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NUMERICAL SOLUTION OF INVERSE HEAT TRANSFER PROBLEMS BY PARAMETERS ESTIMATION OF ORDINARY DIFFERENTIAL EQUATIONS

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ABSTRACT

In this paper, algorithms for solving of two inverse one-dimensional heat transfer problems are considered. They are: the coefficient inverse problem and the determination of phase interface location in a melting problem. These inverse problems are reduced to parameters estimation of ordinary differential equations (ODE) using a finite element method. The algorithm based on the sensitivity analysis is applied to parameters estimation of the resultant ODE systems. Some results of numerical experiments are given.

INTRODUCTION

It is known that spatial discretization of the initial boundary value problem for a one-dimensional heat equation results in the Cauchy problem for a stiff ODE system. If the heat equation contains some unknown parameters, then as a result, we obtain the ODE system containing unknown parameters.

Actually, there are many effective algorithms for the numerical solution of stiff ODE systems. The Rosenbrock type methods refer to them. These methods have stability properties inherent to implicit methods and, as opposed to implicit methods, they do not require iterations in performance.

In (Gusev, 1983) an effective method of identification of parameters of stiff ODE systems was developed. The unknown parameters of ODE systems are estimated by using the least squares and sensitivity analysis. In addition, the identification method includes the effective Rosenbrock type method of the second order with a variable integration step.

Application of gradient methods for minimization of an objective function results in the necessity of obtaining derivatives of the solution of the ODE system with respect to the parameters. These derivatives are referred to as *sensitivity functions*. We name the ODE system, for which it is required to determine parameters, as the *basic system*. The sensitivity functions can be obtained by a simultaneous solution of the basic system and *sensitivity equations*. The sensitivity equations arise as a result of differentiation of the basic system with respect to parameters.

It follows from the construction of sensitivity equations that dimension of the ODE system considerably grows in computation of sensitivity functions. It is also known, that solution of ODE's by a Rosenbrock type method demands at each integration step the solution of linear equations systems of the same dimension as that of the ODE system .

The proposed approximation of the numerical solution of the basic system, being included in sensitivity equations, enables to solve block diagonal systems of linear equations thus considerably redusing the execution time.

THE PARAMETERS ESTIMATION METHOD OF ODE SYSTEM

Let us consider a Cauchy problem of an ODE system

$$\begin{aligned} \dot{y} &= f(y,t,p), \\ y(0,p) &= y_0, \end{aligned} \tag{1}$$

where $y, y_0 \in R^n$; $p \in R^m$ is a vector of parameters.

Let us denote $Z = (z_1, \ldots, z_s)^T$ a vector of observables. We assume, the components of Z to be suffuciently smooth functions of the solution to system (1). Let us designate Z_k^* values of the vector of observations at the times $t_k, k = 1, \ldots, s$, which are obtained as a result of measurements.

The estimated parameters are obtained as a result of minimization of the following function

$$\Phi(p) = \frac{1}{2} \sum_k (\Delta z_k)^T W_k (\Delta z_k), \tag{2}$$

where $\Delta z_k = z_k^* - z(y(t_k, p))$, W_k is the matrix of weight multipliers.

The components of the gradient of (2) can be calculated under the formula

$$\frac{\partial \Phi}{\partial p_i} = - \sum_k (\Delta z_k)^T W_k \frac{\partial z(y(t_k))}{\partial y} \frac{\partial y}{\partial p_i}(t_k, p) \tag{3}$$

The derivatives $\frac{\partial y}{\partial p_i}(t_k, p)$ are called sensitivity functions and can be obtained from the following ODE system

$$\begin{aligned} &\dot{y} = f(y, t, p), \\ &\dot{y}_{p_i} = f_y y_{p_i} + f_{p_i}, \\ &y(0, p) = y_0, \\ &y_{p_i}(0, p) = 0, \end{aligned} \tag{4}$$

where f_y is the Jacobian matrix of system (1). We suppose in (4) y_0 do not depend on p.

The considered method of computation of sensitivity functions is based on the use of the following L-stable Rosenbrock type method of the second order for solving nonautonomous ODE systems (Gusev, 1983)

$$\begin{aligned} &y_{n+1} = y_n + ak_1 + (1-a)k_2, \\ &[I - ahf_y]k_1 = hf(y_n, t_n + ah), \\ &[I - ahf_y]k_2 = hf(y_n + ak_1, t_n + 2ah), \end{aligned} \tag{5}$$

where h is an integration step, I is the identity matrix, $a = 1 - \frac{1}{\sqrt{2}}$ is a real number parameter.

The Jacobian of (4) has the following form:

$$\begin{pmatrix} f_y & & 0 \\ H_1 & f_y & \\ \vdots & \ddots & \\ H_s & \ldots & f_y \end{pmatrix}, \tag{6}$$

where

$$H_i = \frac{\partial^2 f}{\partial y^2} y_{p_i} + \frac{\partial^2 f}{\partial p_i \partial y}.$$

The reduction of computer costs is carried out in the algorithm by approximation of the basic system solution at points $t_n + ah$, $t_n + 2ah$ and their substitution in the sensitivity equations. Here we make use of the following formulas

$$y(t_k + ah) \approx y_k + ak_1, \quad y(t_k + 2ah) \approx y_k + a(k_1 + k_2), \tag{7}$$

As consequence of using (7) the following block-diagonal matrix participates in computations instead of matrix (6)

$$\begin{pmatrix} f_y & & 0 \\ & f_y & \\ & \ddots & \\ 0 & & f_y \end{pmatrix}.$$

Thus, at each integration step, $2 \times (m+1)$ linear equations systems of n dimension with the matrix $I - ahfy$ are solved instead of solution of two systems of $(m+1) \times n$ dimension.

By Taylor expansion of $y_p(t_n + h)$ and comparing that with expansion of the exact solution, it is easily verified, that formulas (7) do not bring an essential error in computation of sensitivity functions.

For the purpose of minimization of (2) it is possible to use the quickest descent or conjugate gradients methods with iterative regularization (Aliphanov, 1988).

In numerical calculations we used a variant of a quasi-Newton algorithm with iterative regularization. Calculation of a matrix closed to the Hessian in this algorithm is made under the recalculation formulas (Gill, 1971)

$$B^{k+1} = B^k + \frac{1}{\alpha_k z^T e^k} \cdot z z^T + \frac{1}{(g^k)^T e^k} \cdot g^k (g^k)^T, \tag{8}$$

where $z^k = g^{k+1} - g^k$; g^k is the gradient at the k -iteration; e^k is the direction of one-dimensional search at the k-th iteration determined from the equality $B^k e^k = -g^k$; α_k is a step along the direction of e^k. In this algorithm the matrix B^k holds in the form of the Cholesky decomposition $B^k = L^k D^k (L^k)^T$, where D^k is a diagonal matrix. The elements of D^k are "refreshed", if they are less than some given $\varepsilon > 0$. It allows us to avoid an excessive increase of the norm of the inverse matrix to B^k.

ESTIMATION OF COEFFICIENTS IN ONE-DIMENSIONAL HEAT EQUATION

We consider the following initial boundary value problem

$$
\begin{aligned}
&c(u)u_t = (\lambda(u)u_x)_x, \\
&(x,t) \in G \equiv \{(x,t) | 0 < x < l, 0 < t < T\}, \\
&u(x,0) = u_0, \\
&-\lambda(u)u_x|_{x=0} = \psi(t), \\
&u_x|_{x=l} = 0
\end{aligned} \tag{9}
$$

The inverse problem consists in definition of the functions $u(x,t)$, $c(u)$, $\lambda(u)$, if the density of the heat flow $\psi(t)$ and temperature values at the boundaries $u(0,t) = f_0(t)$, $u(l,t) = f_r$, and, may be, temperature values at some internal points $u(x_i,t) = f_i(t)$, $i = 1,\ldots,r-1$, $0 < x_i < l$ are known. The given inverse problem has the unique solution if conditions of monotony of heating and smoothness of the functions $\psi(t)$, $f_0(t)$, $f_1(t)$ hold (Muzilev, 1980).

Let us assume the coefficients $c(u)$, $\lambda(u)$ of the heat equation to be rather smooth functions, and it is possible to parametrize them $c(u) = \sum_i^{m_1} c_i g_i(u)$, $\lambda(u) = \sum_i^{m_2} \lambda_i g_i(u)$. For example, as $g_i(u)$ it is possible to take u^i or B-splines. Using discretization of the heat equation by the Galerkin method employing piecewise basic functions we arrive at the ODE system of the form

$$
\begin{aligned}
&A(y,\bar{c})\dot{y} - B(y,t,\bar{\lambda}) = 0, \quad y \in R^N, \\
&y(0) = y_0,
\end{aligned} \tag{10}
$$

where N is the number of mesh points, A is a square symmetric three-diagonal matrix, $\bar{c} = (c_1,\ldots,c_{m_1})^T$, $\bar{\lambda} = (\lambda_1,\ldots,\lambda_{m_2})^T$ are parameters of the ODE system subject to definition, y_0 is the vector of u_0 values on the grid.

A more detailed description of application of the Galerkin method to problem (9) is considered in (Gusev, 1989). A change of the solution of the ODE system (10) at one integration step with the use of method (5) can be expressed as the following

$$
\begin{aligned}
&y_{n+1} = y_n + ak_1 + (1-a)k_2, \\
&k_1 = hD^{-1}A^{-1}(y_n,\bar{c})B(t_n + ah, y_n, \bar{\lambda}), \\
&k_2 = hD^{-1}A^{-1}(y_n,\bar{c})B(t_n + 2ah, y_n, \bar{\lambda}), \\
&D = I - ah[A^{-1}(y_n,\bar{c})B(t_n, y_n, \bar{\lambda})]_y,
\end{aligned} \tag{11}
$$

where $[A^{-1}B]_y = A^{-1}B_y - A^{-1}A_yA^{-1}B$.

In a similar way, it is possible to consider the reduction of a boundary inverse heat transfer problem to the problem of parameters estimation of an ODE system. A more interesting illustration of our technique is given in the next section.

ESTIMATION OF PHASE INTERFACE LOCATION IN A MELTING PROBLEM

The following one-dimensional melting problem is considered

$$
\begin{aligned}
&c_L u_t = (\lambda_L(u_l)_x)_x, \qquad 0 < x < \xi(t), && (12)\\
&c_S u_t = (\lambda_S u_x)_x, \qquad \xi(t) < x < l, && (13)\\
&u(\xi(t),t) = u_m, && (14)\\
&-\rho\mathcal{L}\dot{\xi} = \lambda_S u_x - \lambda_L(u_l)_x, \quad x = \xi(t), && (15)\\
&u_l(0,t) = f_0(t), && (16)\\
&u(l,t) = f_l(t), && (17)\\
&u(x,0) = u_0(x), \qquad 0 < x < l, && (18)\\
&\xi(0) = 0, && (19)
\end{aligned}
$$

where u, u_l are temperature values of the solid and the liquid phases, respectively;
c_L, c_S are the volumetric heat capacity coefficients of the liquid and the solid phases;
λ_L, λ_S are the heat conduction coefficients of the liquid and the solid phases;
$f_0(t)$, $f_l(t)$ are the temperature dependences of t at $x = 0$ and at $x = l$, respectively;
$\mathcal{L}$ is the latent melting heat;
$\xi(t)$ is the change of the phase interface location;
$u_0(x)$ is the initial temperature, i.e. at $t = 0$, $x \in (0,l)$;
u_m is the fusion temperature.

It is supposed that the functions $f_l(t)$, $u_0(x))$ are known, and, also, we have f_{ij}, $j = 1,\ldots,r$ - measurements of temperature at the points z_i, $I = 1,\ldots,r$ of the solid phase. The inverse problem consists in definition of the functions $u(x,t)$, $\xi(t)$ satisfying equations (12) - (19).

Let us consider the approximation of $\xi(t)$ by B-splines. We denote: k – the given order of B-splines for approximation of $\xi(t)$, M – the number of intervals of splitting of $[0,T]$. Let us set a sequence of nodes $\{t_i\}_{i=1}^{2(k-1)+M-1}$ such that

$$
\begin{aligned}
&t_1 \le t_2 \le \ldots \le t_k = 0, \\
&t_i < t_{i+1}, \quad i = k,\ldots,k+M, \\
&T = t_{k+M} \le \ldots \le t_{2(k-1)+M+1}.
\end{aligned}
$$

For each unit t_i $(i = 1, \ldots, k + M - 1)$ we set $B_{i,k}$ as a normalized B-spline of the k-th order determined in (de Boor, 1985) by means of the k-th divided difference of the function $B_k(t, x) = (t - x)_+^{k-1}$, namely,

$$B_{i,k}(x) = (t_{i+k} - t_i)[t_i, \ldots, t_{i+k}]b_k,$$

where $[t_i, \ldots, t_{i+k}]g$ is a designation of divided difference of the function g (de Boor, 1985).

Let us consider the problem of the determination of the phase interface location as problem of definition of the coefficients p_i of the following linear combination

$$\hat{\xi}(t) = \sum_{i=1}^{m} p_i B_{i,k}(t), \quad m = M + k - 1, \tag{20}$$

such, that the following functional

$$F(p_1, \ldots, p_m) = \frac{1}{2}\Bigg(\sum_{j=1}^{r} \sum_{\{i:\, z_i > \hat{s}(t_j)\}} \big(u(z_i, t_j) - f_{ij}\big)^2 + \alpha_1 \sum_{\{i:\, z_i \le \hat{s}(T)\}} \big(\hat{s}(\tau_i) - z_i\big)^2 \Bigg), \tag{21}$$

has the minimal value with substitution of (20) into (12) – (15). In (21), we denote by τ_i the times of the achievement (known from the experiment, if any) by the phase interface location of the points z_i which are dispositions of the temperature detectors. The second summand in (21) allows for a useful information on the ahievement by $\xi(t)$ of the points z_i. If it is known from the heat experiment that the phase interface location has not achieved any point z_i, then we set $\alpha_1 = 0$.

As well as in (Zabaras, 1989) we have introduced into the minimized functional a regularizing addend for the improvement of stability of the inverse problem solution. The addend is defined by

$$\Phi_1(p_1, \ldots, p_m) = \alpha_2 \sum_{j=1}^{r} \beta_j \left(\frac{d\hat{s}}{dt}(t_j) \right)^2, \tag{22}$$

where β_j are weight multipliers, α_2 is a regularization parameter, which depends on measurement errors.

It is necessary to note, that when the direct problem is solved the moving phase interface location is defined by some given vector of parameters. Therefore in calculations we use only one of the two Stephan conditions, namely, condition (14).

We use a moving finite element method in solution of the direct problem. Let us consider its application in more detail.

We set on $[\xi(t), l]$ a mesh $G = \{s_i\}_{i=1}^{N}$ which has extreme points, coinciding with the ends of this closed segment, i.e. $s_1 = \xi(t)$, $s_N = l$. There are many ways to set movements of the other nodes.

Let us take, for example, uniform disposition of nodes on $[\xi(t), l]$ at anyone $t \in [0, T]$. Then distribution of $s_i(t)$, $i = 2, \ldots, N-1$, is determined by the nodes s_1, s_N and can be calculated as follows:

$$s_i(t) = \xi(t) + \frac{\big(l - \xi(t)\big)\,(i-1)}{N-1}, \qquad i = 2, \ldots, N-1. \tag{23}$$

We define on the grid G the basic piecewise linear functions:

$$\varphi_i(x,t) = \begin{cases} \frac{x - s_{i-1}}{h} & \text{when } s_{i-1} < x < s_i \\ \frac{s_{i+1} - x}{h} & \text{when } s_i < x < s_{i+1} \\ 0 & \text{in other cases} \end{cases} \tag{24}$$

where $i = 2, \ldots, N-1$;

$$\varphi_1(x,t) = \begin{cases} \frac{s_2 - x}{h} & \text{when } s_1 < x < s_2, \\ 0 & \text{in other cases;} \end{cases} \tag{25}$$

$$\varphi_N(x,t) = \begin{cases} \frac{x - s_{N-1}}{h} & \text{when } s_{N-1} < x < s_N, \\ 0 & \text{in other cases.} \end{cases} \tag{26}$$

According to the moving finite element method the numerical solution of the initial boundary value problem (12)-(19) is determined as

$$u(x,t) = \sum_{i=2}^{N-1} y_i(t)\varphi_i(x,t) + u_m\varphi_1(x,t) + f_l(t)\varphi_N(x,t). \tag{27}$$

As a result, we have the Cauchy problem for an ODE system, which is dependent on parameters $p_1, \ldots, p_m$

$$A(y,t,p)\dot{y} = B(y,t,p), \qquad (28)$$
$$y(0) = y_0, \qquad p = (p_1,\ldots,p_m)^T.$$

The formulas for solution of system (28) and the corresponding sensitivity equations by the Rosenbrock method can be obtained by analogy with (11).

NUMERICAL EXPERIMENTS

Estimation of $c(u), \lambda(u)$ in a one-dimensional heat equation

The process of heating of an unlimited plate of thickness equal to 1cm under the influence of light radiation is considered. It is supposed that at one side the plate is insulated. It is required to determine the volumetric capacity and the heat conduction of the material as functions of temperature by using temperature measurements at both sides of the plate and inside it at distances of 0.3cm and 0.6cm from the heated side and by the known function specifying a heat flow. The heat transfer process inside the plate is described by the following one-dimensional heat equation

$$c(u)u_t = (\lambda(u)u_x)_x, \qquad (29)$$
$$0 < x < l(=1cm), \quad 0 < t \le T(=540s)$$

with the initial and the boundary conditions:

$$u(x,0) = u_0(=300K),$$
$$\lambda(u)u_x|_{x=0} = \epsilon\varsigma(f(t) - u^4(0,t)),$$

where $\epsilon = 0.8$ is emmisivity, $\varsigma = 5.669 \cdot 10^{-12}\frac{\mathrm{W}}{\mathrm{cm^2K^4}}$ is the Boltzmann constant, $f(t) = (t/0.6 + 300)^4$;

$$u_x|_{x=l} = 0. \qquad (30)$$

It is supposed in this example that the temperature dependence of c, λ is well described by polynomials of the third or the lesser degree. Specifically, these polynomials are the following

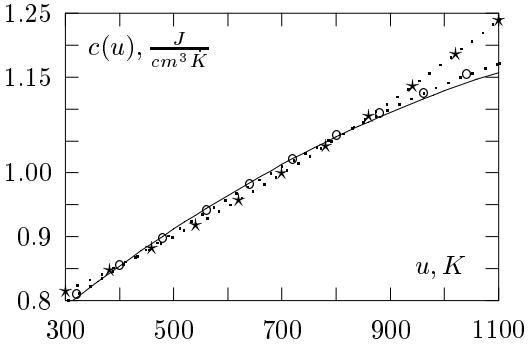

Figure 1. ESTIMATION OF THE VOLUMETRIC CAPACITY COEFFICIENT: ——- - exact solution; · · · o · · · - $\sigma = 5K$; · · · ⋆ · · · - $\sigma = 10K$

$$c(u) = 0.5745 + 0.7955 \cdot 10^{-3}u - 0.2416 \cdot 10^{-6}u^2, \qquad (31)$$
$$\lambda(u) = 0.1228 \cdot 10^{-1} +$$
$$0.7430 \cdot 10^{-5}u + 0.6220 \cdot 10^{-11}u^3 \qquad (32)$$

The temperature "measurements" were simulated as a result of solution of the given initial boundary value problem with $c(u)$, $\lambda(u)$ taken from (31), (32). Random disturbances were added to the simulated values of temperature for ivestigation of the influence of measurement errors on the accuracy of determination of c, λ. The random errors were simulated with the help of a pseudorandom numbers generator. They were normally distributed with zero average and standard deviation 5 K, 10 K.

The constant values of $c = 0.7\frac{\mathrm{J}}{\mathrm{cm^3 \cdot K}}$, $\lambda = 0.03\frac{\mathrm{W}}{\mathrm{cm \cdot K}}$ were taken as initial before minimization.

The results of restoration of $c(u), \lambda(u)$ are given in Fig. 1, 2. In calculation of the gradient of the objective function in the example, the dimension of the ODE system has in 9 times increased in comparison with the ODE system, which was solved in calculation of the objective function. Houever, the computer time for calculation of the gradient has less than in 3 times increased ; $t_{\nabla\Phi} = 2.85$ s in comparison with $t_\Phi = 1.05$ s on Pentium 75. It confirms the efficiency of the used technique.

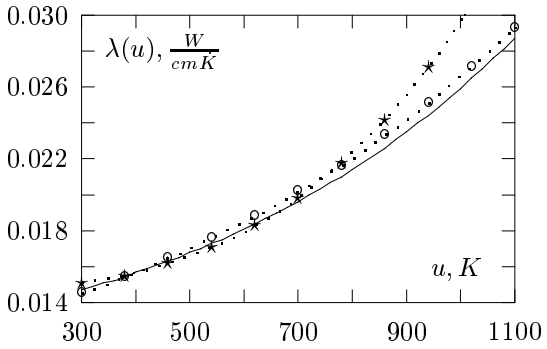

Figure 2. ESTIMATION OF THE HEAT CONDUCTIVITY COEFFICIENT: ——- - exact solution; $\cdots\circ\cdots$ - $\sigma = 5K$; $\cdots\star\cdots$ - $\sigma = 10K$

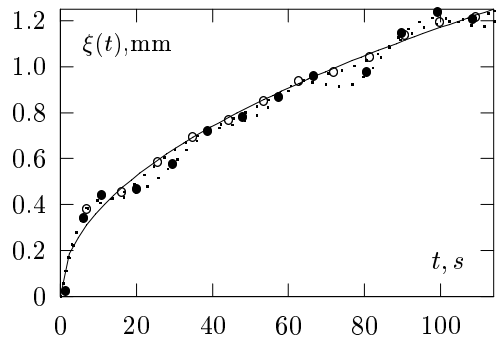

Figure 3. ESTIMATION OF THE PHASE INTERFACE LOCATION: ——- - exact solution; $\cdots\circ\cdots$ – $\sigma = 0.01\ ^\circ C$; $\cdots\bullet\cdots$ – $\sigma = 0.05\ ^\circ C$;

The numerical determination of the change of the phase interface location

As an example of the inverse melting problem we consider the problem of determination of the change of the phase interface location of an unlimited plate of ice. We used the following data of the experiment: the thickness of the plate is 5 mm; the initial temperature of ice is $-5\ ^\circ C$; when $t > 0$ the plane $X = 0$ is supported with constant temperature $u_h = +5\ ^\circ C$.

In (Carslaw, 1964) the analytical solution of one-dimensional two-phase melting problem with constant thermal properties is given. The temperature fields in the liquid and the solid phases are described by the equations

$$u_l = u_h - \frac{u_h - u_m}{\mathrm{er}\, f(\psi)} - \mathrm{er}\, f\left(\frac{x}{2\sqrt{a_L \cdot t}}\right), \qquad (33)$$

$$u = \frac{u_m}{\mathrm{er}\, f^*(\psi \cdot r)} - \mathrm{er}\, f^*\left(\frac{x}{2\sqrt{a_S \cdot t}}\right), \qquad (34)$$

where $\mathrm{er}\, f(z) = \frac{2}{\pi^{1/2}} \int_0^z e^{-t^2} dt$, $\mathrm{Er}\, f^*(z) = 1 - \mathrm{er}\, f(z)$, ψ is the root of the equation

$$\psi = \frac{\bar{c}_L(u_h - u_m)}{\pi^{1/2} L}\left(\frac{\exp\left(-\psi^2\right)}{\mathrm{er}\, f(\psi)} - \frac{\lambda_L r u_m \cdot \exp\left(-\psi^2 r^2\right)}{\lambda_S (u_h - u_m) \mathrm{er}\, f^*(\psi r)}\right). \qquad (35)$$

Here we use the following notations: a_L, a_S are diffusivities of liquid and solid phases; $\bar{c}_L$ is mass capacity of water; $r = (a_S/a_L)^{1/2}$. The analytical solution of the melting boundary problem is obtained as $\xi(t) = 2\psi\sqrt{a_L t}$.

Equation (35) was numerically solved and the value $\psi = 1,541\,27 \cdot 10^{-4}$ was obtained . The temperature values at $z_1 = 1,25$; $z_2 = 5$ mm are calculated by formula (34). The temperature values at $z_2 = 5$ mm were used as boundary conditions when the direct problem was solved. At $T = 114$ s the phase interface location attained the position $x = 1,25$ mm.

In order to calculate "temperature measurements", the simulated measurement errors were added to temperature values calculated by formula (34). The errors was normal distributed with zero average and standard deviations $\sigma = 0.01;\ 0.05\ ^\circ C$.

For approximation of the change of the phase interface location we set 12 normalized B-splines of the fourth order. Here, the uniform grid on $[0, T]$ was used. As the initial values of parameters, the coefficients of B-spline were taken, which approximated by the least squares the line segment connecting the points $(0, 0)$ and (T, z_1). Numerical results for different standard deviations of errors are given in Fig. 3.

CONCLUSION

The method of solution of the inverse heat transfer problems is proposed. This method is based on reducing the inverse problem to the ODE system with unknown parameters. The method, developed by the author, is used for estimation of the unknown parameters of the ODE system. It provides the effective calculation of sensitivity functions. The results of solution of two one-dimensional inverse problems confirm the utility and the efficiency of the proposed

method.

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