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CALCULATION OF HEAT AND MOISTURE DISTRIBUTION IN THE POROUS MEDIA LAYER

H. KALIS and I. KANGRO

Institute of Mathematics Latvian Academy of Sciences and University of Latvia

Akadēmijas laukums 1, LV-1524 Rīga, Latvia

E-mail: kalis@lanet.lv

Rēzekne Higher Education Institution, Department of engineering science

Atbrīivošanas aleja 90, LV-4601, Rēzekne, Latvija

E-mail: kangro@cs.ru.lv

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Abstract. In this paper we study the problem of the diffusion of one substance through the pores of a porous material which may absorb and immobilize some of the diffusing substances with the evolution or absorption of heat. The transfer of moisture and the heat are described by the model. The system of two partial differential equations (PDEs) is derived, one equation expresses the rate of change of concentration of water vapour in the air spaces and the other the rate of change of temperature. The obtained initial–boundary value problem is approximated by using the finite volume method. This procedure allows us to reduce the 2D transfer problem described by a system of PDEs to initial value problem for a system of ordinary differential equations (ODEs) of the first order.

Key words: Finite-volume method, mathematical models, porous media flows

1. The Mathematical Model

The interest to studies of hydrodynamic flow and heat transfer through a porous media is increased due to its vast applications such as the drying in porous solids and soils, drying of wood and paper, soil mechanics, porous heat pipes, paper machines, liquid composite moulding. Many mathematical models are developed for the analysis of such processes, for example mathematical models of moisture movement in wood, when the wood is considered as porous media [1, 2, 3, 8]. Basically these models can be classified into three categories: empirical curve-fitting equations, moisture diffusion equations, and fundamental heat and mass transfer equations. Historically, most models are based on the moisture diffusion equation. The using of diffusion equation is usually restricted to the drying below the fiber saturation point, where only water vapor and bound water are involved and transported by molecular diffusion. However, over the last decades the development of more accurate and general models becomes more popular [2, 3, 8]. In such models the wood is consider as a porous medium and multiphase flow and heat transfer is taken into account. In certain porous media applications the working fluid heat generation (source) or absorption (sink) effects are important [5]. In this paper we study the heat and moisture transfer processes in the porous media layer, described in [4].

We shall further assume linear dependence on both temperature and moisture content and write

$$M = const + \sigma C - \omega T, \tag{1.1}$$

where C is the concentration of water vapour in the air spaces, M is the amount of moisture absorbed by unit mass of fiber, σ and ω are constants. We shall consider the equilibrium uptake of moisture by a fiber to be related to water vapour concentration and temperature T by the linear relation (1.1).

Let us consider an element of a porous material. We can derive two equations, one expressing the rate of change of concentration and the other describing the rate of change of temperature. The PDE defining water vapour diffusion is given in the following form

$$mgD\frac{\partial^2 C}{\partial x^2} = m\frac{\partial C}{\partial t} + (1-m)\rho_s\frac{\partial M}{\partial t}, \quad x \in [0, L], \ \ t > 0, \tag{1.2}$$

where D is the diffusion coefficient for moisture in air, m is the fraction of the total volume of the material occupied by air and $(1-m)$ is the fraction of the porous material occupied by fiber of density ρ_s, $2L$ is the thickness of the layer of the porous media (due to symmetry conditions

$$\left.\frac{\partial C}{\partial x}\right|_{x=L} = 0, \quad \left.\frac{\partial T}{\partial x}\right|_{x=L} = 0$$

we consider only a half of this layer), t is the time. If $m = 1$, then the equation (1.2) is diffusion equation for the concentration without fibers. The parameter g, follows from the fact that the diffusion process goes not along straight air channels but through a matrix of intertwined fibers and any diffusion of mass along the fibers is also allowed.

The rate at which the temperature of the element changes is determined by the heat conduction through air and fibers and the heat evolved when moisture is absorbed by fibers. The heat diffusion PDEs can be rewritten in the following form:

$$c\rho\frac{\partial T}{\partial t} = K\frac{\partial^2 T}{\partial x^2} + q\rho\frac{\partial M}{\partial t}, \tag{1.3}$$

where c is the specific heat of the fibers, K, ρ is the heat conductivity and the density of the porous material, q is the heat evolved when the water vapour is absorbed by the fibers.

We notice, that both PDEs (1.2), (1.3), i.e. the vapour and temperature equations, depend on the amount of moisture M in the fibers.

We assume that

1. All coefficients in the PDEs are assumed constant and independent of moisture concentration and temperature.
2. The heat of sorption q is assumed independent of regain, though in practice it it can depend on it.
3. Hysteresis of sorption is neglected.
4. The relative volumes occupied by fiber and air are assumed to be constant as diffusion proceeds, i.e. m is assumed to be constant.
5. The influence of capillarity in the air spaces is not taken into account.

By eliminating M from (1.1), we get the system of two PDEs

$$\begin{cases} D^T \dfrac{\partial^2 T}{\partial x^2} = \dfrac{\partial T}{\partial t} - \nu \dfrac{\partial C}{\partial t}, \\ D^C \dfrac{\partial^2 C}{\partial x^2} = \dfrac{\partial C}{\partial t} - \lambda \dfrac{\partial T}{\partial t}, \end{cases} \tag{1.4}$$

where

$$D^T = \frac{K}{\rho(c + q\omega)}, \quad D^C = \frac{Dmg}{m + (1-m)\rho_s \sigma},$$
$$\nu = \frac{q\sigma}{c + q\omega}, \quad \lambda = \frac{(1-m)\omega\rho_s}{m + (1-m)\rho_s\sigma}.$$

For $t = 0$ we give the initial condition:

$$T(x,0) = T_0(x), \quad C(x,0) = C_0(x), \tag{1.5}$$

where T_0, C_0 are known functions.

2. Reduction to Non-connected Diffusion Equations

Let us assume that Dirichlet boundary conditions (BDc) are formulated on the exterior surfaces $x = 0$

$$T(0,t) = \phi_1(t), \quad C(0,t) = \phi_2(t), \tag{2.1}$$

where ϕ_1, ϕ_2 are given functions. Then it follows from [4] that simple diffusion PDEs

$$\frac{1}{\mu_i} \frac{\partial^2 V_i}{\partial x^2} = \frac{\partial V_i}{\partial t}, \quad i = 1, 2 \tag{2.2}$$

can be obtained for functions $V_1 = C - m_2 T,\ V_2 = T - m_1 C$, here

$$m_1 = \frac{1 - \mu_1 D^C}{\lambda}, \quad m_2 = \frac{1 - \mu_2 D^T}{\nu},$$

and μ_1, μ_2 are the roots of the quadratic equation

$$\left(\mu - \frac{1}{D^T}\right)\left(\mu - \frac{1}{D^C}\right) = \frac{\lambda\nu}{D^C D^T}.$$

They can be written in the following form

$$\mu_1 = (d_1 + d_2)/d_3, \quad \mu_2 = (d_1 - d_2)/d_3, \quad d_1 = D^T + D^C,$$
$$d_3 = 2D^T D^C, \quad d_2 = \sqrt{(D^C - D^T)^2 + 4\lambda\nu D^T D^C}, \quad \lambda\nu \in (0,1).$$

Let us assume that solutions $V_i(x,t)$ of diffusion equations (2.2) subject to initial and boundary conditions (1.5), (2.1) are obtained. Then solving for T and C we get

$$T = \frac{\gamma}{V_2 + m_1 V_1}, \quad C = \frac{\gamma}{V_1 + m_2 V_2}, \tag{2.3}$$

where $\gamma = 1 - m_1 m_2$.

3. Solution of the Initial-Boundary Problem for the Diffusion Equation in Infinite Layer

If $L = \infty$, then functions T_0, C_0, ϕ_1, ϕ_2 in (1.5), (2.1) are constants and $T|_\infty = T_0$, $C|_\infty = C_0$, then we get solutions of diffusion equations (2.2) in the following form:

$$V_1(x,t) = \Phi_1 + (V_{10} - \Phi_1)\,\mathrm{erf}\left(\frac{\sqrt{\mu_1}x}{2\sqrt{t}}\right),$$
$$V_2(x,t) = \Phi_2 + (V_{20} - \Phi_2)\,\mathrm{erf}\left(\frac{\sqrt{\mu_2}x}{2\sqrt{t}}\right),$$

where

$$V_{10} = C_0 - m_2 T_0, \quad V_{20} = T_0 - m_1 C_0,$$
$$\Phi_1 = \phi_2 - m_2\phi_1, \quad \Phi_2 = \phi_1 - m_1\phi_2, \quad \mathrm{erf}\,(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-y^2}dy.$$

Solutions T and C follow from (2.3).

4. The Finite-Difference Scheme for Diffusion Equations

Let us consider the case of finite layer($L \neq \infty$). We solve diffusion equations (2.2) with BDc $V_i|_{x=0} = \Phi_i$, $\frac{\partial V_i}{\partial x}|_{x=L} = 0$, and initial conditions $V_i|_{t=0} = V_{i0}$, $i = 1,2$ by using the following explicit finite-difference scheme(FDS):

$$\begin{cases} V_j^{m+1} = V_j^m + r/\mu(V_{j-1}^m - 2V_j^m + V_{j+1}^m), \\ V_0^m = \Phi, \quad V_{N+1}^m = V_{N-1}^m, \quad V_j^0 = V_0(x_j), \quad j = \overline{1,N},\ m = \overline{0,M}, \end{cases} \tag{4.1}$$

where V_j^m is the approximate value of $V_i(x_j, t_m), i = 1, 2,$

$$x_j = jh, \quad Nh = L, \quad t_m = m\tau, \quad r = \tau/h^2,$$

h, τ are the corresponding space and time steps in the uniform grid

$$\Phi = \Phi_i, \quad V_0 = V_{i0}, \quad i = 1, 2.$$

The stability condition for FDS (4.1)is given by

$$\tau = \frac{k_0 h^2}{2} \min(\mu_1, \mu_2), \quad k_0 < 1.$$

5. The Finite-Difference Scheme for System of Two PDEs

If BDc on the exterior surfaces $x = 0$ are different (the second or the third) kind, then it is not possible to obtain the PDEs (2.2). The initial-boundary value problem for the system of two PDEs (1.4) can be written in the following matrix-vector form:

$$\begin{cases} \dfrac{\partial W}{\partial t} = A \dfrac{\partial^2 W}{\partial x^2}, \\ \dfrac{\partial W}{\partial x}\Big|_{x=L} = 0, \quad W|_{t=0} = W_0, \quad W|_{x=0} = \phi, \end{cases} \tag{5.1}$$

where

$$A = \frac{1}{1 - \lambda\nu} \begin{vmatrix} D^T & \nu D^C \\ \lambda D^T & D^C \end{vmatrix}$$

is the matrix of the second order, $W = (T, C)^T$, $W_0 = (T_0, C_0)^T$, $\phi = (\phi_1, \phi_2)^T$ are the vectors, $0 < \lambda\nu < 1$. Then the vector finite-difference scheme is given by

$$\begin{cases} W_j^{m+1} = W_j^m + rA\big(W_{j-1}^m - 2W_j^m + W_{j+1}^m\big), \\ W_0^m = \phi, \quad W_{N+1}^m = W_{N-1}^m, \quad W_j^0 = W_0, \quad j = \overline{1, N}. \end{cases} \tag{5.2}$$

The stability condition for the vector FDS (5.2) can be written as

$$\tau = \frac{k_0 h^2}{2} ||A||^{-1}, \quad k_0 < 1, \quad ||A|| = ||A||_\infty. \tag{5.3}$$

If BDc are of the second kind, then it is necessary to add other finite-difference equations. As an example, if $C|_{x=0} = 1$, $\dfrac{\partial T}{\partial x}|_{x=0} = 0$, then the difference equation at grid point $x_0 = 0$ is added

$$T_0^{m+1} = T_0^m + 2rD^T(T_1^m - T_0^m). \tag{5.4}$$

The stability condition for this equation $\tau = k_0 h^2/(2D^T)$ follows from (5.4).

If BDc are given in the form $T|_{x=0} = 1$, $\dfrac{\partial C}{\partial x}|_{x=0} = 0$, then we formulate the following difference equation

$$C_0^{m+1} = C_0^m + 2rD^C(C_1^m - C_0^m),$$

with the stability condition $\tau = k_0 h^2/(2D^C)$.

6. The System of Ordinary Differential Equations

The system of PDEs (5.1) can be rewritten in the following form:

$$A\frac{\partial^2 W}{\partial x^2} = \dot{W},$$

where $\dot{W} = \dfrac{\partial W}{\partial t}$. Using the method of finite volumes we obtain the following exact vector finite-difference scheme with respect to grid points $x_1 = L/2$, $x_2 = L$, $h = L/2$ for the given function $\dot{W}$ [6, 7]:

$$\begin{cases} Ah^{-1}(W_2 - 2W_1 + W_0) = R_1^+ + R_1^-, \\ -Ah^{-1}(W_2 - W_1) = R_2^-, \end{cases} \tag{6.1}$$

where

$$R_1^- = \frac{1}{h}\int_0^h x\dot{W}_1(x,t)dx = hJ_3, \qquad R_1^+ = \frac{1}{h}\int_h^L (L-x)\dot{W}_2(x,t)dx = hJ_1,$$

$$R_2^- = \frac{1}{h}\int_h^L (x-h)\dot{W}_2(x,t)dx = hJ_2, \quad J_1 = \int_0^1 (1-\bar{x})V_2(\bar{x})d\bar{x},$$

$$J_2 = \int_0^1 \bar{x}V_2(\bar{x})d\bar{x},\ \bar{x} = (x-h)/h, \qquad V_2(\bar{x}) = \dot{W}_2(h + h\bar{x}, t);$$

$$J_3 = \int_0^1 \bar{x}V_1(\bar{x})d\bar{x},\ \bar{x} = x/h, \qquad V_1(\bar{x}) = \dot{W}_1(h\bar{x}, t).$$

In the non-stationary case one must approximate integrals $J_k,\ k = 1,2,3$ with quadrature formulas in the following way:

$$J_k = A_1^{(k)}V_2(0) + A_2^{(k)}V_2(1) + A_3^{(k)}V_2'(1) + r_k, \quad k = 1,2, \tag{6.2}$$

$$J_3 = A_1^{(3)}V_1(0) + A_2^{(3)}V_1(1) + r_3, \tag{6.3}$$

$$r_k = \frac{h^3}{3!}\frac{\partial^3 \dot{W}_2(\xi_k, t)}{\partial x^3}C_k, \quad \xi_k \in (h, L), \quad (k = 1,2),$$

$$r_3 = \frac{h^2}{2!}\frac{\partial^2 \dot{W}_1(\xi_3, t)}{\partial x^2}C_3, \quad \xi_3 \in (0, h).$$

Here r_k are vector-errors terms, $A_n^{(k)},\ C_k(k, n = 1,2,3)$ are indefinite coefficients. Using the power functions $\bar{x}^i, i = 0,1,\dots$ in (6.2)–(6.3) for the fixed coordinate of vectors $V_1(\bar{x}), V_2(\bar{x})$ we get the systems of linear algebra equations for $A_n^{(k)}$:

$$\begin{cases} 1/[(i+1)(i+2)] = A_1^{(1)}0^i + A_2^{(1)} + iA_3^{(1)}, \\ 1/i+2 = A_1^{(2)}0^i + A_2^{(2)} + iA_3^{(2)}, \quad i = \overline{0,2}, \\ 1/i+2 = A_1^{(3)}0^i + A_2^{(3)}, \quad i = \overline{0,1}, \end{cases} \tag{6.4}$$

where $0^i = 1$ for $i = 0$. Calculations shows that solutions of the corresponding systems (6.4) are given by

$$A_1^{(1)} = A_2^{(1)} = \frac{1}{4}, \quad A_3^{(1)} = -\frac{1}{12}, \quad A_1^{(2)} = \frac{1}{12}, \quad A_2^{(2)} = \frac{5}{12},$$
$$A_3^{(2)} = -\frac{1}{12}, \quad A_1^{(3)} = \frac{1}{6}, \quad A_2^{(3)} = \frac{1}{3}.$$

Constants C_k in the residual r_k are determined using power functions $\bar{x}^2$, $\bar{x}^3$:

$$C_1 = \frac{1}{20}, \quad C_2 = -\frac{1}{30}, \quad C_3 = -\frac{1}{12}.$$

Using vector difference equations (6.1) and the right-side integral's approximations (6.2), (6.3) with neglected error terms $r_k, k = \overline{1,3}$ we have the following initial value problem for vector system of linear ODEs of the first order $(\dot{u}_0 = 0)$:

$$\begin{cases} \frac{1}{4}\dot{W}_1 + \frac{1}{4}\dot{W}_2 + \frac{1}{3}\dot{W}_1 = \frac{A}{h^2}\Big(W_2 - 2W_1 + W_0\Big), \\ \frac{1}{12}\dot{W}_1 + \frac{5}{12}\dot{W}_2 = -\frac{A}{h^2}\Big(W_2 - W_1\Big), \\ W_1(0) = \phi(h), \quad W_2(0) = \phi(L). \end{cases} \tag{6.5}$$

7. Some Numerical Results

We consider two processes in the porous layer without inner temperature by using the following parameters:

$$L = 0.5, \ D^T = 10^{-3}, \ D^C = 10^{-4}, \ M = 50000, \ N = 50, \ \lambda\nu = 0.9,$$

1) the drying process(D): $T_0 = 0, \ C_0 = 1, \ \phi_1 = 1, \ \phi_2 = 0,$

2) the moister process(M): $T_0 = 0, \ C_0 = 0, \ \phi_1 = 0, \ \phi_2 = 1.$

The results of calculations for FDS are obtained by MATLAB. For the FDS (4.1) and for both grid functions $V_i, i = 1,2$ we consider matrix $V = zeros(2, N1), \ N1 = N + 1$, then MATLAB operator for calculations in every time step is written in following form:

$$V(:,2:N1) = V(:,2:N1) + r * B * ((V :,1:N) - 2 * V(:,2:N1) + (V(:,3:N1)V(:,N)),$$

where B is a diagonal-matrix with the elements μ_1^{-1}, μ_2^{-1}. For the vector FDS (5.2) this MATLAB operator is similar with $B = A$.

The results of calculations for ODEs are obtained by MAPLE. In Table 1 the values of

$$C_1 = C|_{x=0.25}, \ T_1 = T|_{x=0.25}, \ C_2 = C|_{x=0.5}, \ T_2 = T|_{x=0.5}$$

Table 1. The values of C and T for $x = 0.25, x = 0.5$ at time $t = 114.6$.

Process	λ	ν	C_1	T_1	C_2	T_2
1(M)	0.9	1.0	0.1603	0.0846	0.085	0.0923
2(M)	0.1	9.0	0.1603	0.7627	0.085	0.8311
3(M)	9.0	0.1	0.1603	0.0085	0.085	0.0092
4(D)	0.1	9.0	0.9244	0.1603	1.007	0.0850
5(D)	0.9	1.0	1.6020	0.8383	1.746	0.8238
6(D)	1.0	0.9	1.6870	0.8467	2.839	0.8330

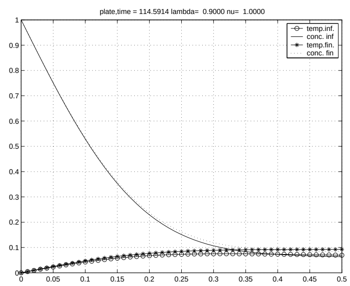

Figure 1. The moister process $\lambda = 0.9, \nu = 1.0$

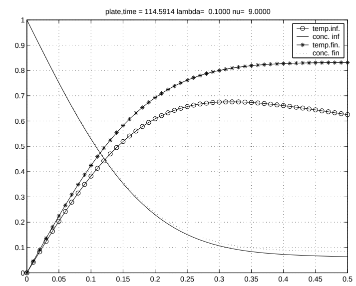

Figure 2. The moister process $\lambda = 0.1, \nu = 9.0$

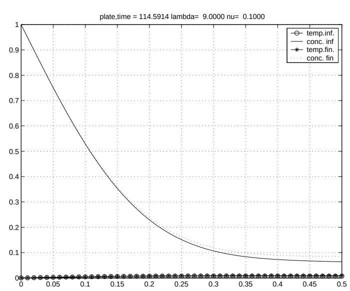

Figure 3. The moister process $\lambda = 9.0, \nu = 0.1$

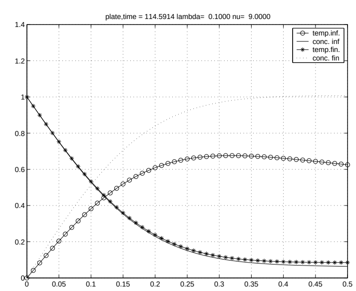

Figure 4. The draying process $\lambda = 0.1, \nu = 9.0$

are presented for $t = 114.5914, M = 50000$. Comparing the solutions of ODEs system (6.5) and FDS (4.1), (5.2), we see that for $C_i, T_i, i = 1; 2$ two digits remain the same.

In Fig.1–6 we present the concentration and temperature distributions in the porous layer depending on the space coordinate x and on the parameters λ, ν at time moment $t = 114.5914$. In the legends the following notation is used:

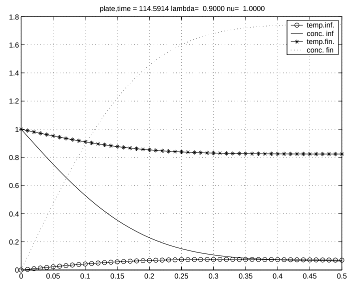

Figure 5. The draying process $\lambda = 0.9, \nu = 1.0$

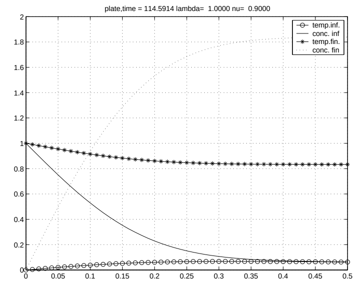

Figure 6. The draying process $\lambda = 1.0, \nu = 0.9$

1) $\circ - \circ - \circ$ for the temperature curve in infinite layer of $x \in [0, 0.5]$,
2) $* - * - *$ for the temperature curve in corresponding finite layer,
3) ——— for the concentration curve in infinite layer,
4) $\cdots\cdots$ for the concentration curve in finite layer.

For the moister process in Fig.1–3 we can see, that if parameter ν is increased and water vapour is absorbed by porous material, then inside the layer heat is evolved, this produces a considerable increase in temperature.

For the draying process in Fig.4–6 we can see, that for increasing values of parameter λ and the temperature inside the layer the concentration of water vapour in the air spaces also can be increased.

8. Conclusions

1. For the modelling of transfer of moisture and heat in porous layer the system of two PDEs is considered. It is used for determination of the concentration C of water vapour in the air spaces and the temperature T.
2. In the case of BDs of the first kind this system is transformed to two independent PDEs.
3. The initial-boundary value problems for the system of PDEs and for the separate PDEs are solved by using the explicit vector finite-difference scheme.
4. The 2D problem of the system of PDEs with constant coefficients is approximated by the initial value problem for a system of ODEs of the first order.
5. Such a procedure allows us to obtain a simple engineering algorithm for solving mass transfer equations for different substances in layered domain.
6. The results of the numerical experiments give us some new physical conclusions about the drying and moister processes in porous material.

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