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Structural difference model of unsteady high temperature processes

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The paper provides an overview of numerical methods for solving boundary value problems, with excretion of their characteristic weaknesses in nonstationary problems with high gradients of the desired function, as well as an overview of the newest inclusion geometric information methods in analytical structures for numerical and analytical methods of solution. It is proposed a numerical-analytical structural-difference approach to high-speed nonstationary temperature processes. The series of numerical experiments were carried out, which showed high accuracy of the proposed method.

Key words: *discrete mathematical model boundary-value problem, analytic structure of solution, nonstationary temperature processes.*

Наводиться огляд чисельних методів розв’язання крайових задач, з виділенням їх характерних недоліків при вирішенні нестаціонарних задач з високими градієнтами цільової функції, а також огляд новітніх методів включення геометричній інформації в аналітичну структуру, для чисельно-аналітичних методів рішення. Запропоновано чисельно-аналітичний структурно-різницевий підхід до вирішення високошвидкісних нестаціонарних теплових процесів. Виконано ряд обчислювальних експериментів, які показали високу точність запропонованого методу.

Ключові слова: *дискретна математична модель, крайова задача, аналітичні структури розв’язку, нестаціонарні теплові процеси.*

Приводится обзор численных методов решения краевых задач, с выделением их характерных недостатков при решении нестационарных задач с высокими градиентами искомой функции, а так же обзор новейших методов включения геометрической информации в аналитическую структуру, для численно-аналитических методов решения. Предложен численно-аналитический структурно-разностный подход к решению высокоскоростных нестационарных тепловых процессов. Проделан ряд вычислительных экспериментов, которые показали высокую точность предложенного метода.

Ключевые слова: *дискретная математическая модель, краевая задача, аналитические структуры решения, нестационарные тепловые процессы.*

1. Review of methods for solving boundary value problems

For the solution of boundary value problems of heat conduction, mechanics, electrodynamics and other fields for areas with non-canonical forms and curvilinear parts of boundaries the numerical methods most widely used are following:

- The finite difference method [1-3];
- The finite element method [4, 5];
- The integral equations method [6, 7];
- The variational-difference methods [8-10];
- Combination of several methods [11-12];

In the finite difference method boundary value problem for the differential equation reduces to a system of algebraic equations. When approximating the boundaries that do not coincide with the coordinate curves, particularly for desired functions large gradients, the method gives significant errors. To overcome this limitation curvilinear orthogonal coordinates [13] (also required the approximation of boundaries) and local curvilinear nonorthogonal coordinates [14, 15], which are related to the shape of the body are used (in that case need to create algorithms for the calculation in each area, and there is a risk to get physically inadequate decision).

In the integral equations method the original partial differential equations are replaced by the integral equation in region extent. The boundary is divided into a finite number of isothermal parts, and there is no problem to satisfy the boundary conditions. Unfortunately, the method faced with difficulties based on principles of the mathematical nature in solving nonstationary problems with strong nonlinearity parameters.

The finite element method for nonlinear nonstationary problems still needs to be improved in comparison with more developed method of finite differences.

There is general lack of numerical methods for solving boundary value problems: discrete approximation is used to both differential equations solution and boundary conditions accounting. In problems where the unknown function has a large gradient at the boundary, this leads to a growing of nonlinear superposition error and becoming higher than the allowable error.

Thus, for problems with high gradients of unknown function, promising development is not numerical, but numerical-analytical methods. However, as noted by G. I Marchuk, H Ortega, R. Schechter and other scientist, here there are difficulties associated with the construction of the basis (coordinate) functions for each point in time, which is exactly satisfying the nonstationary boundary conditions.

2. Review of methods for including geometric information in the structure of solutions

To create a structure for solving boundary value problems in the numerical-analytical methods it is required a description of the boundaries of the complicated regions. The equation of the complicated boundaries can be constructed using R-functions (RFM or R-Function Method) [16], PS-functions [17,18] and S-functions [19] by means of known equations of simple regions Development of numerical functions, through which it became possible to build in an implicit form of the boundary equations, started with the creation of R-functions by V. L. Rvachev . The complete system of R-functions is given by eq. (2.1):

$$\mu_1 \wedge_\sim \mu_2 = (1+\sim)^{-1}\left(\mu_1+\mu_2-\sqrt{\mu_1^2+\mu_2^2-2\sim\mu_1\mu_2}\right);$$
$$\mu_1 \vee_\sim \mu_2 = (1+\sim)^{-1}\left(\mu_1+\mu_2+\sqrt{\mu_1^2+\mu_2^2-2\sim\mu_1\mu_2}\right); -1 \le \sim \le 1. \qquad (2.1)$$

R-functions gave a good account of oneself as a method of analytical geometry, suitable for describing complex geometric objects. However, they have some grave disadvantages that occur when using R-functions in the basis functions in the analytical structure. The structure, obtained with they help, is unphysical, since there is not possible to describe the boundaries curvature using R-functions. The define coefficients of the Ritz's algebraic system which is obtained of calculation of double integrals over the research region, are equal to infinity.

R-functions’ potentialities are restricted by analytical geometry, for solving boundary value problems it is necessary to solve completely the inverse problem of differential geometry. And that means not only to write the equation of the border, which are "normalized" on the region boundary, but also accurately account for the curvature of the boundary. In this regard, A. P. Slesarenko in 1972 had proposed PS-function (2.2) [17], which allow strictly solve the inverse problem within the bounds of differential geometry. Furthermore, PS-functions are "loaded" with additional variables, which make the W support function "plate-shaped" , this property let to build the analytical structures of solutions whose behavior are physically adequately in the regions adjacent border as well as in the regions’ main body. If $\beta = 2$ in the PS-functions, they coincide with the R- functions for $\alpha = 0$. If $\beta \geq 4$ PS-functions allow you to accurately account for the curvature of the boundary.

$$\mu_1 \underset{PS}{\wedge} \mu_2 = \mu_1 + \mu_2 - \sqrt{\mu_1 \quad + \mu_2 \quad} ; \quad = 2N.;$$

$$\mu_1 \underset{PS}{\vee} \mu_2 = \mu_1 + \mu_2 + \sqrt{\mu_1 \quad + \mu_2 \quad} ; n = 0.5 \quad - 1; \tag{2.2}$$

$$\mu_{1,2} = f_{1,2}(1 + \sim_1 f_{1,2} + \sim_2 f_{1,2}{}^2 + \sim_3 f_{1,2}{}^3 + \sim_4 f_{1,2}{}^4 + ... + \sim_n f_{1,2}{}^n).$$

The necessitate to consider structural elements of complex shape, and physical processes which should be described adequately in the vicinity of the corner points, had led to the creation of S-functions (2.3). As there are no things in a real world with mathematical sharp corners, some exact solutions are unphysical in the neighborhood of the corner points (For example, the exact solution of Blasius problem for semi-infinite plate in axial flow of a laminar flow of a viscous incompressible fluid [20], the exact solution of the problem of determining the magnetic field between two magnets semi-infinite cylindrical shape [21]). S-functions allow us to construct continuous functions with continuous derivatives, and describe the real boundary of the body in the asymptotic approximation with the desired degree of accuracy; they might turn an unphysical precise mathematical description into an actual description of the boundary:

$$\mu_1 \underset{S}{\wedge} \mu_2 = -b + a^{\mu_1} + a^{\mu_2} - \sqrt{a^{\quad \cdot \mu_1} + a^{\quad \cdot \mu_2}}; \quad 1 \leq b \leq 2 - \sqrt{2};$$

$$\mu_1 \underset{S}{\vee} \mu_2 = -2 - a^{(\mu_1+\mu_2)0,5} + a^{\mu_1} + a^{\mu_2} + \sqrt{a^{\quad \cdot \mu_1} + a^{\quad \cdot \mu_2}}; \quad a > 1. \tag{2.3}$$

3. Problem definition of the research

Disadvantages of the solution of boundary value problems by numerical methods are most manifest in the modeling of high-speed high-gradient temperature processes. Such models are required in high-tech engineering fields such as space and nuclear, where it’s needed a solution with high accuracy.

We will consider the problem of heat conduction with nonstationary boundary conditions (3.1):

$$\begin{aligned} & c(t)\rho \cdot T(x,y,t)_t' = \lambda(t)\left(T(x,y,t)_{xx}'' + T(x,y,t)_{yy}''\right) + F_s(x,y,t); \\ & \left(\pm T(x,y,t)_x' + h(t)T(x,y,t)\right)\Big|_{x=\pm 1,} = h(t)T_e(x,y,t);\ T(x,y,0) = \varphi(x,y); \\ & \left(\pm T(x,y,t)_x' + h(t)T(x,y,t)\right)\Big|_{y=\pm 1} = h(t)T_e(x,y,t);\ x,y \in \Omega\ ,\ \ 0 < t < \infty. \end{aligned} \tag{3.1}$$

where the functions c (t), λ (t), h (t) describe the time variation of the specific heat of material structural element, its thermal conductivity, and the relative heat transfer coefficient, respectively, ρ – structural element density, T_e – environment temperature, Fs – sources.

We pass on to dimensionless quantities of position and time (3.2)

$$\begin{aligned} & c(t) = c_0\gamma(t);\ \lambda(t) = \lambda_0\sigma(t);\ \ h(t) = \alpha \cdot \lambda^{-1};\ a = c_0\rho \cdot \lambda_0^{-1};\ \ Bi(t) = h(t)l; \\ & x_1 = x \cdot l^{-1};\ \ y_1 = y \cdot l^{-1};\ Fo = atl^{-2};\ T(x,y,0) = \varphi(x,y); \end{aligned} \tag{3.2}$$

$$\begin{aligned} & \gamma(Fo)T(x,y,Fo)_{Fo}' = \sigma(Fo)\left(T(x,y,Fo)_{xx}'' + T(x,y,Fo)_{yy}''\right) + F_s(x,y,Fo)l^2 \cdot a^{-1}; \\ & \left(\pm T(x,y,Fo)_x' + Bi(Fo)T(x,y,Fo)\right)\Big|_{x=\pm 1} = Bi(Fo)T_e(x,y,Fo);\ \ x,y \in \Omega\ ; \\ & \left(\pm T(x,y,Fo)_y' + Bi(Fo)T(x,y,Fo)\right)\Big|_{y=\pm 1} = Bi(Fo)T_e(x,y,Fo);\ \ 0 < Fo < \infty. \end{aligned}$$

The numerical-analytical approach is offered to the solution of unsteady heat conduction problems based on the joint application of difference schemes of high order of accuracy, analytical structures and PS-functions.

4. Numerical-analytical approach to structural-difference modeling of the high-speed temperature processes

We will consider the application of structural-difference method to the solution of heat conduction problem with nonstationary boundary conditions for an infinite rectangular prism (4.1) -1≤x≤1, -1≤y≤1:

$$\begin{aligned} & T(x,y,Fo)_{Fo}' = \Delta T(x,y,Fo) + F(x,y,Fo);\ T(x,y,0) = \varphi(x,y); \\ & \left(\pm T(x,y,Fo)_x' + Bi(Fo)T(x,y,Fo)\right)\Big|_{x=\pm 1} = Bi(Fo)T_e(x,y,Fo);\ x,y \in \Omega\ ; \\ & \left(\pm T(x,y,Fo)_y' + Bi(Fo)T(x,y,Fo)\right)\Big|_{y=\pm 1} = Bi(Fo)T_e(x,y,Fo);\ 0 < Fo < \infty. \end{aligned} \tag{4.1}$$

The exact solution of the model problem we choose in the form of eq. (4.2):

$$\begin{aligned} & T_{ex}(x,y,Fo) = T_e(Fo) + (\theta(x,Fo) - f_1(x)\psi(x,Fo)_x' f_1(x)_x' + f_1(x)Bi(Fo) \times \\ & \psi(x,Fo)) \times (\chi(y,Fo) - f_2(y)\chi(y,Fo)_y' f_2(y)_y' + f_2(y)Bi(Fo)\chi(y,Fo)); \end{aligned} \tag{4.2}$$

The structure of the solutions (4.3) [22] for the problem (4.1) exactly satisfies the time-dependent boundary conditions and has a modular construction, any analytical dependence of Biot number and ambient temperature may be substituted in it.

$$T(x,y,Fo) = \omega_0(x,y,Fo) + \sum_{k,l} C_{k,l}\,\varphi_{k,l}(x,y,Fo)\ , \tag{4.3}$$

where $c_0(x,y,Fo) = Tcp(Fo)$; $^{-}(x,y) = T_{ex}(x,y,0)$;

$$F(x,y,Fo) = T_{\tau}(x,y,Fo)_{Fo}{}' - \left(T_{ex}(x,y,Fo)_{xx}{}'' + T_{ex}(x,y,Fo)_{yy}{}''\right);$$

$$i_{k,l}(x,y,Fo) = P_k(x)P_l(y) - W_1(x,y)\left[\left(P_k(x)_x{}' P_l(y)DW_1(x,y) - Bi(Fo)P_k(x)P_l(y)\right)\Big|_{x=\pm 1}\right] -$$

$$- W_2(x,y)\left[\left(P_l(y)_y{}' P_k(x)DW_2(x,y) - Bi(Fo)P_k(x)P_l(y)\right)\Big|_{y=\pm 1}\right];$$

$C_{k,l}$ – an unknown coefficients; $\Phi_0(x,y,Fo)$ – function, which is exactly satisfy the nonstationary inhomogeneous boundary conditions; $\chi_{k,l}(x,y,Fo)$ – basis functions, which exactly satisfy the nonstationary homogeneous boundary conditions; $P_k(x)$, $P_l(y)$ – normalized Chebyshev polynomials; $W_l(x,y)$ and $W_2(x,y)$ – PS-functions for an infinite rectangular prism of square section, DW1(x,y) and DW2(x,y) – derivatives of $W_l(x,y)$ and $W_2(x,y)$ in x and y, respectively, with a fixed value $DW_l(x,y)$ and $DW_2(x,y)$ on the border.

Information about the geometry area is defined by PS-functions (4.4):

$$W_1(x,y) = \mu_1(x) + (2\mu_2(y))^2 - \sqrt{\mu_1(x) \quad + (2\mu_2(y))^2} \; ; \qquad (4.4)$$

$$W_2(x,y) = \mu_2(y) + (2\mu_1(x))^2 - \sqrt{\mu_2(y) \quad + (2\mu_1(x))^2} \; ;$$

$$\mu_1(x) = f_1(x)\left(1 + \sim_1 \cdot f_1(x) + \sim_2 \cdot f_1(x)^2 + ... + \sim_n \cdot f_1(x)^n\right),$$

$$\mu_2(y) = f_2(y)\left(1 + \sim_1 \cdot f_2(y) + \sim_2 \cdot f_2(y)^2 + ... + \sim_n \cdot f_2(y)^n\right);$$

$$f_1(x) = 0.5(1 - x^2), \; f_2(y) = 0.5(1 - y^2), \; n = 0.5 \cdot \quad -1; \quad = 2N$$

Figure 1 shows the $W_1(x,y)$ support function of β=2; 4 and 8 which satisfying the zero curvature at the boundary of an infinite prism of square section and provides the best approximation properties of an analytic structures.

The discrete mathematical models are constructed using the finite-difference schemes [22]: "leapfrog" (4.5) and the "box" (4.6)

$$\left(T_{Fo}{}'\right)_{3\,i,j}^{\;s} = \left(aT\right)_{9\,lf.i,j}^{\;s} \qquad (4.5)$$

$$\left(T_{Fo}{}'\right)_{3\,i,j}^{\;s} = \left(aT\right)_{9\,b.i,j}^{\;s}, \qquad (4.6)$$

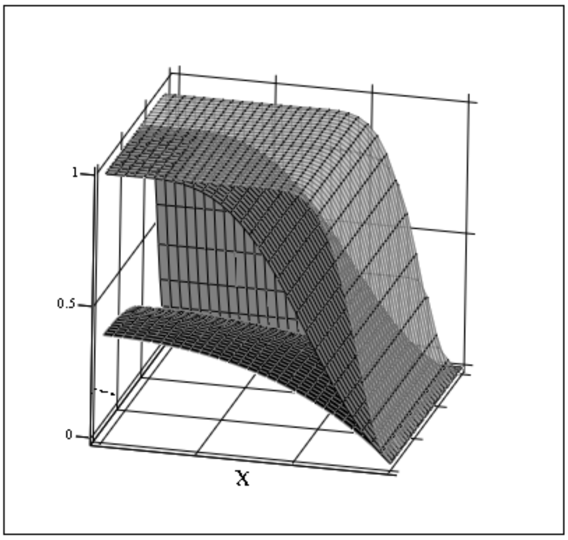


Fig. 1. The W1(x,y) support function of =2 (lower graph), =4 (middle graph), =8 (upper graph)

where $\left(T_{Fo}'\right)^{s}_{3\,i,j} = \left(T^{s}_{i,j} - T^{s-1}_{i,j}\right)\cdot Fo^{-1},\ s = 1,2;\ \left(T_{Fo}'\right)^{s}_{i,j} = \left(T^{s-2}_{i,j} - 4\cdot T^{s-1}_{i,j} + 3\cdot T^{s}_{i,j}\right)\times$

$\times\left(2\cdot Fo\right)^{-1},\ s > 2;\ (\Delta T)^{s}_{9\,lf.\,i,j} = \left(12h^{2}\right)^{-1}\left(-T^{s}_{i-2,j} - T^{s}_{i,j-2} - T^{s}_{i+2,j} - T^{s}_{i,j+2} +\right.$

$\left. +16\left(T^{s}_{i-1,j} + T^{s}_{i,j-1} + T^{s}_{i+1,j} + T^{s}_{i,j+1}\right) - 60T^{s}_{i,j}\right);\ (\Delta T)^{s}_{9\,b.\,i,j} = \left(6h^{2}\right)^{-1}\left(T^{s}_{i-1,j-1} +\right.$

$\left. + T^{s}_{i+1,j+1} + T^{s}_{i-1,j+1} + T^{s}_{i+1,j-1} + 4\left(T^{s}_{i-1,j} + T^{s}_{i,j-1} + T^{s}_{i+1,j} + T^{s}_{i,j+1}\right) - 20T^{s}_{i,j}\right)$.

A necessary spectral Neumann stability conditions [22] $|\lambda(\mu,\nu,r)| \le 1$ for the schemes (4.5) - (4.6), respectively:

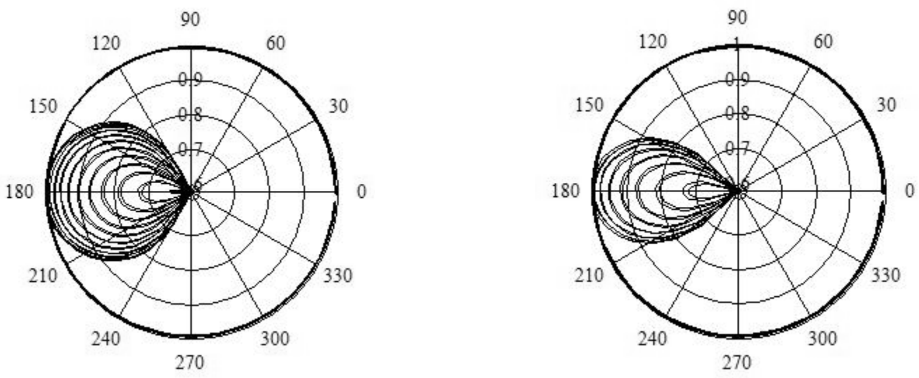
$$\lambda_{3-9\,lf.}(\mu,\nu,r) = 6^{-1}\cdot\left[4 + 2r\cdot A(\mu,\nu) \pm \sqrt{\left(4 + 2r\cdot A(\mu,\nu)\right)^{2} - 12}\right]; \qquad (4.7)$$

$$\lambda_{3-9\,b.}(\mu,\nu,r) = 6^{-1}\cdot\left[4 + 2r\cdot B(\mu,\nu) \pm \sqrt{\left(4 + 2r\cdot B(\mu,\nu)\right)^{2} - 12}\right]; \qquad (4.8)$$

where $A(\mu,\nu) = 12^{-1}\cdot\left[-\cos(2\mu) - \cos(2\nu) + 16\left(\cos(\mu) + \cos(\nu)\right) - 60\right]$;

$B(\mu,\nu) = 6^{-1}\cdot\left[\cos(\mu)\cos(\nu) + 4(\cos(\mu) + \cos(\nu)) - 20\right]$, $r = \Delta Fo\cdot h^{-2}$.

The maximum value of the r parameter, which complied with the necessary stability condition: r = 0,511 for the scheme (4.5), r = 0,889 for the scheme (4.6). Figure 2 shows the spectra of the complex $\lambda(\mu;\nu;r)$ for the schemes (4.5) and (4.6), satisfying the necessary spectral Neumann stability conditions.



a *b*

Fig. 2. The spectrum of λ(«;¬;r):(a) – scheme (4.5), r = 0,889;
(b) – scheme (4.6), r = 0,511

For each point of time we will obtain a discrete model in the form of equations. In matrix form equation (8) is given by: $B\overline{C} = \overline{G}$. To go to an algebraic system of equations of the form nxn, multiply both sides by the transposed matrix B^T: $B^T B\overline{C} = B^T\overline{G}$.

From the resulting linear system of equations it is easy to find the unknown coefficients of the basis functions. To interpolate them over the τ (4.9)

$$² = e^{-P_1 \cdot Fo}, \quad (4.9)$$

where P1 – the rate of heating and cooling, we will find the values of the coefficients of basis functions for the entire region $² \in [0;1]$. Thus, we obtain an approximate value of the temperature over the whole duration of time (4.10):

$$T(x, y, ²) = T_e(x, y, ²) + \sum_{k,l} C_{k,l}(²)\, ¡_{k,l}(x, y, ²)\,. \quad (4.10)$$

5. The results of numerical experiments

The series of numerical experiments is conducted in the range from 0.001Fo to 0.02Fo, which is characterized by the large gradients of the target function. In all numerical experiments the time step was 0.001Fo, were used 55 coordinate functions, α_1=0.25.

Numerical experiment 1 The parameters of the exact solution, environment temperature and Biot number: $¨(x) = \exp(-x^2)$, $\cdot\,(y) = \exp(-y^2)$, $Te(Fo) = 120(1 - J_0(Fo \cdot 500))$, $Bi(Fo) = 70(\sin(500Fo) + 1)$. Figure 3a shows graphs of temperature of infinite prism of square section (Ω region).

Table 1 shows the temperature in Ω region at three points of time. Temperatures calculated approximately are given at the top cells of the table, the exact temperature are given at the bottom cells. Calculations were carried out on difference scheme with three layers in time and nine points by coordinates, type "box", 900 knots, β=4.

Table 1. Numerical experiment 1. The temperature in Ω region at three points of time and the maximum relative error of calculation

Fo	Temperature	(0;0)	(0.5;0.5)	(1;1)	ε max, %
0.01	approximate	2793,083	960,8108	7,528908	0,502025
	exact	2793,101	960,8001	7,518958	
0.1	approximate	147,2439	143,4807	141,4281	0,015416
	exact	147,2538	143,4799	141,4469	
0.2	approximate	437,11	248,6085	149,6357	0,020259
	exact	437,1288	248,6061	149,6476	

<u>Numerical experiment 2</u> The parameters of the exact solution, environment temperature and Biot number: ¨ $(x)=\frac{1+100\cdot x^2}{1+0.1\cdot x^2}$, · $(y)=\frac{1+100\cdot y^2}{1+0.1\cdot y^2}$, $T_e(Fo)=10000\cdot\left(1-e^{-Fo}\right)$, $Bi(Fo)=e^{-10\cdot Fo}$. Figure 3b shows graphs of temperature in Ω region at the moment 0.02Fo. Table 2 shows the temperature in Ω region, difference scheme has 900 knots, β=8.

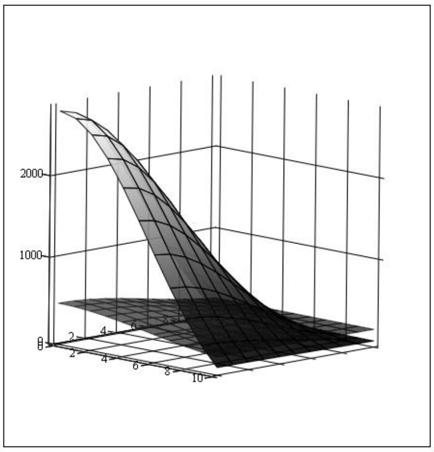
Table 2. Numerical experiment 2. The temperature in Ω region at three points of time, calculated using the difference schemes the "leapfrog" (3-9 lf) and the "box" (3-9 b), the maximum relative error of calculation

Fo	*difference scheme*	(0;0)	(0.5;0.5)	(1;1)	ε max, 10^{-3} %
0.01	3-9 lf.	12,196087	2798,053955	9282,056545	0,758424
	3-9 b	12,195341	2798,053643	9282,054198	0,767263
	exact	12,574497	3279,109000	9462,714000	–
0.1	3-9 lf.	101,827401	2983,914064	9504,085562	1,558383
	3-9 b.	101,826284	2983,913430	9504,063103	1,205007
	Exact	101,826284	2983,913430	9504,063103	–
0.2	3-9 lf.	200,518805	3202,403626	9765,789659	1,989289
	3-9 b.	200,517572	3202,402690	9765,751910	1,449082
	exact	200,517572	3202,402690	9765,751910	–

<u>Numerical experiment 3</u> The parameters of the exact solution, environment temperature and Biot number: ¨ $(x)=\left(\cos(x\cdot ® \cdot 2/3)+2\right)$, · $(y)=\left(\cos(y\cdot ® \cdot 2/3)+2\right)$, $T_e(Fo)=10000\cdot\left(1-e^{-0.5Fo}\right)$, $Bi(Fo)=e^{-230\cdot Fo}$. Figure 3c shows graphs of temperature in Ω region at the moment 0.01Fo. Table 3 shows the temperature in Ω region, depending on the support function's coefficients, by the example of temperature at the moment 0.01Fo. Calculations were carried out on difference scheme with three layers in time and nine points by coordinates, type "box", 400 knots.

Table 3. Numerical experiment 3. The temperature in Ω region and maximum relative error of calculation on the support function's coefficients at the moment 0.01Fo

Fo	Coefficients	(0; 0)	(0.5;0.5)	(0.9;0.9)	ε max, %
0.01	β=2	372,4742	80,17161	61,23909	0,029677
	β=4	372,4785	80,1695	61,23814	0,017820
	β=6	372,4781	80,1676	61,23457	0,016436
	Exact	372,4826	80,16862	61,23158	



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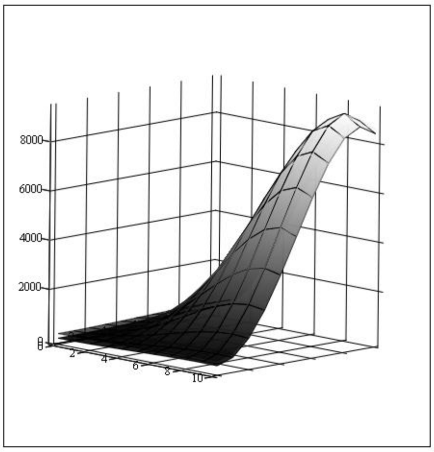

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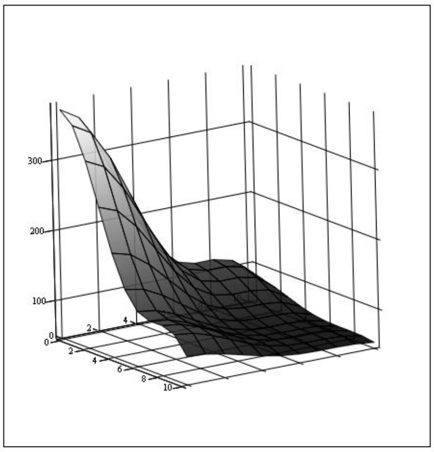

c

Fig. 3. The temperature at Ω region:
(a) Numerical experiment 1. The temperature at the moment 0.001Fo (lower graph) and at the moment 0.02Fo (upper graph);
(b) Numerical experiment 2. The temperature at the moment 0.02Fo;
(c) Numerical experiment 2. The temperature at the moment 0.01Fo

6. Summary

Structure-difference method combines the advantages of numerical methods and at the same time free from their shortcomings. It allows you to accurately account for nonstationary boundary conditions for any given time-depending functions in the boundary conditions, physical and geometrical characteristics of the body, is effective for the solution of unsteady boundary-value problems of desired function , with high gradients both in time and coordinates.

Models constructed on the basis of the method allows, without rebuilding the structures, to assess the desired function on the entire range of admissible parameters, which can be defined as an analytic function. Thus, it is possible to do qualitative analysis of the fine structure of dynamic processes, including such complex processes as the thermophysical processes with unsteady boundary conditions.

On the basis of structural-difference models can be created a database of the temperature behavior of structural elements of various shapes, materials and functions. The information in this database, thanks to interpolation of the coefficients of basis functions, can be stored in succinct format, which provides data compression.

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