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THERMAL ABLATION MODELING VIA THE BIOHEAT EQUATION AND ITS NUMERICAL TREATMENT

Abstract. The phenomenon of thermal ablation is described by Pennes' bioheat equation. This model is based on Newton's law of cooling. Many approximate methods have been considered because of the importance of this issue. We propose an implicit numerical scheme which has better stability properties than other approaches.

1. Introduction. Thermal ablation is a low invasive technique which eliminates cancerous tissue using high temperature. To this end, an electrode tip is inserted into the cancerous tissue and radio-frequency energy is supplied. This results in a local temperature increase and the destruction of the tumor tissue. The problem is to control the area that is damaged. For this purpose, it is helpful to construct a model which takes into account modification of thermal parameters of the tissue, and effects of cooling, either by blood or saline introduced into a heated area. The model must give a possibility to destroy tissue depending on the position of the electrodes and the time of treatment. The maximal temperature must be less than 92°C to avoid vaporization, whereas it must be less than 43°C in large vessels in order to prevent cell death. The main goal is to optimize the power input which destroys cancerous tissues.

The model is well described mathematically in [2]. In [7] the authors discuss an analytical approach under the assumption of sinusoidal heat flux on the skin. In [3] there are exact solutions for a fairly general class of Pennes-type problems. In [8] the authors approximate a bioheat equation by means of a second-order finite difference scheme which is a combination of the explicit

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and implicit Euler schemes. In [1] we consider the one-dimensional case, while this article is devoted to a three-dimensional model. The boundary conditions in [1] are of the first order, so error estimates are still quite weak. Moreover, the explicit Euler method component makes solutions more sensitive to any initial-data perturbations. We propose an implicit scheme, which by its nature is of the first order but has much better properties. What is more, we are convinced that our scheme gives an opportunity to perform reliable computations even though the coefficients k, Q_b, Q_m, and Q_z are discontinuous. This improvement significantly increases the possibility of practical applications.

The paper is organized as follows. We first formulate an implicit difference scheme for Pennes' equation. Next, we study the properties of this scheme, in particular its stability, which clearly implies convergence. Finally, we give some numerical examples and conclude with several remarks on multidimensional generalizations.

2. Formulation of the problem. Newton's law of cooling states that the rate of change of the temperature of an object is proportional to the difference between its own temperature and the ambient temperature. More specifically: *The rate of heat loss of a body is proportional to the difference in temperatures between the body and its surroundings.* In symbols, the rate of change of the temperature dT/dt is proportional to the difference between the object temperature $T = T(t)$ and the ambient temperature T_a:

$$\frac{dT}{dt} = -r(T - T_a).$$

Then one can consider Pennes' equation, i.e. the law of cooling with diffusion. In the one-dimensional case it has the form

$$c\rho\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2} + Q_b + Q_m + Q_z.$$

The biological interpretation of the coefficients of this equation is as follows: $c\,[\mathrm{J/kgK}]$ is the specific heat of tissue, $\rho\,[\mathrm{kg/m^3}]$ the tissue density, $T\,[\mathrm{K}]$ the tissue temperature, $k\,[\mathrm{W/mK}]$ the thermal conductivity of tissue, $Q_b\,[\mathrm{W/m^3}]$ a term which accounts for the effects of perfusion, $Q_m\,[\mathrm{W/m^3}]$ the metabolic heat generation term, and $Q_z\,[\mathrm{W/m^3}]$ the power density delivered by an external source.

The coefficients c, ρ, k, Q_b, Q_m, and Q_z may depend on x and T, which is coherent with experimental data. The Q_z may also depend on time (for example during the heating interval). We restrict our attention to a simplified case $Q_b = -r(T - T_a)$ and consider the three-dimensional problem

$$\begin{aligned}(2.1)\qquad & c(x,T)\rho(x,T)\frac{\partial T}{\partial t}\\ &\quad = \nabla\cdot(k(x,T)\nabla T) + Q_m(x,T) + Q_z(t,x,T) - r(T - T_a) \quad \text{on } \Omega,\end{aligned}$$

where $x = (x^1, x^2, x^3) \in \Omega \subset \mathbb{R}^3$. The respective initial-boundary conditions depend on the region Ω, the electrode and the surrounding tissue. We have

$$T(0,x) = \omega_0(x), \quad \text{where} \quad 0 < T_a \le \omega_0(x) \le T_0, \tag{2.2}$$

and

$$T(t,0) = T_0, \qquad \frac{\partial T}{\partial \boldsymbol{n}} = 0 \quad \text{on } \partial\Omega, \tag{2.3}$$

where $\boldsymbol{n}$ is the unit normal vector to the boundary, $\omega_0(0) = T_0$.

From the mathematical point of view the functions $Q_m(x,T)$ and $Q_z(t,x,T)$ can be grouped into one function $Q(t,x,T)$. Denote $c(x,T)\rho(x,T)$ by $\hat{\rho}(x,T)$. Thus we consider

$$\hat{\rho}(x,T)\frac{\partial T}{\partial t} = \nabla \cdot (k(x,T)\nabla T) + Q(t,x,T) - r(T - T_a).$$

We discretize the problem on a regular mesh. Assume that $\Delta t > 0$, $\Delta x_l > 0$ for $l = 1,2,3$. Denote the nodes value by $t_n = n\Delta t$, $n \in \mathbb{Z}$, and $x_j = (x_j^1, x_j^2, x_j^3) = (j_1\Delta x_1, j_2\Delta x_2, j_3\Delta x_3)$ for $j = (j_1, j_2, j_3) \in \mathbb{Z}^3$. The set of all nodes is denoted by $Z_h = \{(t_n, x_j)\colon (n,j) \in \mathbb{Z}^{1+3}\}$. Denote $E_h = \bar{\Omega} \cap Z_h$, $E_h^* = \bar{\Omega}^c \cap Z_h$, where $\bar{\Omega}^c$ is the complement of $\bar{\Omega}$. Assume that $k(x,T)$ is a 3×3 diagonal matrix. Then the respective scheme looks as follows:

$$\begin{aligned} &\hat{\rho}(x_j, T_j^{n-1})\frac{T_j^n - T_j^{n-1}}{\Delta t} \\ &= \sum_{l=1}^{3}\Bigg(k_l(x_j, T_j^{n-1})\frac{T_{j+e_l}^n - 2T_j^n + T_{j-e_l}^n}{\Delta x_l^2} + \frac{\partial k_l(x_j, T_j^{n-1})}{\partial x^l}\,\frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l} \\ &\quad + \frac{\partial k_l(x_j, T_j^{n-1})}{\partial T}\left(\frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l}\right)^2\Bigg) + Q(t_{n-1}, x_j, T_j^{n-1}) - r(T_j^n - T_a), \end{aligned} \tag{2.4}$$

where $T_j^n = T(t_n, x_j)$, $j = (j_1, j_2, j_3)$, $x_j = (x_j^1, x_j^2, x_j^3)$ and $e_1 = (1,0,0)$, $e_2 = (0,1,0)$, $e_3 = (0,0,1)$. The respective boundary conditions depend on the region, the electrode and the surrounding tissue:

$$T_j^0 = \omega_0(x_j) \tag{2.5}$$

and

$$T_0^n = T_0, \qquad T_j^n = (I_hT)(t_n, R(x_j)) \quad \text{on } E_h^*, \tag{2.6}$$

where I_h is the interpolation operator (see [4]) and R is the reflection operator (reflection with respect to the boundary). Define a difference operator $\mathcal{L}_h$

on E_h as follows:

$$
\begin{aligned}
\mathcal{L}_h T_j^n &= \hat\rho(x_j, T_j^{n-1})\frac{T_j^n - T_j^{n-1}}{\Delta t}\\
&\quad - \sum_{l=1}^{3}\biggl(k_l(x_j, T_j^{n-1})\frac{T_{j+e_l}^n - 2T_j^n + T_{j-e_l}^n}{\Delta x_l^2} + \frac{\partial k_l(x_j, T_j^{n-1})}{\partial x^l}\,\frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l}\\
&\quad + \frac{\partial k_l(x_j, T_j^{n-1})}{\partial T}\left(\frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l}\right)^2\biggr) - Q(t_{n-1}, x_j, T_j^{n-1}) + r(T_j^n - T_a).
\end{aligned}
$$

Then equation (2.4) is equivalent to $\mathcal{L}_h T_j^n = 0$. Assume that $0 < k_0 \le k_l(x,T) \le k_1$ for $l = 1,2,3$, $0 < \rho_0 \le \hat\rho(x,T) \le \rho_1$, $0 \le Q(t,x,T) \le Q_1$ and the Lipschitz conditions

$$
\begin{gathered}
|\hat\rho(x,T) - \hat\rho(x,\tilde T)| \le L_{\hat\rho}|T - \tilde T|,\\
|k(x,T) - k(x,\tilde T)| \le L_k|T - \tilde T|,\\
\left|\frac{\partial k_l(x_j, T_j^{n-1})}{\partial x^l} - \frac{\partial k_l(x_j, \tilde T_j^{n-1})}{\partial x^l}\right|, \left|\frac{\partial k(x,T)}{\partial T} - \frac{\partial k(x,\tilde T)}{\partial T}\right| \le \bar L_k|T - \tilde T|,\\
|Q(t,x,T) - Q(t,x,\tilde T)| \le L_Q|T - \tilde T|
\end{gathered}
$$

hold for some $L_{\hat\rho} > 0$, $L_k > 0$, $\bar L_k > 0$ and $L_Q > 0$. It is obvious that the following lemma requires only a few of the above assumptions.

LEMMA 2.1 (Estimate). *Under the above assumptions the solution of* (2.4)–(2.6), *for a sufficiently small discretization parameter* Δx, *satisfies the estimate*

$$
T_a \le T_j^n \le Q_1\frac{\rho_1 + r\Delta t}{r\rho_0}\left[1 - \frac{1}{\left(1 + \frac{r\Delta t}{\rho_1}\right)^n}\right] + \frac{T_0 - T_a}{\left(1 + \frac{r\Delta t}{\rho_1}\right)^n}
$$

in a class of functions with first order difference quotients with respect to x *bounded by a constant* M_1 *independent of* Δx.

Proof. It is convenient to simplify the notation as follows:

$$
\begin{aligned}
&k_{l,j}^{n-1}(T) = k_l(x_j, T_j^{n-1}), \qquad k_{l,l,j}^{n-1}(T) = \frac{\partial k_l(x_j, T_j^{n-1})}{\partial x^l},\\
&k_{T,l,j}^{n-1}(T) = \frac{\partial k_l(x_j, T_j^{n-1})}{\partial T},\\
&\hat\rho_j^{n-1}(T) = \hat\rho(x_j, T_j^{n-1}), \qquad Q_j^{n-1}(T) = Q(x_j^{n-1}, T_j^{n-1}).
\end{aligned}
\tag{2.7}
$$

In this proof we skip T, e.g. we write $k_{l,j}^{n-1}$ insead of $k_{l,j}^{n-1}(T)$. From the initial condition we have $T_j^0 \ge T_a$ (cf. (2.2)). We will prove by induction on n that $T_j^n \ge T_a$. Assume that this holds for $n-1$ and suppose, on the contrary, that there exists j such that $T_j^n < T_a$. We choose j such that $T_j^n = \min_i T_i^n$ and j is the least in the lexicographical order. Since $Q_j^{n-1} \ge 0$, $T_j^{n-1} - T_a \ge 0$

and $\mathcal{L}_h T_j^n = 0$, it follows that

$$(T_j^n - T_a)\hat{\rho}_j^{n-1}\frac{1}{\Delta t} - \sum_{l=1}^{3}\Bigg\{k_{l,j}^{n-1}\frac{T_{j+e_l}^n - 2T_j^n + T_{j-e_l}^n}{\Delta x_l^2} + \frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l}\left(k_{l,l,j}^{n-1} + k_{T,l,j}^{n-1}\frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l}\right)\Bigg\} + r(T_j^n - T_a) \geq 0$$

for sufficiently small Δx_l, because $k_{l,l,j}^{n-1} + k_{T,l,j}^{n-1}\frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l}$ is bounded by $L_k(1 + M_1)$. This contradicts $T_j^n - T_a < 0$.

Now we will prove the upper bound. Rewrite the equation $\mathcal{L}_h T_j^n = 0$ as

$$\begin{aligned}(T_j^n - T_a)&\left(\hat{\rho}_j^{n-1}\frac{1}{\Delta t} + r + 2\sum_{l=1}^{3}\frac{k_{l,j}^{n-1}}{\Delta x_l^2}\right)\\ &= \sum_{l=1}^{3}\Bigg(k_{l,j}^{n-1}\frac{T_{j+e_l}^n - T_a}{\Delta x_l^2} + k_{l,j}^{n-1}\frac{T_{j-e_l}^n - T_a}{\Delta x_l^2}\\ &\qquad + \frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l}\left(k_{l,l,j}^{n-1} + k_{T,l,j}^{n-1}\frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l}\right)\Bigg)\\ &\quad + Q_j^{n-1} + (T_j^{n-1} - T_a)\hat{\rho}_j^{n-1}\frac{1}{\Delta t}.\end{aligned}$$

Since this holds for all j, we can consider j for which $T_j^n = \max_i T_i^n$. Once again using the boundedness of first order difference quotients, we obtain

$$\begin{aligned}(T_j^n - T_a)&\left(\hat{\rho}_j^{n-1}\frac{1}{\Delta t} + r + \sum_{l=1}^{3}\frac{2k_{l,j}^{n-1}}{\Delta x_l^2}\right)\\ &\leq \sum_{l=1}^{3}\left(2k_{l,j}^{n-1}\frac{T_j^n - T_a}{\Delta x_l^2}\right) + Q_j^{n-1} + (T_j^{n-1} - T_a)\hat{\rho}_j^{n-1}\frac{1}{\Delta t}\end{aligned}$$

for $k_0 \geq \Delta x_l L_k(1 + M_1)/2$, which simplifies to

$$(T_j^n - T_a)\left(\hat{\rho}_j^{n-1}\frac{1}{\Delta t} + r\right) \leq Q_j^{n-1} + (T_j^{n-1} - T_a)\hat{\rho}_j^{n-1}\frac{1}{\Delta t}.$$

Thus

$$T_j^n - T_a \leq \frac{Q_j^{n-1}}{\hat{\rho}_j^{n-1}\frac{1}{\Delta t} + r} + (T_j^{n-1} - T_a)\frac{\hat{\rho}_j^{n-1}\frac{1}{\Delta t}}{\hat{\rho}_j^{n-1}\frac{1}{\Delta t} + r},$$

hence

$$\begin{aligned}T_j^n - T_a &\leq \frac{Q_1}{\rho_0\frac{1}{\Delta t} + r} + (T_j^{n-1} - T_a)\frac{\rho_1\frac{1}{\Delta t}}{\rho_1\frac{1}{\Delta t} + r}\\ &\leq \frac{Q_1}{\rho_0\frac{1}{\Delta t}} + (T_j^{n-1} - T_a)\frac{1}{1 + \Delta t\frac{r}{\rho_1}}.\end{aligned}$$

Thus

$$T_j^n - T_a \le Q_1 \frac{\Delta t}{\rho_0} \sum_{i=1}^{n} \frac{1}{\left(1+\frac{r\Delta t}{\rho_1}\right)^{i-1}} + (T_j^0 - T_a)\frac{1}{\left(1+\frac{r\Delta t}{\rho_1}\right)^{n}}$$
$$\le Q_1 \frac{\rho_1 + r\Delta t}{r\rho_0}\left[1 - \frac{1}{\left(1+\frac{r\Delta t}{\rho_1}\right)^{n}}\right] + \frac{T_0 - T_a}{\left(1+\frac{r\Delta t}{\rho_1}\right)^{n}}.$$

Observe that the boundary values are interpolated from internal ones, so the inequalities are also satisfied. ■

Remark 2.2. Observe that $T_j^n - T_a$ can be approximately estimated by

$$Q_1 \frac{\rho_1}{r\rho_0}(1 - e^{-tr/\rho_1}) + (T_0 - T_a)e^{-tr/\rho_1}, \qquad t = t_n.$$

We formulate a stability theorem. Note that it implies convergence.

Theorem 2.3 (Stability). *Under the above assumptions, if $\omega_0 \in C^2$ and $k \in C^{1,2}$, then the scheme* (2.4)–(2.6) *is stable in any class of solutions with bounded first order difference quotients with respect to t and x, and bounded second order difference quotients with respect to x.*

Proof. Suppose that T_j^n is a solution of (2.4)–(2.6) with the first and second order difference quotients bounded by M_1 and M_2 respectively. Consider the perturbed scheme (2.4)–(2.6), i.e.

$$\mathcal{L}_h \tilde{T}_j^n = \xi_j^n$$

with perturbations ξ_j^n such that

$$\max_{j,n} |\xi_j^n| := \|\xi\| \to 0 \quad \text{as } h \to 0.$$

Suppose that the difference quotients of $\tilde{T}$ have the same estimates M_1, M_2. Denote $\varepsilon_j^n = \tilde{T}_j^n - T_j^n$. We use the same notation (2.7) as in the proof of Lemma 2.1. Then we have the error equation

$$\mathcal{L}_h \tilde{T}_j^n - \mathcal{L}_h T_j^n = \hat{\rho}_j^{n-1}(\tilde{T})\frac{\varepsilon_j^n - \varepsilon_j^{n-1}}{\Delta t} + \frac{T_j^n - T_j^{n-1}}{\Delta t}(\hat{\rho}_j^{n-1}(\tilde{T}) - \hat{\rho}_j^{n-1}(T))$$
$$-\sum_{l=1}^{3}\left\{\varepsilon_{j+e_l}^n\left[\frac{k_{l,j}^{n-1}(\tilde{T})}{\Delta x_l^2} + \frac{k_{l,l,j}^{n-1}(\tilde{T})}{2\Delta x_l} + \frac{k_{T,l,j}^{n-1}(\tilde{T})}{2\Delta x_l}\left(\frac{\tilde{T}_{j+e_l}^n - \tilde{T}_{j-e_l}^n}{2\Delta x_l} + \frac{T_{j+e_l}^n - T_{j-e_l}^n}{2\Delta x_l}\right)\right]\right.$$

$$+\varepsilon^n_{j-e_l}\left[\frac{k^{n-1}_{l,j}(\tilde T)}{\Delta x_l^2}-\frac{k^{n-1}_{l,l,j}(\tilde T)}{2\Delta x_l}+\frac{k^{n-1}_{T,l,j}(\tilde T)}{2\Delta x_l}\left(\frac{\tilde T^n_{j+e_l}-\tilde T^n_{j-e_l}}{2\Delta x_l}+\frac{T^n_{j+e_l}-T^n_{j-e_l}}{2\Delta x_l}\right)\right] - 2\varepsilon^n_j\frac{k^{n-1}_{l,j}(\tilde T)}{\Delta x_l^2}\Bigg\}$$

$$-\sum_{l=1}^{3}\Bigg\{(k^{n-1}_{l,j}(\tilde T)-k^{n-1}_{l,j}(T))\frac{T^n_{j+e_l}-2T^n_j+T^n_{j-e_l}}{\Delta x_l^2} + (k^{n-1}_{l,l,j}(\tilde T)-k^{n-1}_{l,l,j}(T))\frac{T^n_{j+e_l}-T^n_{j-e_l}}{2\Delta x_l} + (k^{n-1}_{T,l,j}(\tilde T)-k^{n-1}_{T,l,j}(T))\left(\frac{T^n_{j+e_l}-T^n_{j-e_l}}{2\Delta x_l}\right)^2\Bigg\}$$

$$-Q^{n-1}_j(\tilde T)+Q^{n-1}_j(T)+r\varepsilon^n_j+\xi^n_j.$$

Hence we get the estimate

$$|\varepsilon^n_j|\left(\frac{\hat\rho^{n-1}_j(\tilde T)}{\Delta t}+\sum_{l=1}^{3}\left(k^{n-1}_{l,j}(\tilde T)\frac{2}{\Delta x_l^2}\right)+r\right)$$
$$\le |\varepsilon^{n-1}_j|\frac{\hat\rho^{n-1}_j(\tilde T)}{\Delta t}+\sum_{l=1}^{3}\Bigg(|\varepsilon^n_{j+e_l}|\left(\frac{k^{n-1}_{l,j}(\tilde T)}{\Delta x_l^2}+\frac{|k^{n-1}_{l,l,j}(\tilde T)|}{2\Delta x_l}+\frac{|k^{n-1}_{T,l,j}(\tilde T)|}{\Delta x_l}M_1\right) + |\varepsilon^n_{j-e_l}|\left(\frac{k^{n-1}_{l,j}(\tilde T)}{\Delta x_l^2}-\frac{|k^{n-1}_{l,l,j}(\tilde T)|}{2\Delta x_l}+\frac{|k^{n-1}_{T,l,j}(\tilde T)|}{\Delta x_l}M_1\right)\Bigg)$$
$$+\sum_{l=1}^{3}\big(|k^{n-1}_{l,j}(\tilde T)-k^{n-1}_{l,j}(T)|M_2+|k^{n-1}_{l,l,j}(\tilde T)-k^{n-1}_{l,l,j}(T)|M_1 + |k^{n-1}_{T,l,j}(\tilde T)-k^{n-1}_{T,l,j}(T)|M_1^2\big)$$
$$+|Q^{n-1}_j(\tilde T)-Q^{n-1}_j(T)|+M_1|\hat\rho^{n-1}_j(\tilde T)-\hat\rho^{n-1}_j(T)|+|\xi^n_j|.$$

If Δx_l are small enough, we have

$$|\varepsilon^n_j|\left(\frac{\hat\rho^{n-1}_j}{\Delta t}+r\right) \le |\varepsilon^{n-1}_j|\left(\frac{\hat\rho^{n-1}_j}{\Delta t}+\sum_{l=1}^{3}(L_kM_2+\bar L_kM_1+\bar L_kM_1^2)+L_Q+M_1L_{\hat\rho}\right)+|\xi^n_j|.$$

Thus

$$\|\varepsilon^n\|\left(\frac{\hat\rho^{n-1}_j}{\Delta t}+r\right) \le \|\varepsilon^{n-1}\|\left(\frac{\hat\rho^{n-1}_j}{\Delta t}+3L_kM_2+3\bar L_kM_1+3\bar L_kM_1^2+L_Q+M_1L_{\hat\rho}\right)+\|\xi\|.$$

Therefore we obtain

$$\|\varepsilon^n\| \le \|\varepsilon^{n-1}\| \frac{\frac{\hat\rho_j^{n-1}}{\Delta t} + 3L_k M_2 + 3\bar L_k M_1 + 3\bar L_k M_1^2 + L_Q + M_1 L_{\hat\rho}}{\frac{\hat\rho_j^{n-1}}{\Delta t} + r} + \frac{\|\xi\|}{\frac{\hat\rho_j^{n-1}}{\Delta t} + r}.$$

If we add appropriate perturbed boundary conditions, in the simplest case we obtain the estimate

$$\begin{aligned}\|\varepsilon^n\| \le \|\varepsilon^0\| &\frac{1}{\left(1 + \frac{\Delta t(r-(3L_k M_2+3\bar L_k M_1+3\bar L_k M_1^2+L_Q+M_1 L_{\hat\rho}))}{\rho_1+\Delta t(3L_k M_2+3\bar L_k M_1+L_Q+M_1 L_{\hat\rho})}\right)^n}\\ &+ \frac{\|\xi\|}{\frac{\rho_0}{\Delta t}+r}\left(1 - \frac{1}{\left(1 + \frac{\Delta t(r-(3L_k M_2+3\bar L_k M_1+3\bar L_k M_1^2+L_Q+M_1 L_{\hat\rho}))}{\rho_1+\Delta t(3L_k M_2+3\bar L_k M_1+L_Q+M_1 L_{\hat\rho})}\right)^n}\right)\\ &\times \frac{\rho_1 + r\Delta t}{\Delta t(r - (3L_k M_2 + 3\bar L_k M_1 + 3\bar L_k M_1^2 + L_Q + M_1 L_{\hat\rho}))}.\end{aligned}$$

This yields the desired assertion. ∎

3. Numerical simulations. The numerical simulations are performed using the proposed scheme. The model assumptions are as follows: the time of simulations is 600 [s], $T_0 = 363$ [K], $\omega_0(x)$ is assumed to change linearly from T_0 at $x = 0$ to T_a at the distance equal to 0.005 [m]. The time step is $\Delta t = 6$ [s], while the space step is $\Delta x_l = 0.0005$ [m] for $l = 1, 2$. The region consists of the rectangle $[-0.01, 0] \times [-0.01, 0.01]$ with two semicircles of radius 0.01 attached at the points $(x, y) = (-0.01, 0)$ and $(x, y) = (0, 0)$. The material parameters are taken from [6], so $c\rho = 3.9 \cdot 10^6$ [J/m^{3}K], while two cases of the parameter $k(x, T)$ are considered. In the first case $k_l(x, T) = 0.55$ [W/mK], $l = 1, 2$, so it is constant (independent of x and T), while in the other case

$$k_l(x,T) = \begin{cases} 0.55\,[\mathrm{W/mK}] & \text{for } T < 322\,[\mathrm{K}],\\ 0.55 - 0.13(T-322)/11\,[\mathrm{W/mK}] & \text{for } 322\,[\mathrm{K}] \le T \le 333\,[\mathrm{K}],\\ 0.42\,[\mathrm{W/mK}] & \text{for } T > 333\,[\mathrm{K}],\end{cases}$$

for $l = 1, 2$. Based on [2] the value of T_a is equal to 310 [K], while $r = 0.1$ [1/s].

The results of numerical simulations are presented in the following figures. Figure 1 shows the initial distribution of the temperature for both models.

Figure 2 shows the temperature distribution for $t = 600$ [s] for the case of constant value of $k(x, T)$, while Figure 3 shows the temperature distribution for $t = 600$ [s] for $k(x, T)$ variable. Figure 4 shows the difference between the temperature distribution for $t = 600$ [s] obtained for both cases of $k(x, T)$.

4. Conclusions. (1) Our boundary condition (2.6) is very stable with respect to nonconstant perturbations of the boundary heat flux. This property fails for the discrete boundary condition in [8].

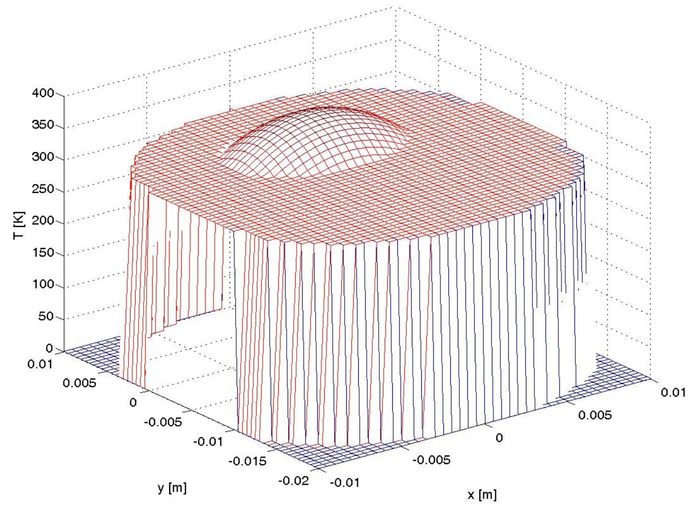

Fig. 1. The initial temperature distribution

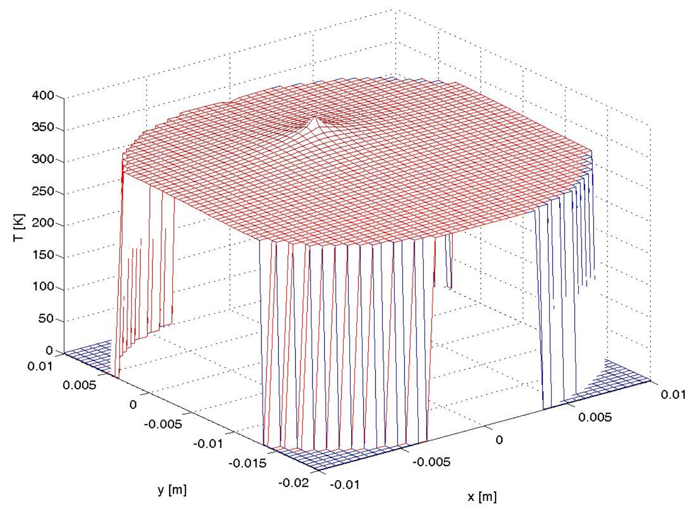

Fig. 2. The temperature distribution for $t = 600\,[\mathrm{s}]$ for $k(x,T)$ constant

(2) The assumption concerning bounded first and second order difference quotients in Theorem 2.3 is reasonable, because the parabolic operator has strongly dissipative and smoothing properties. In practice this numerical method behaves very well, even in the case of irregular data.

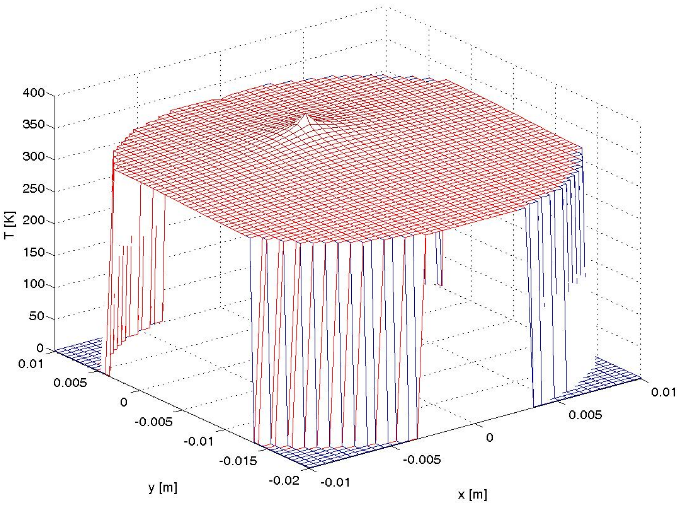

Fig. 3. The temperature distribution for $t = 600\,[\mathrm{s}]$ for $k(x, T)$ varying

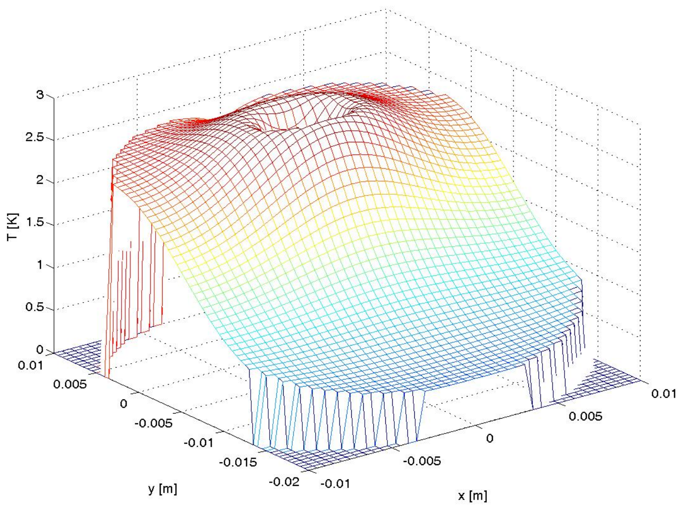

Fig. 4. The difference between the temperature distributions for $t = 600\,[\mathrm{s}]$ obtained for the two cases of $k(x, T)$

(3) In [1] we considered a simplified one-dimensional model, which assumes the radial symmetry of the three-dimensional model. In this paper we allow the full three-dimensional model with general geometry, other than

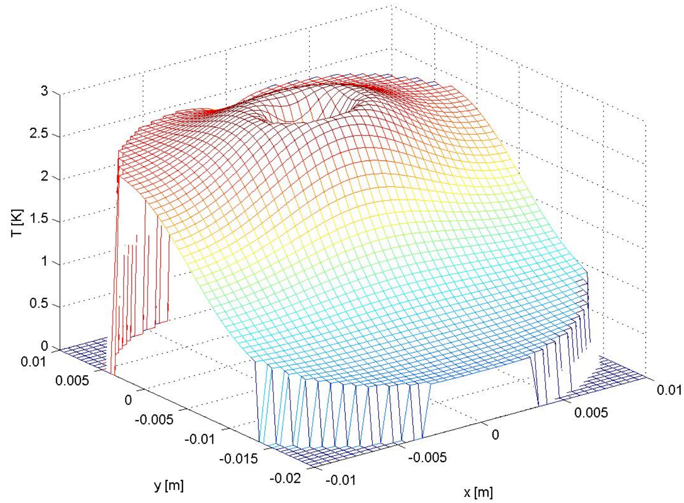

Fig. 5. The difference between the temperature distributions for $t = 600\,[\mathrm{s}]$ obtained for the two cases of $k(x,T)$ for (4.1)

radially (spherically) symmetric. This leads to strong nonlinearities comparable with $\|\nabla T\|^2$, which makes the approximation problem more difficult.

(4) Observe that one can allow a full diffusion coefficient matrix $k(x,T)$, which permits considering different thermal properties in different directions.

(5) We have also tested FDM's based on the divergence form (2.1), where $\nabla \cdot (k(x,T)\nabla T)$ is approximated by

(4.1)
$$\sum_{l=1}^{3} \frac{1}{\Delta x_l}\left(k(x_{j+.5e_l}, T^{n-1}_{j+.5e_l}) \frac{T^n_{j+e_l} - T^n_j}{\Delta x_l} - k(x_{j-.5e_l}, T^{n-1}_{j-.5e_l}) \frac{T^n_j - T^n_{j-e_l}}{\Delta x_l} \right);$$

see Figure 5. Such schemes behave very well in all numerical experiments, but it turned out that their theoretical treatment is rather technical. Similar difference schemes describing the host–parasite dynamics were considered in [5].

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