Nanofiber textiles –problem of FEM modelling the coupled heat and moisture transfer

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Abstract: - Nanofiber technology is an important branch of the growing discipline - nanotechnology. Nanofiber textiles are finding increasing number of applications in filtration industry, particularly in processes involving remediation technologies. Materials in nanofiber form do not only lead to superior functions due to the nano-effect, but also provide a means to deliver additional qualities to higher order structures. Model described in this article was developed to solve tasks of coupled heat and moisture transfer. By this model, can be tested the influence of different parameters (material of fibers, design of fiber structure) on the textile performance and get a lot of information without producing the real textile.

Key-Words: - FEM, unsteady heat flow, unsteady moisture flow, nanofiber textiles
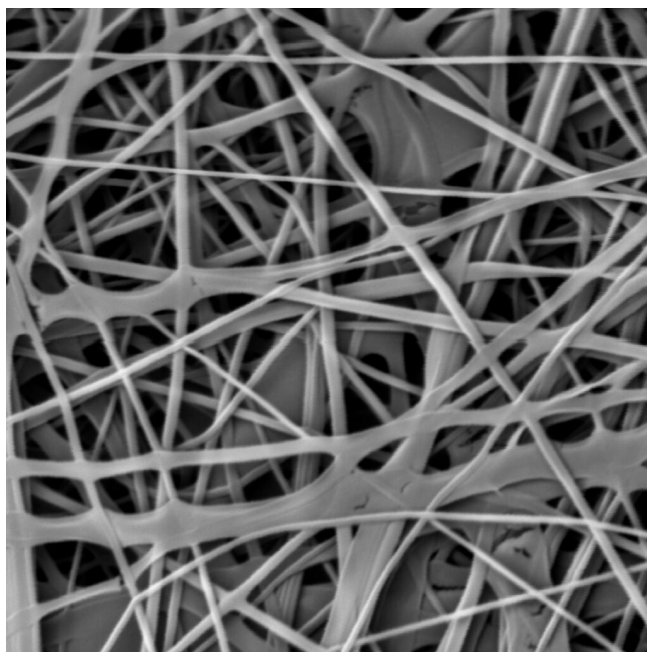
1 Introduction

SEM MAG: 20.00 kx   DET: BE Detector
HV: 30.0 kV   DATE: 04/13/04   5 µm   Vega ©Tescan / TU Liberec
Figure 1 Nanofiber structure
The authors thank to colleagues from Department of Nonwoven Textiles at Technical University of Liberec for permit to published this picture

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

$$c_v(T,C_a,C_f)\frac{\partial T}{\partial t} - \lambda(T,C_a,C_f)\frac{\partial C_f}{\partial t} = \nabla.(K(T,C_a,C_f)\nabla T)$$

$$\varepsilon\frac{\partial C_a}{\partial t} + (1-\varepsilon)\frac{\partial C_f}{\partial t} = \nabla.(D_a(T,C_a,C_f)\frac{\varepsilon}{\tau}\nabla T)$$

$$\frac{1}{\varepsilon}\frac{\partial C_f}{\partial t} = \left(\frac{C_a}{C_a^{100}} + \frac{C_f}{C_f^{100}}\right)\gamma(T,C_a,C_f) \tag{1}$$

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 of water vapor by fiber (it gives information on interaction forces between the water vapor 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^{100}_a water vapor concentration for 100% relative humidity (RH) in air, C^{100}_f water vapor concentration for 100% RH in fiber and γ is a general function, for example [4]

$$\gamma = k_1\left(1 - e^{\left(k_2\left|\frac{C_a}{C^{100}_a} - \frac{C_f}{C^{100}_f}\right|\right)}\right). \qquad (2)$$

The assumption of instantaneous thermal equilibrium between the fibers and the air in the inter-fiber space does not therefore lead to a significant error. Equations (1a) and (1b) are not linear and they contain three unknowns T, C_a and C_f. The equation (1c) was derived by Henry [5] 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

$$\begin{aligned} T(\vec{x},t) &= T_D(t) \\ C_a(\vec{x},t) &= C^a_D(t) \end{aligned} \qquad \vec{x} \in \Gamma_1 \text{ in time } (0,t^*), \quad (3)$$

Neumann BC are

$$\begin{aligned} \frac{\partial T}{\partial x}(\vec{x},t).n &= \alpha(t) \\ \frac{\partial C_a}{\partial x}(\vec{x},t).\vec{n} &= \beta(t) \end{aligned} \qquad \vec{x} \in \Gamma_2 \text{ in time } (0,t^*), \quad (4)$$

Newton BC are

$$\begin{aligned} \frac{\partial T}{\partial \vec{x}}(\vec{x},t).n + \sigma_T(t)(T - T_D(t)) &= 0 & \sigma_T(t) > 0 \\ \frac{\partial C_a}{\partial \vec{x}}(\vec{x},t).n + \sigma_{C_a}(t)(C_a - C^a_D(t)) &= 0 & \sigma_{C_a}(t) > 0 \end{aligned} \qquad (5)$$
$$\vec{x} \in \Gamma_3 \text{ in time } (0,t^*),$$

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

$$\begin{aligned} T(\vec{x},0) &= T_0 \\ C_a(\vec{x},0) &= C^a_0 \quad \vec{x} \in \Omega \quad . \\ C_f(\vec{x},0) &= C^f_0 \end{aligned} \qquad (6)$$

2.1 Weak formulation

To use the finite element method, the weak formulation has to be derived. The problem is discreted in the space variable $\boldsymbol{x} = \{x,y,z\}$. Let be $H_0(\Omega) = \{f \in W^1_2(\Omega), f|_\Gamma = 0\}$ the space of testing functions. Further, is denoted the scalar products as $(\varphi,\psi) = \int_\Omega \varphi\psi d\Omega$, $\langle\varphi,\psi\rangle = \int_\Gamma \varphi\psi d\Gamma$.

Equations (1a), (1b) and (1c) are multiplied by testing function $w \in H_0(\Omega)$, integrated over Ω. Then a Green formula is used and substitution of boundary conditions gives integral identities

$$c_v\left(\frac{\partial T}{\partial t},w\right) - \lambda\left(\frac{\partial C_f}{\partial t},w\right) = \langle K\nabla T.n, w\rangle - (K\nabla T, \nabla w)$$
$$\varepsilon\left(\frac{\partial C_a}{\partial t},w\right) + (1-\varepsilon)\left(\frac{\partial C_f}{\partial t},w\right) = \left\langle\frac{\varepsilon}{\tau}D_a\nabla C_a.n, w\right\rangle - \left(\frac{\varepsilon}{\tau}D_a\nabla C_a, \nabla w\right) \qquad (7)$$
$$\frac{1}{\varepsilon}\left(\frac{\partial C_f}{\partial t},w\right) = \left(\frac{C_a}{C^{100}_a}\gamma, w\right) - \left(\frac{C_f}{C^{100}_f}\gamma, w\right)$$

The problem is solved in time interval $I = <0, t^*>$. Then $T^*, C^*_a, C^*_f \subset AC(I, W^1_2(\Omega))$ is denoted as the function fulfilling the Dirichlet BC (3). Let

$$\begin{aligned} T(\vec{x},t) &= T^*(\vec{x},t) + T_0(\vec{x},t), \\ C_a(\vec{x},t) &= C^*_a(\vec{x},t) + C_{a0}(\vec{x},t), \\ C_f(\vec{x},t) &= C^*_f(\vec{x},t) + C_{f0}(\vec{x},t), \end{aligned} \qquad (8)$$

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 (1a), (1b) and (1c) with boundary conditions (3), (4) and (5) and initial conditions (6) in time interval I, if they fulfil the identities (7) for arbitrary $w \in H_0(\Omega)$. Existence of integrals in (7) is allowed by finiteness of functions ε, τ, D_a, K a γ.
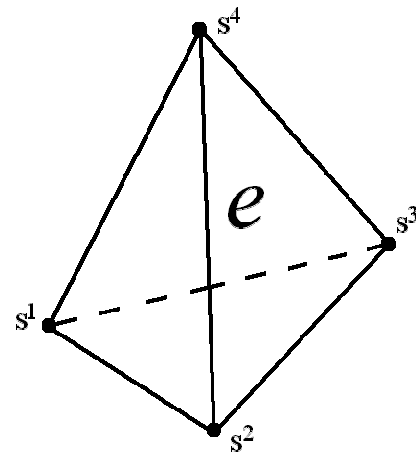

Figure 2 Element of discretization

2.2   Spatial discretization

For spatial discretization the tetrahedrons with linear base functions are used (see figure 2).

Area Ω is then approximated by the set Ω^h,

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

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, $w_i = \alpha^i_0 + \alpha^i_1 x_1 + \alpha^i_2 x_2 + \alpha^i_3 x_3$, $i=1,2,3,4$. They fulfill the condition $w_i(s^j) = \delta_{ij}$. The approximation of weak solution is looked for in the form (r is number of nodes)

$$T^h(\vec{x}, t) = \sum_{i=1}^{r} T^i(\vec{x}, t) w_i(\vec{x}),$$

$$C_a^h(\vec{x}, t) = \sum_{i=1}^{r} C_a^i(\vec{x}, t) w_i(\vec{x}), \qquad (9)$$

$$C_f^h(\vec{x}, t) = \sum_{i=1}^{r} C_f^i(\vec{x}, t) w_i(\vec{x}),$$

Coefficients $T^i(t)$, $C_a^i(t)$, $C_f^i(t)$ are values of unknowns at the nodes of discretization in time t. The approximations (9) are entered into identities (7). Then is searched for their fulfilment for all base functions w_j, $j \in r$. The resulting system of ordinary differential equations has the block structure

$$\begin{pmatrix} \mathbf{B}_T & 0 & \mathbf{C}_T \\ 0 & \mathbf{B}_{C_a} & \mathbf{C}_{C_a} \\ 0 & 0 & \mathbf{B}_{C_f} \end{pmatrix} \frac{d}{dt} \begin{pmatrix} \mathbf{T} \\ \mathbf{C}_a \\ \mathbf{C}_f \end{pmatrix} + \begin{pmatrix} \mathbf{A}_T & 0 & 0 \\ 0 & \mathbf{A}_{C_a} & 0 \\ 0 & \mathbf{C}_{C_f} & \mathbf{A}_{C_f} \end{pmatrix} \begin{pmatrix} \mathbf{T} \\ \mathbf{C}_a \\ \mathbf{C}_f \end{pmatrix} = \begin{pmatrix} \mathbf{R}_T \\ \mathbf{R}_{C_a} \\ \mathbf{R}_{C_f} \end{pmatrix}, \quad (10)$$

where

$$[A_T]_{i,j} = K(\nabla \omega_i, \nabla \omega_j) \quad [A_{C_a}]_{i,j} = \frac{D_a \varepsilon}{\tau}(\nabla \omega_i, \nabla \omega_j) \quad [A_{C_f}]_{i,j} = \frac{\gamma}{C_f^{100}}(\omega_i, \omega_j)$$

$$[B_T]_{i,j} = c_v(\omega_i, \omega_j) \quad [B_{C_a}]_{i,j} = \varepsilon(\omega_i, \omega_j) \quad [B_{C_f}]_{i,j} = \frac{1}{\varepsilon}(\omega_i, \omega_j)$$

$$[C_T]_{i,j} = \lambda(\omega_i, \omega_j) \quad [C_{C_a}]_{i,j} = (1-\varepsilon)(\omega_i, \omega_j) \quad [C_{C_f}]_{i,j} = -\frac{\gamma}{C_a^{100}}(\omega_i, \omega_j)$$

$$[R_T]_i = \frac{D_a \varepsilon}{\tau}(\beta, \nabla \omega_i) \quad [R_{C_a}]_i = K(\alpha, \omega_i) \quad [R_{C_f}]_i = 0$$

$$[T]_i = T^i(t) \quad [C_a]_i = C_a^i(t) \quad [C_f]_i = C_f^i(t)$$

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 (10) with initial conditions (6) 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, γ).

2.1   Time discretization

The implicit scheme for approximation of time derivatives is used,

$$\left. \frac{\partial f}{\partial t} \right|_{t=n} \equiv \frac{f_{n+1} - f_n}{\Delta t} \quad , \qquad (11)$$

This scheme provides sufficient numerical stability. Then the system (10) can be rewriten more simply,

$$\mathbf{D}\dot{\mathbf{X}} + \tilde{\mathbf{D}}\mathbf{X} = \mathbf{R} \quad , \qquad (12)$$

where

$$\mathbf{D} = \begin{pmatrix} \mathbf{B}_T & 0 & \mathbf{C}_T \\ 0 & \mathbf{B}_{C_a} & \mathbf{C}_{C_a} \\ 0 & 0 & \mathbf{B}_{C_f} \end{pmatrix}, \quad \tilde{\mathbf{D}} = \begin{pmatrix} \mathbf{A}_T & 0 & 0 \\ 0 & \mathbf{A}_{C_a} & 0 \\ 0 & \mathbf{C}_{C_f} & \mathbf{A}_{C_f} \end{pmatrix}, \quad (13)$$

$$\mathbf{X} = \begin{pmatrix} \mathbf{T} \\ \mathbf{C}_a \\ \mathbf{C}_f \end{pmatrix} \quad , \qquad \mathbf{R} = \begin{pmatrix} \mathbf{R}_T \\ \mathbf{R}_{C_a} \\ \mathbf{0} \end{pmatrix} \quad . \qquad (14)$$

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

$$\tilde{\mathbf{D}}^{(n)} = \tilde{\mathbf{D}}(\tilde{\mathbf{X}}^{(n+1)}), \quad \mathbf{R}^{(n)} = \mathbf{R}(\tilde{\mathbf{X}}^{(n+1)}) \quad . \qquad (15)$$

Consequently, the problem

$$\mathbf{D} \frac{\mathbf{X}^{(n+1)} - \mathbf{X}^{(n)}}{\Delta t} + \tilde{\mathbf{D}}^{(n)} \mathbf{X}^{(n+1)} = \mathbf{R}^{(n)} \quad , \qquad (16)$$

was solved and the variation between the solution $\mathbf{X}^{n+1}$ and the guess $\tilde{\mathbf{X}}^{n+1}$ was watched. For the large variation, the solution $\mathbf{X}^{n+1}$ was used as new estimate $\tilde{\mathbf{X}}^{n+1}$ (for first iteration is used $\tilde{\mathbf{X}}^{n+1} \equiv \tilde{\mathbf{X}}^n$). This process was repeated several times until only small variation are reached. 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,

$$\left(\mathbf{D} + \Delta t \tilde{\mathbf{D}}^{(n)}\right)\mathbf{X}^{(n+1)} = \mathbf{R}^{(n)}\Delta t + \mathbf{D}\mathbf{X}^{(n)} \quad . \tag{17}$$

If denoted

$$\mathbf{R}^{(n)}\Delta t + \mathbf{D}\mathbf{X}^{(n)} = \tilde{\mathbf{R}}^{(n)} \quad , \tag{18}$$

the linear system can be written in block structure,

$$\begin{pmatrix} \mathbf{B}_T + \Delta t \mathbf{A}_T{}^{(n)} & 0 & \mathbf{C}_T \\ 0 & \mathbf{B}_{C_a} + \Delta t \mathbf{A}_{C_a}{}^{(n)} & \mathbf{C}_{C_a} \\ 0 & \Delta t \mathbf{C}_{C_f}{}^{(n)} & \mathbf{B}_{C_f} + \Delta t \mathbf{A}_{Cf}{}^{(n)} \end{pmatrix}\begin{pmatrix} \mathbf{T}^{(n+1)} \\ \mathbf{C}_a^{(n+1)} \\ \mathbf{C}_f^{(n+1)} \end{pmatrix} = \tilde{\mathbf{R}}^{(n)} \tag{19}$$

3 Tuned Solution of SLE

For solution of nanofiber structures, very small elements for spatial discretization of area Ω (see figures 3 and 4) must be used. This requirement leads to fine computation mesh and to the need of solving the large linear system. Applicability of FEM systems primarily depends on the effectiveness of solution this large set of linear equations (SLE).

This model leads to large, nonsymmetrical, sparse SLE. Solvig of this type of SLE is complicated and very time
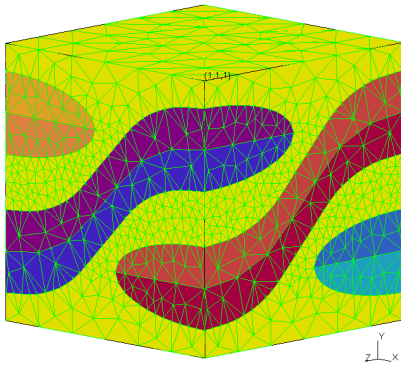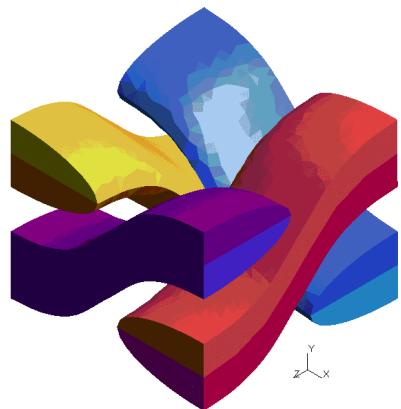

Figure 3 Full mesh

Figure 4 Mesh without air elements

consuming. Any possibility to save the time of solution is useful.

Big change in approach to solve SLE was done by [2]. Application of ideas published in this article allows parallelism, decreases the time required to solve SLE and increases the precision of results. Solution of three smaller tasks is better then solution of the one large.

In the first step, equation (19) is simplified, then blocks of global matrix and vectors of solution and right hand side is relabeled as

$$\begin{pmatrix} \mathbf{A}_1 & 0 & \mathbf{B}_1 \\ 0 & \mathbf{A}_2 & \mathbf{B}_2 \\ 0 & \mathbf{B}_3 & \mathbf{A}_3 \end{pmatrix}\begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \\ \mathbf{X}_3 \end{pmatrix} = \begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \\ \mathbf{R}_3 \end{pmatrix} \quad . \tag{20}$$

Blocks A_1, A_2, A_3, B_1, B_2 and B_3 have the same structure, the same positions of nonzero items. Blocks A_1, A_2, A_3 are positive definite.

The block X_3 can be formalized from 3rd row and put it to 2nd row. Then is obtained

$$\left(\mathbf{A}_2 - \mathbf{B}_2\mathbf{A}_3^{-1}\mathbf{B}_3\right)\mathbf{X}_2 = \mathbf{R}_2 - \mathbf{B}_2\mathbf{A}_3^{-1}\mathbf{R}_3 \quad . \tag{21}$$

The inversion of matrix $\mathbf{A}_3^{-1}$ can be obtained by Cholesky factorization $\mathbf{A}_3^{-1} = \mathbf{L}_{A_3}^{-T}\mathbf{L}_{A_3}^{-1}$ [3]. Then the equation (21) can be rewriten to the final form,

$$\left(\mathbf{A}_2 - \mathbf{B}_2\mathbf{L}_{A_3}^{-T}\mathbf{L}_{A_3}^{-1}\mathbf{B}_3\right)\mathbf{X}_2 = \mathbf{R}_2 - \mathbf{B}_2\mathbf{L}_{A_3}^{-T}\mathbf{L}_{A_3}^{-1}\mathbf{R}_3 \quad . \tag{22}$$

Parenthesis on the left side is known as the Schur's complement. The Schur's complement is a slightly denser than original blocks. There are more nonzero items and structure of these items is general. The iterative method for solution of the unknown block X_2 is used. Very good results (short time, good stability of solution) were achieved by successive over relaxation method.

Because there is insufficient information about behavior of the product in parenthesis, better method could not be used.
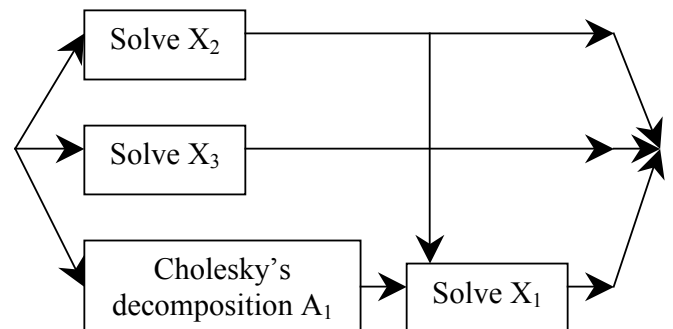

Figure 5 Solution of set of linear equations – schema of splitting of task and distribution of calculation

Concurrently, in the same time, the block X_3 can be solved. The same consecution is used for block X_2 to obtain

$$\left(\mathbf{B}_3 \mathbf{L}_{A_2}^{-T} \mathbf{L}_{A_2}^{-1} \mathbf{B}_2 - \mathbf{A}_3\right)\mathbf{X}_3 = \mathbf{B}_3 \mathbf{L}_{A_2}^{-T} \mathbf{L}_{A_2}^{-1} \mathbf{R}_2 - \mathbf{R}_3 \quad , \quad (23)$$

and the equation is solved by the same sequence as block X_2, where $\mathbf{L}_{A_2}^{-T} \mathbf{L}_{A_2}^{-1} = \mathbf{A}_2^{-1}$.

First row of equation (19) can be modified as

$$\mathbf{X}_1 = \mathbf{L}_{A_1}^{-1} \mathbf{L}_{A_1}^{-T} \left(\mathbf{R}_1 - \mathbf{B}_1 \mathbf{X}_3\right) \quad , \quad\quad (24)$$

where $\mathbf{L}_{A_1}^{-T} \mathbf{L}_{A_1}^{-1} = \mathbf{A}_1^{-1}$.

Equations (22) and (23) can be solved concurrently. Equations (24) depend on variable X_3, but Cholesky factorization of block $\mathbf{A}_1^{-1} = \mathbf{L}_{A_1}^{-T} \mathbf{L}_{A_1}^{-1}$ can be prepared at the same time (with solution of equations (22) and (23)). Then unknown X_1 can be solved by forward and back substitution.

This sequence is shown on the figure 5.

4   Conclusion

In this contribution, the model for solving of the problem of coupled heat and moisture diffusion with sorption in textiles is introduced. Results (see figures 6 to 8) obtained by this model help to understand the processes in textiles.

Special consideration is given to solution of large set of equations. For implementation of numerical model was chosen language JAVA. This project takes advantage of transparent multithreading and easy use of technology RMI – remote method interface – for distribution of the calculations to other computers.

There are areas for further increase of speed in solution of the linear system. Multiplication of matrix can be distributed to more computers. Mentioned algorithms are state-of-the-art.

4   Acknowledgement

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[1] D.Frydrych, P.Ralek: The Solution of Coupled Heat and Moisture Diffusion with Sorption for Textiles, *Algoritmy 2005*, pp. 53-63
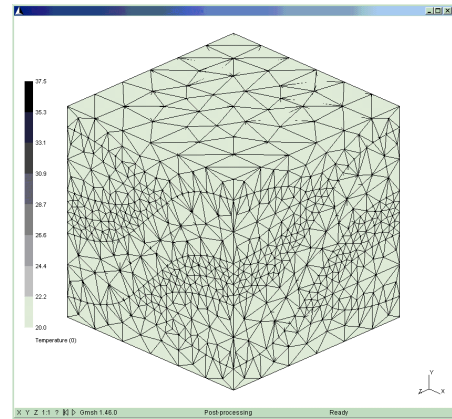

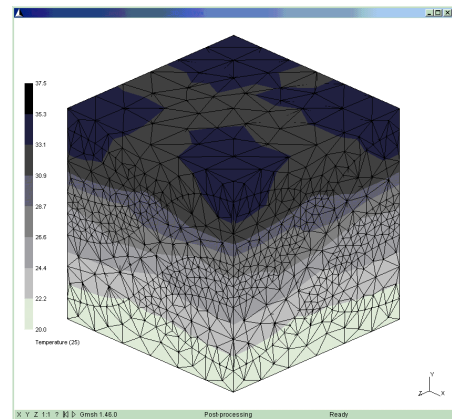Figure 6 Temperature in textiles at time *t = 0* s

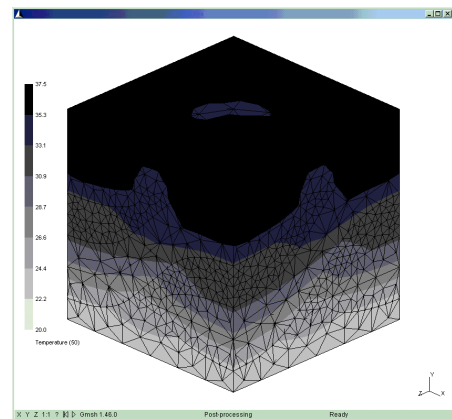Figure 7 Temperature in textiles at time *t = 30* s

Figure 8 Temperature in textiles at time *t = 60* s

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