Proceedings of ALGORITMY 2005
pp. 53–63

THE SOLUTION OF COUPLED HEAT AND MOISTURE DIFFUSION WITH SORPTION FOR TEXTILES *

DALIBOR FRYDRYCH AND PETR RALEK †

Abstract. In this paper, a numerical mathematical model, which deals with the water vapor sorption mechanisms in fabric, is developed. The model describes and predicts the coupled heat and moisture transport in textile materials.

Since the flow rate of moisture diffusing through clothing textiles is too small to be measured directly, the measurement is usually indirect and the interaction between thermal and moisture transport is not considered. In this study, a mathematical model was introduced to describe the moisture migration and thermal transport through porous textiles in order to evaluate the thermal clothing comfort and the interaction between heat and moisture transportation.

The model is based on the energy and moisture conservation equations during the transportation. For numerical solution, the finite elements method is used. The results are enclosed at the end.

Key words. FEM, unsteady heat flow, unsteady moisture flow, diffusion flow, porous textiles

AMS subject classifications. 35J60, 58J35, 80A20

The Solution of Coupled Heat and Moisture Diffusion with Sorption for Textiles

1. Introduction. The mathematical model is introduced in this study to describe the moisture migration and thermal transport through porous textiles in order to evaluate the thermal clothing comfort and the interaction between heat and moisture transportation.

Comparing to the others, mostly one–dimensional models, our model goes much further and takes the structure of the textile fabric into account. It allows the study of the influence between the textile fabric structure and the thermal closing comfort and gives new possibilities for the design process of new textiles.

2. Problem formulation. Heat and mass transportation parameters and the distribution of moisture and temperature within porous textiles are based on the energy and moisture conservation equations during the transportation.

The transfer is described by partial differential equations [1], [3]

$$c_{v(T,C_a,C_f)}\frac{\partial T}{\partial t} - \lambda_{(T,C_a,C_f)}\frac{\partial C_f}{\partial t} = \nabla.\left(K_{(T,C_a,C_f)}\nabla T\right), \tag{2.1}$$

$$\epsilon\frac{\partial C_a}{\partial t} + (1-\epsilon)\frac{\partial C_f}{\partial t} = \nabla.\left(D_{a(T,C_a,C_f)}\frac{\epsilon}{\tau}\nabla C_a\right), \tag{2.2}$$

$$\frac{1}{\epsilon}\frac{\partial C_f}{\partial t} = \left(\frac{C_a}{C_a^{100}} - \frac{C_f}{C_f^{100}}\right)\gamma_{(T,C_a,C_f)}, \tag{2.3}$$

where are: T temperature, C_a water vapor concentration in air, C_f water vapor concentration in fiber, t time, c_v volumetric heat capacity, λ heat of sorption or adsorption

* This work was supported by Czech Ministry of Education under project code MSM 24220001.

†Department of Modelling of Processes, Faculty of Mechatronics and Interdisciplinary Engineering Studies, Technical University of Liberec, Liberec, Czech Republic (dalibor.frydrych@vslib.cz,petr.ralek@vslib.cz).

of water vapor by fiber (it gives information on interaction forces between the water vapour molecules and the sorbent surface–binding energy), K thermal conductivity, ϵ porosity of fiber, D_a diffusion coefficient of water vapor in air, τ effective tortuosity (it is related to the hindrance imposed on diffusing particle by the fibers), C_a^{100} water vapor concentration for 100% relative humidity (RH) in air, C_f^{100} water vapor concentration for 100% RH in fiber and γ is a general function, for example [1]

$$\gamma = k_1 \left(1 - e^{\left(k_2 \left| \frac{C_a}{C_a^{100}} - \frac{C_f}{C_f^{100}} \right| \right)} \right).$$

The assumption of instantaneous thermal equilibrium between the fibers and the air in the inter–fiber space does not therefore leads to an appreciable error. Equations (2.1) and (2.2) are not linear and they contain three unknowns T, C_a and C_f. The equation (2.3) was derived by Henry [4] to obtain an analytical solution by assuming C_f to be linearly dependent on T and C_a, and also that fibers reach equilibrium with adjacent air instantaneously.

The set of boundary conditions (BC) is added, where Dirichlet BC are

$$\begin{aligned} T(x,t) &= T_D(t) \qquad x \in \Gamma_1 \quad \text{in time} \quad (0, \mathrm{t}^*), \\ C_a(x,t) &= C_D^a(t) \qquad x \in \Gamma_1 \quad \text{in time} \quad (0, \mathrm{t}^*). \end{aligned} \tag{2.4}$$

Neumann BC are

$$\begin{aligned} \frac{\partial T}{\partial x}(x,t).\mathbf{n} &= \alpha(t), \qquad x \in \Gamma_2 \quad \text{in time} \quad (0, \mathrm{t}^*), \\ \frac{\partial C_a}{\partial x}(x,t).\mathbf{n} &= \beta(t), \qquad x \in \Gamma_2 \quad \text{in time} \quad (0, \mathrm{t}^*). \end{aligned} \tag{2.5}$$

Newton BC are

$$\begin{aligned} \frac{\partial T}{\partial x}.\mathbf{n} + \sigma_T(t)(T - T_D(t)) &= 0 \qquad \sigma_T(t) > 0, \quad x \in \Gamma_3 \quad \text{in time} \quad (0, \mathrm{t}^*), \\ \frac{\partial C_a}{\partial x}.\mathbf{n} + \sigma_{C_a}(t)(C_a - C_D^a(t)) &= 0 \qquad \sigma_{C_a}(t) > 0, \quad x \in \Gamma_3 \quad \text{in time} \quad (0, \mathrm{t}^*). \end{aligned} \tag{2.6}$$

For initial conditions (IC) the constant functions [2] are usually chosen

$$\begin{aligned} T(x,0) &= T_D \qquad \text{for} \qquad x \in \Omega, \\ C_a(x,0) &= C_D^a \qquad \text{for} \qquad x \in \Omega, \\ C_f(x,0) &= C_D^f \qquad \text{for} \qquad x \in \Omega. \end{aligned} \tag{2.7}$$

2.1. Weak formulation. To use the finite element method, the weak formulation has to be derived. We discretize the problem in the space variable $\mathbf{x} = \{x, y, z\}$. Let be $H_0(\Omega) = \{f \in W_2^1(\Omega),\ f|_\Gamma = 0\}$ the space of testing functions. Further, we denote the scalar products as $(\varphi, \psi) = \int_\Omega \varphi\psi d\Omega$, $\langle \varphi, \psi \rangle = \int_\Gamma \varphi\psi d\Gamma$. We multiply equations (2.1), (2.2) and (2.3) by testing function $w \in H_0(\Omega)$ and integrate them over Ω. Green formula and substitution of boundary conditions gives integral identities

$$c_v \left(\frac{\partial T}{\partial t}, w \right) - \lambda \left(\frac{\partial C_f}{\partial t}, w \right) = \left\langle K \nabla T.\mathbf{n}, w \right\rangle - (K \nabla T, \nabla w),$$

$$\epsilon\left(\frac{\partial C_a}{\partial t}, w\right) + (1-\epsilon)\left(\frac{\partial C_f}{\partial t}, w\right) = \left\langle \frac{\epsilon}{\tau} D_a \nabla C_a.\mathbf{n}, w\right\rangle - \left(\frac{\epsilon}{\tau} D_a \nabla C_a, \nabla w\right), \tag{2.8}$$
$$\frac{1}{\epsilon}\left(\frac{\partial C_f}{\partial t}, w\right) = \left(\frac{\gamma}{C_a^{100}} C_a, w\right) - \left(\frac{\gamma}{C_f^{100}} C_f, w\right).$$

We solve the problem in time interval $I = \langle 0, t^* \rangle$. Let us denote $T^*, C_a^*, C_f^* \subset AC(I, W_2^1(\Omega))$ be the function fulfilling the Dirichlet BC (2.4). Let

$$T(x,t) = T^*(x,t) + T_0(x,t),$$
$$C_a(x,t) = C_a^*(x,t) + C_{a0}(x,t),$$
$$C_f(x,t) = C_f^*(x,t) + C_{f0}(x,t),$$

where $T_0, C_{a0}, C_{f0} \in AC(I, H_0(\Omega))$. Then functions T, C_a, C_f are the weak solution of (2.1), (2.2) and (2.3) with boundary conditions (2.4)-(2.6) and initial conditions (2.7) in time interval I, if they fulfill the identities (2.8) for arbitrary $w \in H_0(\Omega)$. Existence of integrals in (2.8) is allowed by finiteness of functions ϵ, τ, D_a, K a γ.

2.2. Spatial discretization. For spatial discretization, we use tetrahedrons (see Fig. 2.1) with linear base functions. Area Ω is then approximated by the set Ω^h,

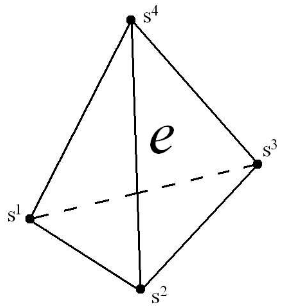

FIG. 2.1. *Element of discretization*

$$\Omega^h = \bigcup_{e \in E^h} e,$$

where E^h is the set of all discretization nodes. On every simplex e with nodes (s^1, s^2, s^3, s^4), four base functions are established, $w_i = \alpha_0^i + \alpha_1^i x_1 + \alpha_2^i x_2 + \alpha_3^i x_3$, $i = 1, 2, 3, 4$. They fulfill the condition $w_i(s^j) = \delta_{ij}$. We look for approximation of weak solution in the form (r is number of nodes)

$$T^h(\mathbf{x},t) = \sum_{i=1}^{r} T^i(t) w_i(\mathbf{x}),$$
$$C_a^h(\mathbf{x},t) = \sum_{i=1}^{r} C_a^i(t) w_i(\mathbf{x}), \tag{2.9}$$
$$C_f^h(\mathbf{x},t) = \sum_{i=1}^{r} C_f^i(t) w_i(\mathbf{x}).$$

Coefficients $T^i(t)$, $C_a^i(t)$, $C_f^i(t)$ are values of unknowns at the nodes of discretization in time t. We substitute approximations (2.9) into identities(2.8) and ask for their fulfilling for all base functions $w_j,\ j \in \hat{r}$. System of ordinary differential equations results, having the block structure

(2.10)

$$\begin{pmatrix} \mathbb{B}_T & 0 & \mathbb{C}_T \\ 0 & \mathbb{B}_{C_a} & \mathbb{C}_{Ca} \\ 0 & 0 & \mathbb{B}_{C_f} \end{pmatrix} \frac{d}{dt} \begin{pmatrix} \mathrm{T} \\ \mathrm{C}_a \\ \mathrm{C}_f \end{pmatrix} + \begin{pmatrix} \mathbb{A}_T & 0 & 0 \\ 0 & \mathbb{A}_{C_a} & 0 \\ 0 & \mathbb{C}_{C_f} & \mathbb{A}_{C_f} \end{pmatrix} \begin{pmatrix} \mathrm{T} \\ \mathrm{C}_a \\ \mathrm{C}_f \end{pmatrix} = \begin{pmatrix} \mathrm{R}_T \\ \mathrm{R}_{C_a} \\ \mathrm{R}_{C_f} \end{pmatrix},$$

where

$$[\mathbb{A}_T]_{i,j} = K(\nabla w_i, \nabla w_j), [\mathbb{A}_{C_a}]_{i,j} = \frac{D_a \epsilon}{\tau}(\nabla w_i, \nabla w_j), [\mathbb{A}_{C_f}]_{i,j} = \frac{\gamma}{C_f^{100}}(w_i, w_j),$$

$$[\mathbb{B}_T]_{i,j} = c_v(w_i, w_j), \quad [\mathbb{B}_{C_a}]_{i,j} = \epsilon(w_i, w_j), \quad [\mathbb{B}_{C_f}]_{i,j} = \frac{1}{\epsilon}(w_i, w_j),$$

$$[\mathbb{C}_T]_{i,j} = \lambda(w_i, w_j),\ [\mathbb{C}_{C_a}]_{i,j} = (1-\epsilon)(w_i, w_j),\ [\mathbb{C}_{C_f}]_{i,j} = -\frac{\gamma}{C_a^{100}}(w_i, w_j)$$

$$[\mathrm{R}_T]_i = \frac{D_a \epsilon}{\tau}\langle \beta, w_i \rangle, \quad [\mathrm{R}_{C_a}]_i = K\langle \alpha, w_i \rangle, \quad [\mathrm{R}_{C_f}]_i = 0,$$

$$[\mathrm{T}]_i = T^i(t), \quad [\mathrm{C_a}]_i = C_a^i(t), \quad [\mathrm{C_f}]_i = C_f^i(t).$$

Values of functions D_a, K, γ in given time are chosen to be piecewise constant on each element (in the manner described further). Values of functions ϵ, τ are also chosen to be piecewise constant on each element, but as material characteristic, independent on time.

3. Numerical model. System (2.10) with initial conditions (2.7) can be solved e.g. by the Euler method. Its advantage is, that it can be used for case, when the system has coefficients depending on unknown quantities ($D_a,\ K,\ \gamma$).

3.1. Time discretization. We use the implicit scheme for approximation of time derivatives,

$$\left.\frac{\partial f}{\partial t}\right|_{t=n} \equiv \frac{f^{n+1} - f^n}{\Delta t},$$

which provides sufficient numerical stability. Let us rewrite the system (2.10) more simply,

$$\mathbb{D}\dot{\mathrm{X}} + \tilde{\mathbb{D}}\mathrm{X} = \mathrm{R},$$

where

$$\mathbb{D} = \begin{pmatrix} \mathbb{B}_T & 0 & \mathbb{C}_T \\ 0 & \mathbb{B}_{C_a} & \mathbb{C}_{C_a} \\ 0 & 0 & \mathbb{B}_{C_f} \end{pmatrix},\ \tilde{\mathbb{D}} = \begin{pmatrix} \mathbb{A}_T & 0 & 0 \\ 0 & \mathbb{A}_{C_a} & 0 \\ 0 & \mathbb{C}_{C_f} & \mathbb{A}_{C_f} \end{pmatrix}$$

$$\mathrm{X} = \begin{pmatrix} \mathrm{T} \\ \mathrm{C}_a \\ \mathrm{C}_f \end{pmatrix},\ \mathrm{R} = \begin{pmatrix} \mathrm{R}_T \\ \mathrm{R}_{C_a} \\ 0 \end{pmatrix}.$$

Values $D_a,\ K,\ \gamma$ in n-th time step were implicitly chosen by substituting the guess $\hat{\mathrm{X}}^{(n+1)}$ in time step $(n+1)$. Matrix $\tilde{\mathbb{D}}$ and right hand side R are time-dependent, more accurately, they depend on values $D_a,\ K,\ \gamma$, which consist in X. For n-th time step, they look

$$\tilde{\mathbb{D}}^{(n)} = \tilde{\mathbb{D}}(\hat{\mathrm{X}}^{(n+1)}),\ \mathrm{R}^{(n)} = \mathrm{R}(\hat{\mathrm{X}}^{(n+1)}).$$

Consequently, the problem

$$\mathbb{D}\,\frac{\mathrm{X}^{(\mathrm{n+1})} - \mathrm{X}^{(\mathrm{n})}}{\Delta t} + \tilde{\mathbb{D}}^{(n)}\mathrm{X}^{(\mathrm{n+1})} = \mathrm{R}^{(n)},$$

was solved and the variation between the solution $X^{(n+1)}$ and the guess $\hat{\mathrm{X}}^{(n+1)}$ was watched. For the large variation, the solution $X^{(n+1)}$ was used as new estimate $\hat{\mathrm{X}}^{(n+1)}$ (for first iteration we used $\hat{\mathrm{X}}^{(n+1)} \equiv \mathrm{X}^{(n)}$). This process was repeated several times and until we got small variation. Then the new initial problem for time step $(n+2)$ was solved.

In particular iteration in n^{th} time step the linear system is solved,

$$(\mathbb{D} + \Delta t\tilde{\mathbb{D}}^{(n)})\mathrm{X}^{(n+1)} = \mathrm{R}^{(n)}\Delta t + \mathbb{D}\mathrm{X}^{(n)}.$$

If we denote

$$\mathrm{R}^{(n)}\Delta t + \mathbb{D}\mathrm{X}^{(n)} = \tilde{\mathrm{R}}^{(n)},$$

the linear system can be written in block structure,

$$\begin{pmatrix} \mathbb{B}_T + \Delta t\mathbb{A}_T^{(n)} & 0 & \mathbb{C}_T \\ 0 & \mathbb{B}_{C_a} + \Delta t\mathbb{A}_{C_a}^{(n)} & \mathbb{C}_{C_a} \\ 0 & \Delta t\mathbb{C}_{C_f}^{(n)} & \mathbb{B}_{C_f} + \Delta t\mathbb{A}_{C_f}^{(n)} \end{pmatrix} \begin{pmatrix} \mathrm{T}^{(\mathrm{n+1})} \\ \mathrm{C}_a^{(n+1)} \\ \mathrm{C}_f^{(n+1)} \end{pmatrix} = \tilde{\mathrm{R}}^{(n)}.$$

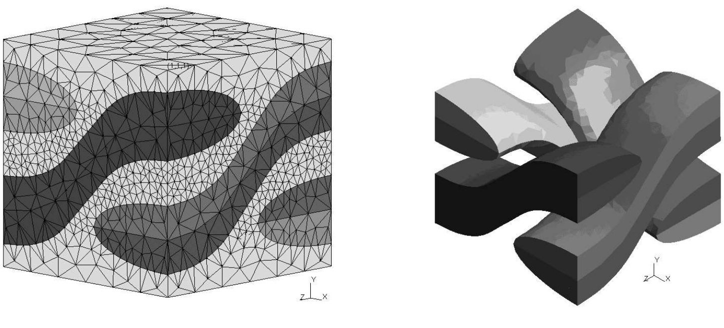

FIG. 3.1. *Full mesh and mesh without air elements*

4. Discussion on the results. For qualitative examination of clothing comfort, the process of the "dressing–up", was chosen. Due to the limited space of the article, we don't present here all results, which describe the heat and moisture penetration in the textile, but only the heat field and heat flow field.

From the textile fabric sample, the smallest volume, which describes its geometrical structure, is chosen. Textiles are usually strong surface structures. Therefore, we can use symmetry (see Fig. 3.1) for the process of heat and moisture transport. Results found on the reference volume form the basis for the models, describing the global behavior of textiles.

4.1. Description of the modelled process. At the beginning, the textile fabric is placed in environment with temperature $T = 20°C$ and relative humidity (RH) $C_a = 50\%$. These values are the initial values of the model (see equation (2.7)). The process of "dressing–up" is performed by the change of boundary condition on the above (inside) boundary. From the point of view of control theory, it is the response to the unit jump. Textile fabric lays free on the human body with temperature $T = 36°C$ and relative humidity (RH) $C_a = 97\%$.

The results, describing arising process, are given on the pictures Fig. 5.1, Fig. 5.2, Fig. 5.3 and Fig. 5.4. Pictures in the left column (sample No. 1) are results for the textile fabric, which absorbs moisture, but does not produce heat of sorption. In the right column (sample No. 2), there are results for the textile fabric with same geometrical characteristics, where absorbing of moisture generates the heat of sorption. The typical material with this behavior is sheep wool. For better comparison, sample No. 1 is also made from sheep wool, but its heat sorption parameter was set zero. Due to the progressive moisture transport in time, the temperature of the sample No. 2 increases. The generated heat of sorption gives it.

After the transient performances, temperature and heat flow stabilize (this stabilization has asymptotic behavior in time). Temperature and the heat flow are the same for both samples (these results are not interesting for us and are not presented here). For both surfaces, the sums of heat flows are computed. From these values and from the progression of heat flow, the clothing comforts of the textile fabrics can be determined. The clothing comfort is subjective parameter, which describes the feelings of human body after dressing the textile fabric - how long persist the uncomfortable feelings (feelings of cold) and how strong they are.

It seems to be very interesting, but difficult problem to set some simple criterion of textile fabric scaling according to the computed parameters. Naturally, the criterion should be to minimize some functional, but the creation of this functional will be difficult (many attributes of textile fabric are subjective).

5. Conclusion. In the paper, the model for solving the problem of coupled heat and moisture diffusion with sorption in textile fabric is introduced. The model works in the area of woven fabrics, knitted fabrics or non-woven fabrics. The fabrics can be non-absorbing (polypropylene) or absorbing (wool) - in this case heat of sorption or adsorption of water vapor can be taken into account.

Model parameters - volumetric heat capacity, thermal conductivity and heat of sorption or adsorption of water vapor are assumed to be nonlinear functions, as well as the relationship describing the rate of water content change in the fibers.

The results from the model allow textile designers to have new insight in mechanism of heat and moisture transport in textile fabrics. The results can be applied in the effective, cheap and fast designing process of new textile fabrics with better customer characteristics.

REFERENCES

[1] Li Y., Luo Z., *An Improved Mathematical Simulation of the Coupled Diffusion of Moisture and Heat in Wool Fabric*, Textile Research Journal, no. 69(10), p. 760 - 768, 1999

[2] Fan J., Wen X., *Heat and Moisture Transfer Through Fibrous Insulation with Phase Change and Mobile Condensates*, HEFAT2000, 1^{st} International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics, 8. - 10. April 2002, South Africa

[3] Li Y., Holcombe B. V., *A Two-Stage Sorption Model of the Coupled Diffusion of Moisture and Heat in Wool Fabrics*, Textile fabricResearch Journal, no. 62(4), p. 211 - 217, 1992

[4] Henry P. S. H., *The Diffusion of Moisture and Heat Through Textiles*, Discuss. Farad. Soc. 3, p. 243 - 257, 1948

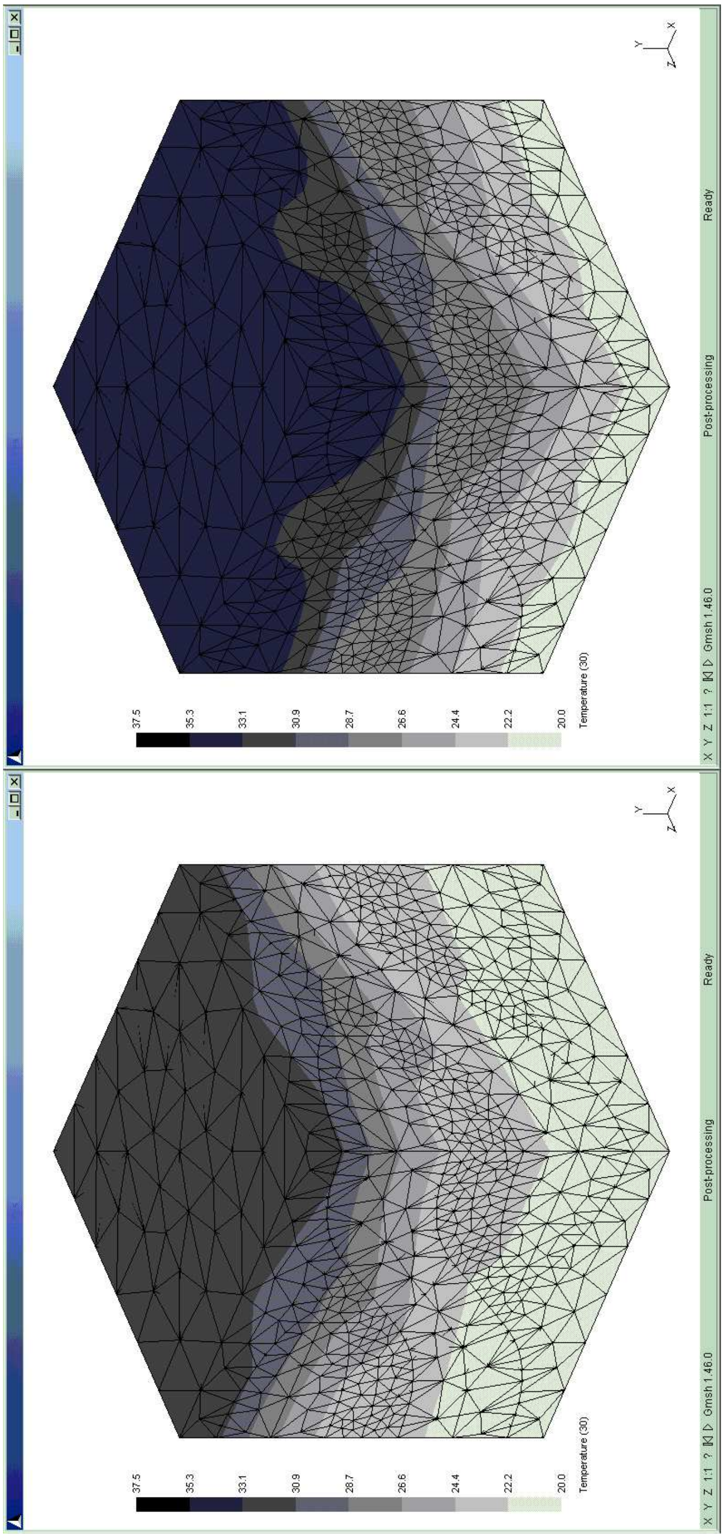

FIG. 5.1. *Temperature in the textiles (woven fabric) at time* $t = 30s$. *Sample No.1. (left/lower column) without heat of sorption; sample No.2. (right/upper column) with heat of sorption.*

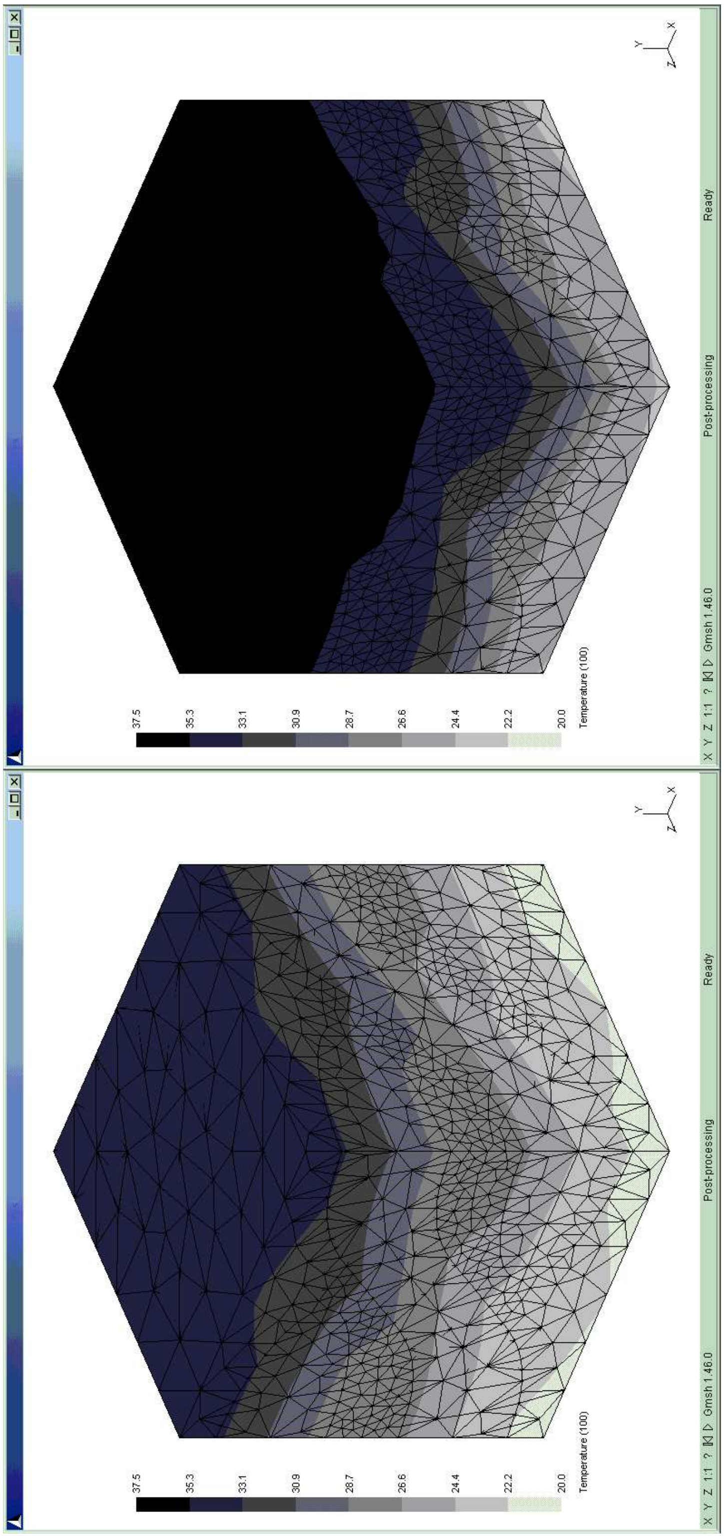

FIG. 5.2. *Temperature in the textiles (woven fabric) at time* $t = 100s$. *Sample No.1. (left/lower column) without heat of sorption; sample No.2. (right/upper column) with heat of sorption.*

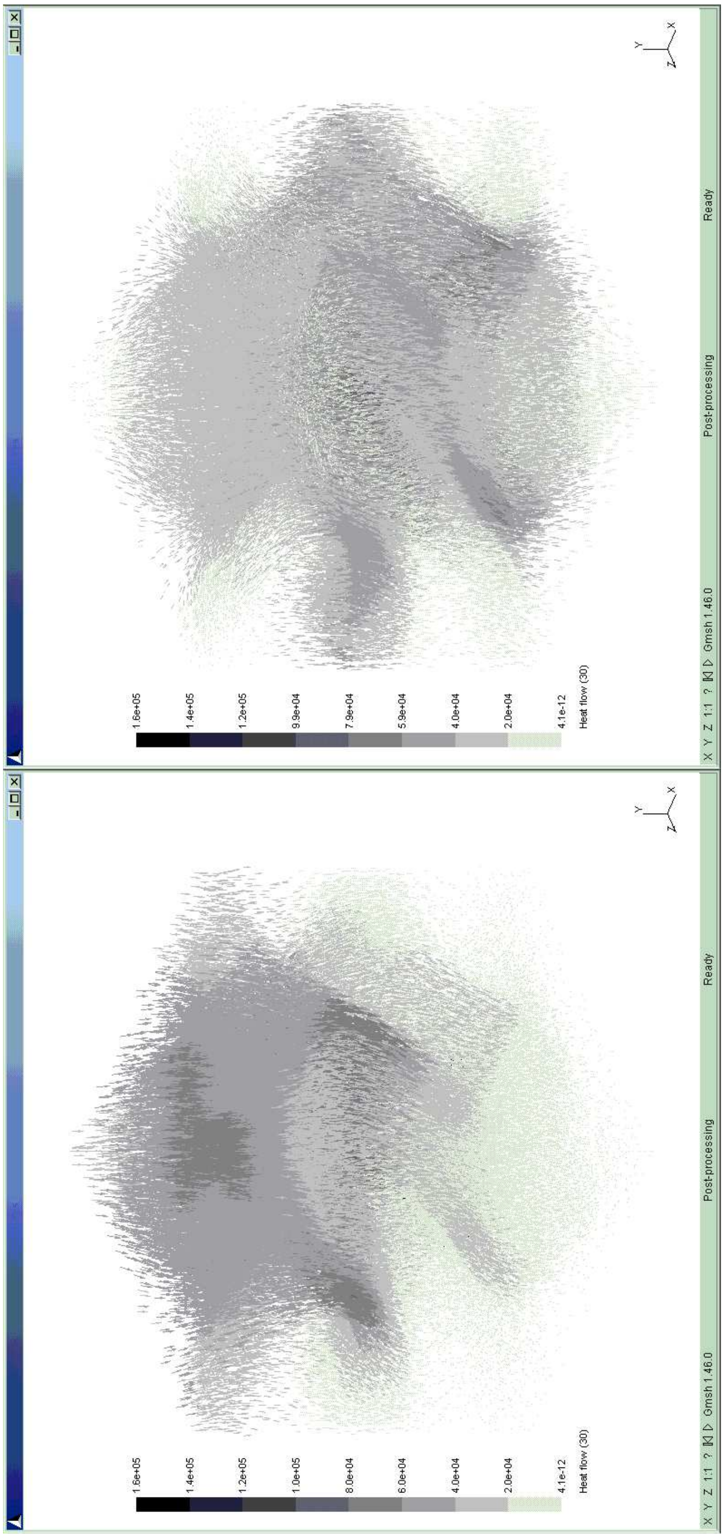

FIG. 5.3. *Heat flow in the textitiles (woven fabric) at time $t = 30s$. Sample No.1. (left/lower column) without heat of sorption; sample No.2. (right/upper column) with heat of sorption.*

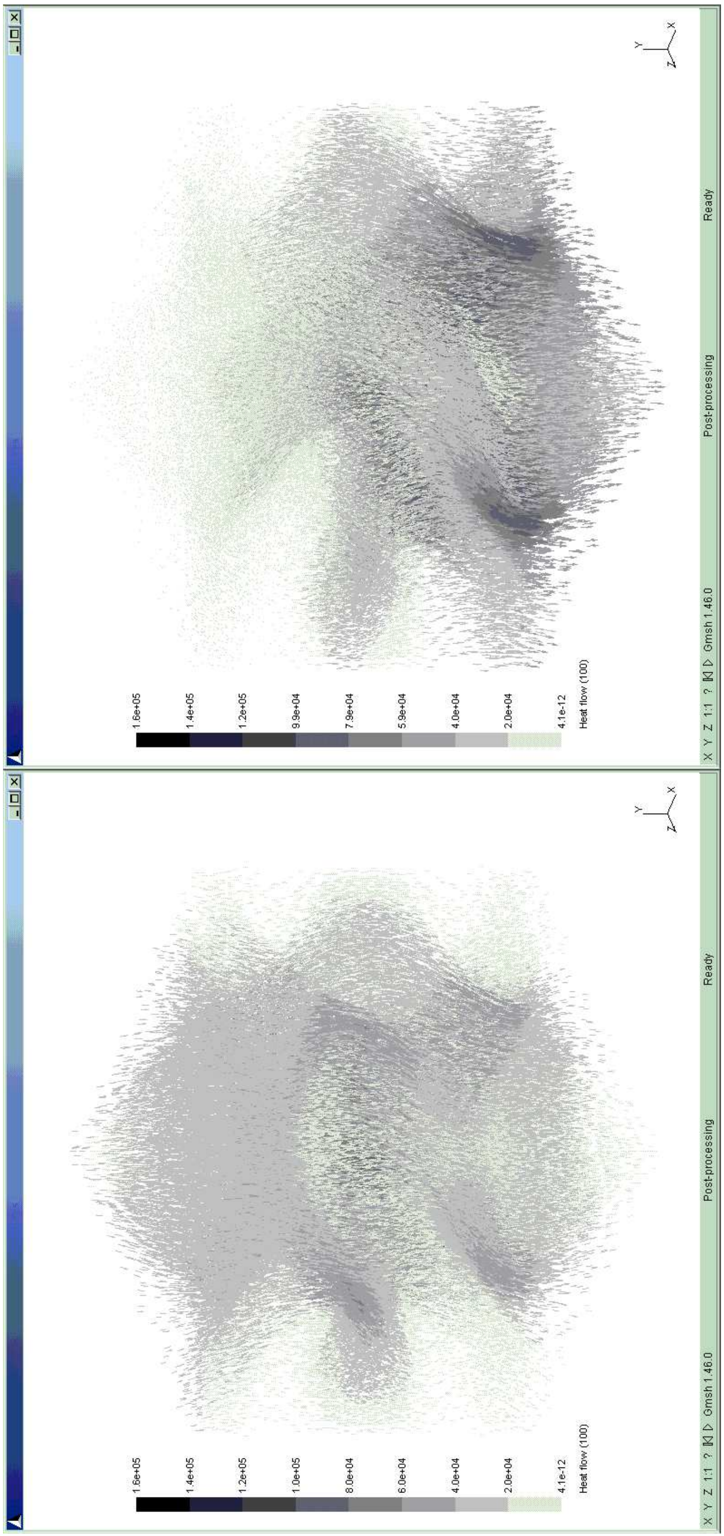

FIG. 5.4. *Heat flow in the textitiles (woven fabric) at time* $t = 100s$. *Sample No.1. (left/lower column) without heat of sorption; sample No.2. (right/upper column) with heat of sorption.*