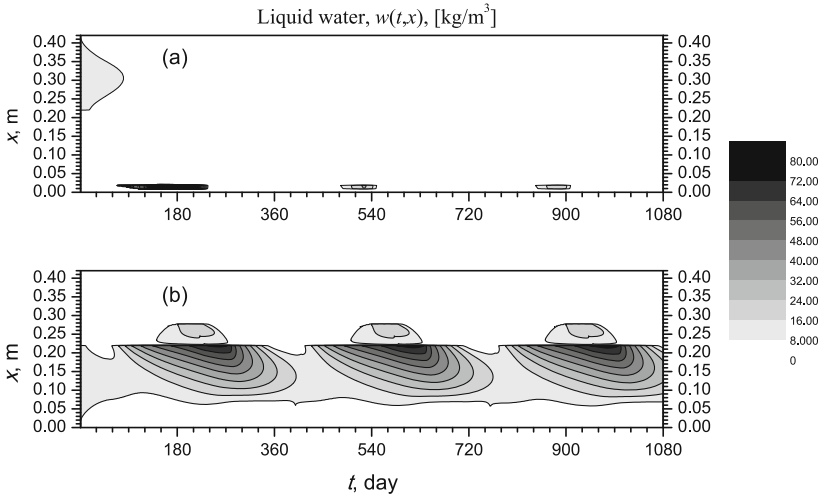


Fig. 3. Space-time plot of water concentration in ‘correct’ (a), and ‘incorrect’ (b) wall.

The graphs of the sorption isotherms and the coefficient β in dependence on ω are shown in Fig. 1, where the experimental measurements, depicted by markers, are connected via polynomial interpolations. In the building interior the constant air temperature and humidity are supposed, $T_{in} = 20\text{ }^\circ\text{C}$, $\varphi_{in} = 0.6$. The temperature and humidity of external air simulate their seasonal variations for Moscow region. The heat exchange coefficients $\alpha_{in} = 31.4$, $\alpha_{ex} = 85.8$, and the vapor exchange coefficients $\gamma_{in} = 0.075$, $\gamma_{ex} = 0.750$.

The initial time moment corresponds to the middle of July with average daily air temperature of 19.3 °C. The initial temperature distribution in wall is linear between 19.3 °C at outer and 20 °C at inner wall surface. The initial moisture concentration is assigned for every wall layer. In our example it was $0.9 \times o(1) = 3.597$ for stucco, $1.5 \times o(1) = 1.775$ for concrete, and $1.5 \times o(1) = 2.813$ for mineral wool. That is, the wall is waterlogged and have to dry.

Figure 2 shows, that (as it should be expected) the fall of temperature in winter time occurs mostly in the heat insulator layer. Hence, during winter the concrete temperature is high in ‘correct’ wall, and low in ‘incorrect’ wall. The vapor condensation proceeds in that regions, where the vapor pressure e becomes higher than the pressure of saturated vapor E . Such a condition is mainly created at low temperatures. Therefore, there are much more possibilities for condensation in ‘incorrect’ wall than in ‘correct’ wall. This is confirmed by Fig. 3.

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