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Numerical simulation of freezing process using the BEM

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The boundary element method is applied for numerical simulation of the freezing process proceeding in biological tissue under the influence of cylindrical cryoprobe. From the mathematical point of view the problem discussed belongs to the group of moving boundaries ones for which the mushy zone sub-region (intermediate phase) is considered. In this paper the mathematical model of the process is formulated using the fixed domain approach and a parameter called the substitute thermal capacity determines the evolution of latent heat. On a stage of numerical computations the generalized variant of the alternating phase truncation method (APTM) is applied and the basic mathematical model is rebuilt by the introduction of the enthalpy function. The boundary element method together with APTM leads to the simple and effective numerical algorithm because the difficulties connected with the non-linear problem modelling can be omitted. In the final part of the paper the results of computations are shown.

1. Introduction

The applications of cryosurgery take place among others for causing a local necrosis of a tissue, the detachment of the bloodless tissue, the destruction of the cancer cells etc. and these methods of treatment are used in dermatology, gynecology, proctology, oncology and also laryngology. In this paper the problem of numerical modelling of freezing process proceeding in domain of biological tissue under the cylindrical cryoprobe action is considered – Fig. 1. From the mathematical point of view the problem discussed is described by the nonlinear Fourier–Kirchhoff equation [2, 3] in which the additional component called the source function appears. The source function determines the evolution of latent heat. In this paper the diffusion equation is transformed to the form corresponding

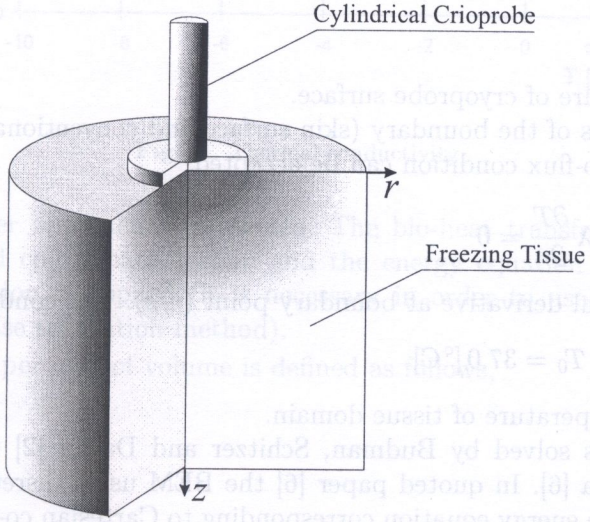

Fig. 1. The domain considered

to one domain method [3, 5, 9]. The basic differential equation is supplemented by assumed boundary and initial conditions. The numerical solution is obtained on the basis of the BEM algorithm for non-steady diffusion problem described in the cylindrical co-ordinate system [1]. In order to take into account the nonlinearities resulting from the temperature-dependent thermophysical parameters of tissue [3], the generalized variant of alternating phase truncation method [7, 8, 10] is applied. This approach requires the 'rebuilding' of the mathematical model to the enthalpy convention. In the final part of the paper the results of numerical simulations are presented and also the more general conclusions are formulated.

2. Governing equations

The freezing process proceeding in domain of biological tissue which can be treated as a binary solution is described by the following energy equation

$$c(T)\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\lambda(T)\frac{\partial T}{\partial r}\right] + \frac{\partial}{\partial z}\left[\lambda(T)\frac{\partial T}{\partial z}\right] + L_V\frac{\partial f_S}{\partial t} \tag{1}$$

where $T = T(r, z, t)$ is the tissue temperature, $c(T)$ is the volumetric specific heat, $\lambda(T)$ is the thermal conductivity, L_V is the latent heat [J/m^3], f_S is the frozen state fraction at the point considered. Assuming the knowledge of the function $f_S = f_S(T)$ in the interval $[T_2, T_1]$ (the border temperatures corresponding to the end and the beginning of freezing process) Eq. (1) can be written in the form

$$\left[c(T) - L_V\frac{\mathrm{d}f_S}{\mathrm{d}T}\right]\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\lambda(T)\frac{\partial T}{\partial r}\right] + \frac{\partial}{\partial z}\left[\lambda(T)\frac{\partial T}{\partial z}\right] \tag{2}$$

or

$$C(T)\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\lambda(T)\frac{\partial T}{\partial r}\right] + \frac{\partial}{\partial z}\left[\lambda(T)\frac{\partial T}{\partial z}\right] \tag{3}$$

where $C(T)$ is the substitute thermal capacity [9]. For 'natural' and frozen sub-regions of tissue, f_S is a constant value (0 or 1) i.e. $\mathrm{d}f_S/\mathrm{d}T = 0$, and Eq. (3) describes the heat transfer process for the whole conventionally homogenous domain.

The functions corresponding to substitute thermal capacity $C(T)$ and thermal conductivity $\lambda(T)$ [3] for the binary solution 24% methyl-cellulose and 76% water which parameters are close to the real parameters of biological tissue are shown in Figs. 2 and 3, respectively. On the contact surface between cryoprobe and skin the 1st type of the boundary condition is assumed, namely

$$(r, z) \in \Gamma_c: \qquad T = T_c \tag{4}$$

where Tc is the temperature of cryoprobe surface.

For the remaining parts of the boundary (skin surface and conventionally assumed limits of the domain considered) the no-flux condition can be accepted

$$(r, z) \in \Gamma_0: \qquad q = -\lambda\frac{\partial T}{\partial n} = 0 \tag{5}$$

where $\partial T/\partial n$ is the normal derivative at boundary point (r, z). The condition

$$t = 0: \qquad T(r, z, 0) = T_0 = 37.0\,[^\circ\mathrm{C}] \tag{6}$$

determines the initial temperature of tissue domain.

A similar problem was solved by Budman, Schitzer and Dayan [2] using the FEM and also by Majchrzak and Ladyga [6]. In quoted paper [6] the BEM using disretization in time has been used, at the same time the energy equation corresponding to Cartesian co-ordinate system has been considered, while the 'cylindrical' component was treated as the additional source function.

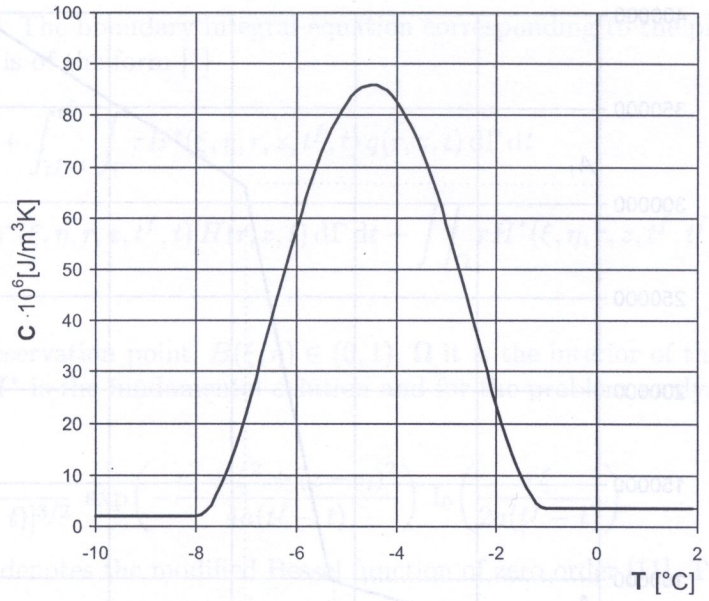

Fig. 2. Substitute thermal capacity

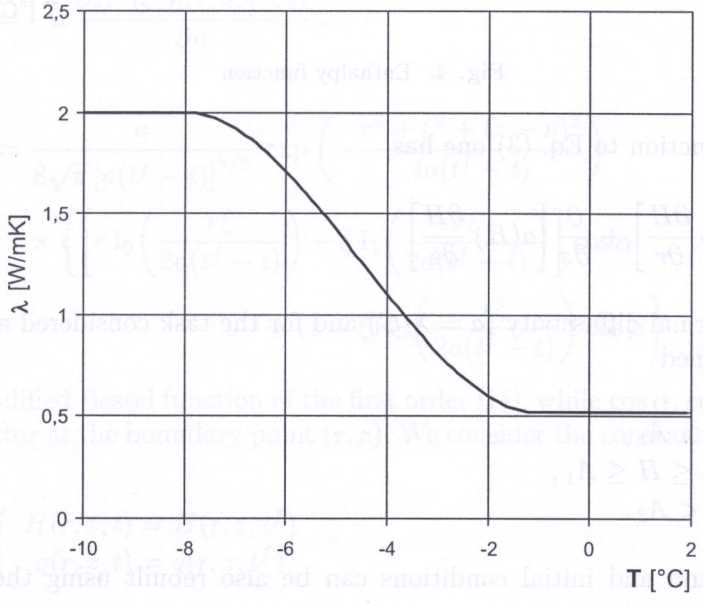

Fig. 3. Thermal conductivity

In this paper the other approach is presented. The bio-heat transfer processes are described directly in the cylindrical co-ordinate system and the energy equation is rebuilt to the form in which the enthalpy function is applied (it is necessary in order to use the numerical procedure called the alternating phase truncation method).

The physical enthalpy per unit of volume is defined as follows,

$$H(T) = \int_{T_r}^{T} C(\mu)\mathrm{d}\mu, \tag{7}$$

where T_r is the arbitrary assumed reference level. The course of enthalpy function is shown in Fig. 4.

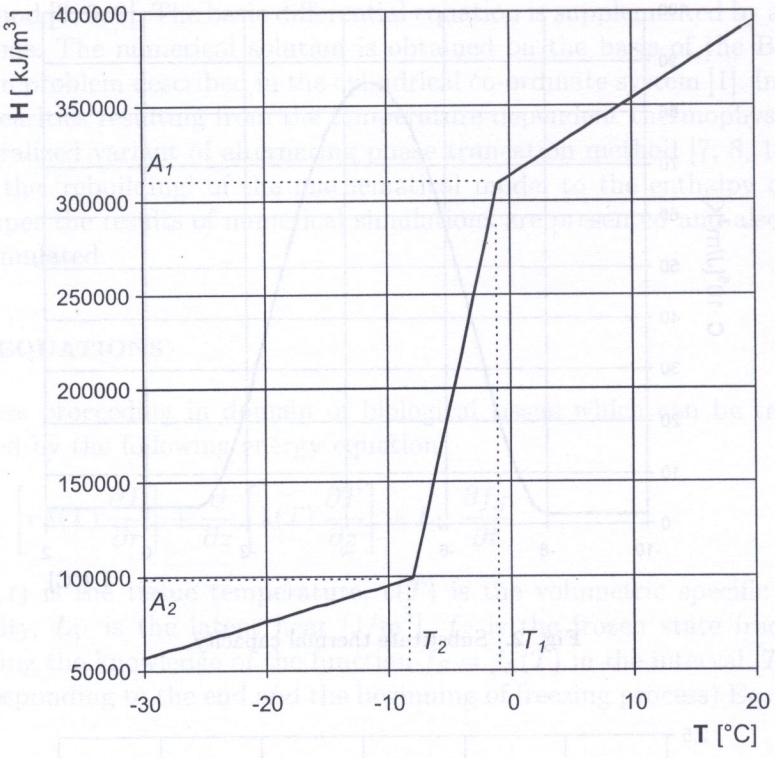

Fig. 4. Enthalpy function

Introducing this function to Eq. (3) one has

$$\frac{\partial H}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[ra(H)\frac{\partial H}{\partial r}\right] + \frac{\partial}{\partial z}\left[a(H)\frac{\partial H}{\partial z}\right] \tag{8}$$

where $a(H)$ is the thermal diffussivity ($a = \lambda/C$) and for the task considered a piece-wise constant function $a(H)$ is assumed

$$a(H) = \begin{cases} a_1\,, & H > A_1\,, \\ a_2\,, & A_2 \le H \le A_1\,, \\ a_3\,, & H < A_2\,. \end{cases} \tag{9}$$

The Dirichlet, Neumann and initial conditions can be also rebuilt using the enthalpy function, namely

$$\begin{cases} (r,z) \in \Gamma_c: & H = H(T_s - wt), \\ (r,z) \in \Gamma_0: & q = -a\dfrac{\partial H}{\partial n} = 0, \\ t = 0: & H = H(T_0). \end{cases} \tag{10}$$

3. Boundary element method for cylindrical domain

In order to construct the BEM algorithm, the time grid

$$0 = t^0 < t^1 < \ldots < t^{f-1} < t^f < \ldots < t^F, \qquad \Delta t = t^f - t^{f-1}, \tag{11}$$

should be introduced. The boundary integral equation corresponding to the problem considered for transition $t^{f-1} \to t^f$ is of the form [1]

$$B(\xi,\eta)H(\xi,\eta,t^f) + \int_{t^{f-1}}^{t^f}\int_\Gamma rH^*(\xi,\eta,r,z,t^f,t)\,q(r,z,t)\,\mathrm{d}\Gamma\,\mathrm{d}t$$
$$= \int_{t^{f-1}}^{t^f}\int_\Gamma rq^*(\xi,\eta,r,z,t^f,t)\,H(r,z,t)\,\mathrm{d}\Gamma\,\mathrm{d}t + \iint_\Omega rH^*(\xi,\eta,r,z,t^f,t^{f-1})\,H(r,z,t^{f-1})\,\mathrm{d}\Omega \tag{12}$$

where (ξ,η) is the observation point, $B(\xi,\eta) \in (0,1)$, Ω it is the interior of the domain considered, $\Gamma = \Gamma_0 \cup \Gamma_c$, while H^* is the fundamental solution and for the problem analyzed it is a function of the form [1, 4]

$$H^* = \frac{1}{4\sqrt{\pi}[a(t^f-t)]^{3/2}}\exp\left(-\frac{r^2+\xi^2+(z-\eta)^2}{4a(t^f-t)}\right)\mathrm{I}_0\left(\frac{r\xi}{2a(t^f-t)}\right) \tag{13}$$

In this formula $\mathrm{I}_0(\cdot)$ denotes the modified Bessel function of zero order [11]. The functions q and q^* in Eq. (12) are equal

$$\begin{aligned} q(r,z,t) &= -a\frac{\partial H(r,z,t)}{\partial n}, \\ q^*(\xi,\eta,r,z,t^f,t) &= -a\frac{\partial H^*(\xi,\eta,r,z,t^f,t)}{\partial n}. \end{aligned} \tag{14}$$

One can find that

$$q^*(\xi,\eta,r,z,t^f,t) = \frac{a}{8\sqrt{\pi}\,[a(t^f-t)]^{5/2}}\exp\left(-\frac{r^2+\xi^2+(z-\eta)^2}{4a(t^f-t)}\right)$$
$$\times\left\{\left[r\,\mathrm{I}_0\left(\frac{r\xi}{2a(t^f-t)}\right) - \xi\,\mathrm{I}_1\left(\frac{r\xi}{2a(t^f-t)}\right)\right]\cos\alpha\right.$$
$$\left. + (z-\xi)\,\mathrm{I}_0\left(\frac{r\xi}{2a(t^f-t)}\right)\cos\beta\right\} \tag{15}$$

where $\mathrm{I}_1(\cdot)$ is the modified Bessel function of the first order [11], while $\cos\alpha$, $\cos\beta$ are the directional cosines of normal vector at the boundary point (r,z). We consider the constant elements with respect to time, namely

$$t \in [t^{f-1},t^f]: \quad \begin{cases} H(r,z,t) = H(r,z,t^f) \\ q(r,z,t) = q(r,z,t^f) \end{cases} \tag{16}$$

and then Eq. (12) takes the form

$$B(\xi,\eta)\,H(\xi,\eta,t^f) + \int_\Gamma rq(r,z,t^f)\,U(\xi,\eta,r,z)\,\mathrm{d}\Gamma$$
$$= \int_\Gamma rH(r,z,t^f)\,W(\xi,\eta,r,z)\,\mathrm{d}\Gamma + \iint_\Omega rH^*(\xi,\eta,r,z,t^f,t^{f-1})\,H(r,z,t^{f-1})\,\mathrm{d}\Omega \tag{17}$$

where

$$U(\xi,\eta,r,z) = \int_{t^{f-1}}^{t^f} H^*(\xi,\eta,r,z,t^f,t)\,\mathrm{d}t \tag{18}$$

and

$$W(\xi,\eta,r,z) = \int_{t^{f-1}}^{t^f} q^*(\xi,\eta,r,z,t^f,t)\,\mathrm{d}t. \tag{19}$$

The integration with respect to time can be done in analytic way. So

$$U(\xi,\eta,r,z) = \frac{1}{2a\sqrt{2\pi r\xi}} \int_{\frac{r\xi}{2a\Delta t}}^{\infty} w^{-\frac{1}{2}} \exp\left(-\frac{sw}{2r\xi}\right) \mathrm{I}_0(w)\,\mathrm{d}w \tag{20}$$

and

$$W(\xi,\eta,r,z) = \frac{1}{2r\xi\sqrt{2\pi r\xi}} \left\{ [r\cos\alpha + (z-\eta)\cos\beta] \int_{\frac{r\xi}{2a\Delta t}}^{\infty} w^{\frac{1}{2}} \exp\left(-\frac{sw}{2r\xi}\right) \mathrm{I}_0(w)\,\mathrm{d}w \right.$$
$$\left. - \xi\cos\alpha \int_{\frac{r\xi}{2a\Delta t}}^{\infty} w^{\frac{1}{2}} \exp\left(-\frac{sw}{2r\xi}\right) \mathrm{I}_1(w)\,\mathrm{d}w \right\}$$

where

$$s = r^2 + \xi^2 + (z-\eta)^2. \tag{21}$$

In order to determine the integrals (20) and (21), the Bessel functions $\mathrm{I}_0(w)$ and $\mathrm{I}_1(w)$ should be written in the form of the series. So

$$\mathrm{I}_0(w) = \begin{cases} \displaystyle\sum_{n=0}^{\infty} \frac{\left(\frac{w}{2}\right)^{2n}}{(n!)^2}, & w \le 3.75, \\ \displaystyle\frac{\exp(w)}{\sqrt{2\pi w}} \left[1 + \sum_{n=1}^{\infty} \frac{f_1(n)}{n!(8w)^n}\right], & w > 3.75, \end{cases} \tag{22}$$

where

$$f_1(n) = 1\ldots(2n-3)^2(2n-1)^2 \tag{23}$$

and

$$\mathrm{I}_1(w) = \begin{cases} \displaystyle\sum_{n=0}^{\infty} \frac{\left(\frac{w}{2}\right)^{2n+1}}{(n!)^2(n+1)}, & w \le 3.75, \\ \displaystyle\frac{\exp(w)}{\sqrt{2\pi w}} \left[1 + \sum_{n=1}^{\infty} \frac{f_2(n)}{n!(8w)^n}\right], & w > 3.75, \end{cases} \tag{24}$$

where

$$f_2(n) = (-1)^n(4-1^2)(4-3^2)\ldots[4-(2n-1)^2]. \tag{25}$$

In this place the following situations should be taken into account. If the lower limit of integration (Eqs. (20), (21)) is greater than 3.75, then the functions I_0 and I_1 should be substituted by series for $w > 3.75$ (formulae (22b) and (24b)). If the lower limit of integration is smaller than 3.75, then the interval of integration should be expressed by the sum

$$\left[\frac{r\xi}{2a\Delta t}, \infty\right) = \left[\frac{r\xi}{2a\Delta t}, 3.75\right] \cup (3.75, \infty) \tag{26}$$

and calculating the first integral we substitute the functions I_0 and I_1 by series (22a) and (24a), while for the second one we use the formulae (22b) and (24b). The details concerning these problems and final formulae can be found in [4]. On the stage of numerical computations the boundary Γ is

divided into N constant boundary elements Γ_j, $j = 1, 2, \ldots, N$, while the interior Ω is divided into L constant internal cells. So, one obtains the following system of algebraic equations ($i = 1, 2, \ldots, N$)

$$B(\xi_i, \eta_i)\, H(\xi_i, \eta_i, t^f) + \sum_{j=1}^{N} G_{ij}\, q(r_j, z_j, t^f) = \sum_{j=1}^{N} \hat{Z}_{ij}\, H(r_j, z_j, t^f) + \sum_{l=1}^{L} P_{il}\, H(r_l, z_l, t^{f-1}) \tag{27}$$

where

$$G_{ij} = \int_{\Gamma_j} r\, U(\xi_i, \eta_i, r, z)\, \mathrm{d}\Gamma_j\,, \tag{28}$$

$$\hat{Z}_{ij} = \int_{\Gamma_j} r\, W(\xi_i, \eta_i, r, z)\, \mathrm{d}\Gamma_j \tag{29}$$

and

$$P_{il} = \int\!\!\int_{\Omega_l} r\, H^*(\xi_i, \eta_i, r, z, t^f, t^{f-1})\, \mathrm{d}\Omega_l\,. \tag{30}$$

The system (27) can be also written in the form

$$\sum_{j=1}^{N} G_{ij}\, q(r_j, z_j, t^f) = \sum_{j=1}^{N} Z_{ij}\, H(r_j, z_j, t^f) + \sum_{l=1}^{L} P_{il}\, H(r_l, z_l, t^{f-1}) \tag{31}$$

where

$$Z_{ij} = \begin{cases} \hat{Z}_{ij}, & i \neq j, \\ -B(\xi_i, \eta_i) = -\sum_{i \neq j} \hat{Z}_{ij}, & i = j. \end{cases} \tag{32}$$

The system of equations (31) allows to determine the enthalpy values on boundary Γ_0 and heat fluxes on Γ_c. The enthalpy field at internal nodes for time t^f is calculated using the formula

$$H(\xi_i, \eta_i) = \sum_{j=1}^{N} Z_{ij}\, H(r_j, z_j, t^f) - \sum_{j=1}^{N} G_{ij}\, q(r_j, z_j, t^f) + \sum_{l=1}^{L} P_{il}\, H(r_l, z_l, t^{f-1}). \tag{33}$$

4. Alternating phase truncation method

The APTM consists in an approximate solution of the freezing problem by conventional reduction of the domain considered to a homogenous one, thermophysical parameters of which are constant. The basic algorithm of this method was reported by Rogers, Berger and Ciment [10], while its generalization by Mochnacki and Kapusta [8] and next by Majchrzak and Mochnacki [7]. The APTM is especially effective as a supplement to the BEM algorithm, because the computations are realized for homogenous domains and generally the problem is reduced to the linear one.

In the paper a situation corresponding to the course of enthalpy presented in Fig. 4 is discussed. Let us consider a multiphase domain Ω being the composition of sub-domains $\Omega_1 \cup \Omega_2 \cup \Omega_3$. The limits of enthalpy corresponding to isotherms T_1 and T_2 are denoted as A_1 and A_2 (see Fig. 4). Additionally, it is assumed that the enthalpy field for time t^{f-1} is known, while the enthalpy for time $t^f = t^{f-1} + \Delta t$ is searched. For every time step Δt three boundary-initial problems are solved. The first concerns the natural state, the second the intermediate phase whereas the last deals with the frozen region. The successive solutions are in a certain way modified.

The first stage of the computations concerns the hottest phase (unfrozen tissue). The given enthalpy distribution in the domain Ω at time t^{f-1} is transformed in this way

$$V_1(r, z, t^{f-1}) = \max\left[A_1\,,\, H(r, z, t^{f-1})\right]. \tag{34}$$

This new pseudo-initial condition corresponds to a structural reduction of the whole area Ω to the unfrozen domain. Next, the transition $t^{f-1} \rightarrow t^f$ is calculated assuming that the diffusion coefficient $a(H) = a_1 = \text{const}$. The solution for time t^f : $V_1^*(r, z, t^f)$ is corrected according to the formula

$$V_1(r, z, t^f) = V_1^*(r, z, t^f) + H(r, z, t^{f-1}) - V_1(r, z, t^{f-1}). \tag{35}$$

If we consider the second stage corresponding to intermediate phase then the results of previous computations $V_1(r, z, t^f)$ are known and they are transformed to the new pseudo-initial condition, namely

$$V_2(r, z, t^{f-1}) = \min\left\{A_1\,,\ \max\left[A_2,\ V_1(r, z, t^f)\right]\right\}. \tag{36}$$

The transition $t^{f-1} \rightarrow t^f$ for the intermediate phase is calculated and the result obtained $V_2^*(r, z, t^f)$ is corrected in following way

$$V_2(r, z, t^f) = V_2^*(r, z, t^f) + V_1(r, z, t^f) - V_2(r, z, t^{f-1}). \tag{37}$$

At the last stage (frozen state) the pseudo-initial condition in the form

$$V_3(r, z, t^{f-1}) = \min\left[A_2\,,\ V_2(r, z, t^f)\right] \tag{38}$$

is assumed and for $a(H) = a_3$ the solution for time t^f : $V_3^*(r, z, t^f)$ is found. The enthalpy field for time t^f results from the formula

$$H(r, z, t^f) = V_3^*(r, z, t^f) + V_2(r, z, t^f) - V_3(r, z, t^{f-1}). \tag{39}$$

The transition $t^{f-1} \rightarrow t^f$ requires the solution of three linear diffusion problems in structurally homogenous domains, but in this way the well known difficulties associated with a strongly nonlinear mathematical model can be eliminated. It should be pointed out that each step of time in the APTM is done three times, i.e. it is necessary to join the boundary conditions adequately because they should act only during one interval Δt. In this connection for two of the stages the boundary Γ should be insulated.

5. Results of computations

The cryoprobe of radius 7.5 [mm] being in ideal thermal contact with biological tissue is considered. The external radius of domain: $R = 15$ [mm], its altitude: $Z = 15$ [mm]. In successive simulations, the cryoprobe surface temperature was assumed as $T_c = -90\,^\circ\text{C}$, $-145\,^\circ\text{C}$ and $-190\,^\circ\text{C}$. The following thermophysical parameters for successive sub-domains have been accepted $a_1 = 1.444 \cdot 10^{-7}$ [m^2/s], $a_2 = 2.673 \cdot 10^{-8}$ [m^2/s], $a_3 = 1.036 \cdot 10^{-6}$ [m^2/s]. The border temperatures between unfrozen region and intermediate phase and between intermediate phase and frozen region are equal $T_1 = -1\,^\circ\text{C}$, $T_2 = -8\,^\circ\text{C}$, respectively. The initial temperature of tissue: $T_0 = 37\,^\circ\text{C}$.

The cylindrical fragment of biological tissue was covered by the mesh containing 40 constant boundary elements and 100 constant internal cells – as in Fig. 5. In order to avoid the singularity for $r = 0$, the axis of symmetry has been surrounded by a small cylinder of radius 10^{-5} [mm]. Along this artificial internal boundary the adiabatic condition can be accepted. Figures 6–8 illustrate the temporary shapes of sub-regions for the cryoprobe surface temperature $T_c = -190\,^\circ\text{C}$ and times 60 [s], 120 [s] and 180 [s].

Summing up, it seems that the composition of the boundary element method and the alternating phase truncation method constitute the very effective tool of numerical simulation of freezing process. The solution obtained in this way is very close to the results presented in [2] and [6], but the FEM application [2] leads to the system of equations with the very big number of unknown parameters, while the solution presented in [6] requires the introduction of additional iterative procedures resulting from the introduction of the artificial heat source in energy equation.

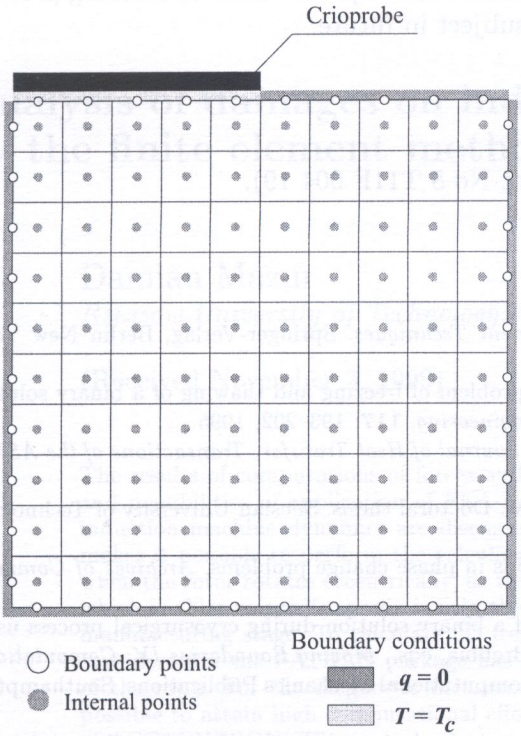

Fig. 5. Discretization of biological tissue domain

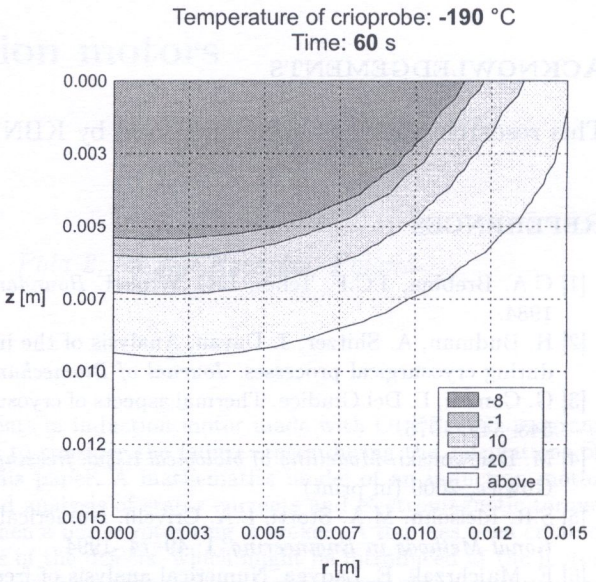

Fig. 6. Position of border isotherms for $T_c = -190\,^{\circ}\mathrm{C}$ (60 [s])

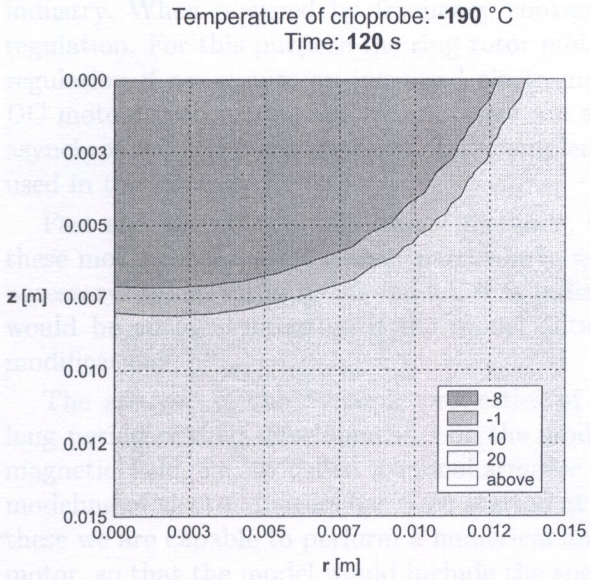

Fig. 7. Position of border isotherms for $T_c = -190\,^{\circ}\mathrm{C}$ (120 [s])

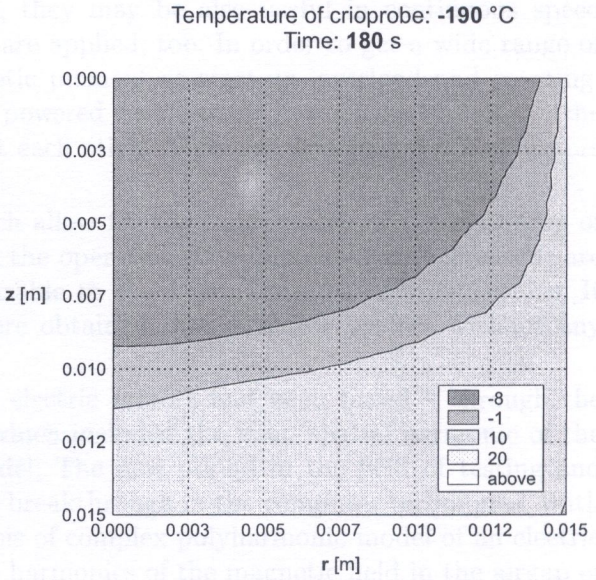

Fig. 8. Position of border isotherms for $T_c = -190\,^{\circ}\mathrm{C}$ (180 [s])

The problem of biological tissue freezing can be also treated as the inverse one. One can analyze the optimal choice of cryoprobe parameters in order to assure the required course of freezing process. The authors of this paper intend to take up also this subject in future.

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