# CONTROL OF AN ERROR OF A FINITE-DIFFERENCE SOLUTION OF THE HEAT-CONDUCTION EQUATION BY THE CONJUGATE EQUATION

## A. K. Alekseev

The results of the calculation of temperature by the finite-difference method can be verified and the value of the remaining error can be estimated by the conjugate problem with a moderate expenditure of computer resources.

**Introduction.** Using the conjugate equations we can calculate variation of an arbitrary functional of the physical field proceeding from local perturbations of the latter [1, 2]. In [3, 4], the conjugate equations are used to verify calculation of a certain objective functional; in [6], this approach is applied to optimization of the computational grid. In what follows, for the finite-difference solution we considered the approach based on estimation of the error by the Taylor series in the Lagrangian form and the conjugate equations in continuous formulation. In contrast to the approaches of [3–5], it allows one not only to verify the solution but also to estimate the accuracy of the result.

Estimation of an Error of Finite-Difference Calculation. We consider the scheme of estimating the error of calculation of temperature at the control point (and decrease of this error) by an example of the finite-difference solution of the one-dimensional equation of heat conduction

$$C\rho \frac{\partial T}{\partial t} - \frac{\partial}{\partial x} \left( \lambda \left( T \right) \frac{\partial T}{\partial x} \right) = 0, \quad (t, X) \in (0 < t < t_{\rm f}, \quad 0 < x < X).$$
<sup>(1)</sup>

The initial conditions are

$$T(0, x) = T_0(x) . (2)$$

The boundaries are thermally insulated:

$$\frac{\partial T}{\partial x}\Big|_{x=0} = 0 , \quad \frac{\partial T}{\partial x}\Big|_{x=X} = 0 . \tag{3}$$

We consider the finite-difference algorithm of second-order accuracy over the time and coordinate; the algorithm coincides with the integro-interpolation method [6] at the constant step of calculation along the coordinate and the thermal conductivity:

$$C\rho \frac{T_k^{n+1/2} - T_k^n}{\tau} - \frac{1}{2} \lambda \frac{T_{k+1}^n - 2T_k^n + T_{k-1}^n}{h_k^2} = 0, \qquad (4a)$$

$$C\rho \frac{T_k^{n+1} - T_k^{n+1/2}}{\tau} - \frac{1}{2} \lambda \frac{T_{k+1}^{n+1} - 2T_k^{n+1} + T_{k-1}^{n+1}}{h_k^2} = 0.$$
(4b)

#### UDC 536.5:519.6

<sup>&</sup>quot;Energiya" Russian Space Corporation, 4a Lenin Str., Korolev, Moscow Region, 141070, Russia; email: aleksey.alekseev@relcom.ru. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 77, No. 1, pp. 146–151, January–February, 2004. Original article submitted August 18, 2003.

We expand the expressions in the vicinity of  $T_k^n$  using the Taylor series in the Lagrangian form, e.g.,  $T_{k+1}^n = T_k^n + h_k \frac{\partial T}{\partial x} + \frac{h_k^2}{2} \frac{\partial^2 T(x_k + \alpha_k^n h_k, t_n)}{\partial x^2}$  (the parameters  $\alpha_k^n \in (0, 1)$  are unknown). Thus, solving finite-difference equations (4), we calculate, instead of (1), its differential approximation

$$C\rho \frac{\partial T}{\partial t} - \frac{\partial}{\partial x} \left( \lambda \left( T \right) \frac{\partial T}{\partial x} \right) + \delta T = 0 , \quad \delta T = \delta T_t + \delta T_x .$$
(5)

We determine the temperature error at a certain control point  $T_{est} = T(t_{est}, x_{est})$  as a function of approximation  $\delta T$ . We denote  $T_{est} = T(t_{est}, x_{est})$  as  $\varepsilon(\delta T)$  and write as a functional

$$\varepsilon \left(\delta T\right) = \iint_{\Omega} T\left(t, x\right) \delta\left(t - t_{\text{est}}\right) \delta\left(x - x_{\text{est}}\right) dt dx .$$
(6)

It is known that the most effective method of calculation of the gradient of the functional is based on use of the conjugate equation [1, 2]. We apply this approach following [7]. The variation of the functional has the form

$$\Delta \varepsilon = \Delta T_{\text{est}} = \iint_{\Omega} \delta T \Psi(x, t) \, dt dx \,. \tag{7}$$

Here  $\Psi$  is the conjugate temperature obtained from the solution of the following (conjugate) problem:

$$C\rho \frac{\partial \Psi}{\partial t} + \lambda \frac{\partial^2 \Psi}{\partial x^2} - \delta \left( t - t_{est} \right) \delta \left( x - x_{est} \right) = 0.$$
(8)

The boundary conditions are

$$\frac{\partial \Psi}{\partial x} \bigg|_{x=0}^{X=1} = 0 , \quad \frac{\partial \Psi}{\partial x} \bigg|_{x=0}^{X=0} = 0 .$$
(9)

The initial condition is

$$C\rho\Psi\left(t,x\right)\left|^{t_{\rm f}}=0.$$
(10)

This problem is solved in the opposite direction with respect to time. From the conjugate equations used in the inverse problems of heat conduction it differs by the form of the source in (8). Usually, problem (8) is solved by the finite-difference method; therefore, it also has a discretization error  $\Psi(x, t) = \Psi_{\text{exact}}(x, t) + \Delta \Psi(x, t)$ . Thus, the error of the functional can be divided into two parts

$$\Delta \varepsilon = \Delta T_{\text{est}} = \iint_{\Omega} \delta T \Psi_{\text{exact}}(x, t) \, dt dx + \iint_{\Omega} \delta T \Delta \Psi(x, t) \, dt dx \tag{11}$$

and can be calculated by expanding finite differences into Taylor series. In this case, the uncertainty related to the last term of the Taylor series and the second part of expression (11) remains.

Estimation of the Error of Approximation of the Spatial Derivative. We use the Taylor series in the Lagrangian form ( $\beta_k^n \in (0, 1)$  and  $\gamma_k^n \in (0, 1)$  are unknown)

$$T_{k+1}^{n} = T_{k}^{n} + h_{k} \frac{\partial T}{\partial x} + \frac{1}{2} h_{k}^{2} \frac{\partial^{2} T}{\partial x^{2}} + \frac{1}{6} h_{k}^{3} \frac{\partial^{3} T}{\partial x^{3}} + \frac{1}{24} h_{k}^{4} \left( \frac{\partial^{4} T(t_{n}, x_{k} + \beta_{k}^{n} h_{k})}{\partial x^{4}} \right) = 0,$$

$$T_{k-1}^{n} = T_{k}^{n} - h_{k} \frac{\partial T}{\partial x} + \frac{1}{2} h_{k}^{2} \frac{\partial^{2} T}{\partial x^{2}} - \frac{1}{6} h_{k}^{3} \frac{\partial^{3} T}{\partial x^{3}} + \frac{1}{24} h_{k}^{4} \left( \frac{\partial^{4} T(t_{n}, x_{k} - \gamma_{k}^{n} h_{k})}{\partial x^{4}} \right) = 0.$$

Approximation of the second derivative can be written as

$$\frac{T_{k+1}^{n} - 2T_{k}^{n} + T_{k-1}^{n}}{h_{k}^{2}} = \frac{\partial^{2}T}{\partial x^{2}} + \frac{1}{24} h_{k}^{2} \left( \frac{\partial^{4}T(x_{k} + \beta_{k}^{n}h)}{\partial x^{4}} + \frac{\partial^{4}T(x_{k} - \gamma_{k}^{n}h)}{\partial x^{4}} \right).$$
(12)

Expression (7) takes on the form

$$\Delta \varepsilon \left(\delta T\right) = -\int_{\Omega} \frac{\lambda}{24} h_k^2 \left( \frac{\partial^4 T \left( x_k + \beta_k^n h \right)}{\partial x^4} + \frac{\partial^4 T \left( x_k - \gamma_k^n h \right)}{\partial x^4} \right) \Psi dx dt .$$
(13)

In the discrete form

$$\Delta \varepsilon \left(\delta T\right) = -\frac{\lambda}{24} \sum_{k=1,i=1}^{N_x,N_t} h_k^2 \left( \frac{\partial^4 T \left(x_k + \beta_k^n h\right)}{\partial x^4} + \frac{\partial^4 T \left(x_k - \gamma_k^n h\right)}{\partial x^4} \right) \Psi_k^n h_k \tau \,. \tag{14}$$

This expression can also be expanded into the Taylor series; in the first order we obtain

$$\Delta \varepsilon \left(\delta T\right) = -\frac{\lambda}{12} \sum_{k=1,i=1}^{N_x,N_t} h_k^3 \frac{\partial^4 T\left(x_k\right)}{\partial x^4} \Psi_k^n \tau - \frac{\lambda}{24} \sum_{k=1,n=1}^{N_x,N_t} h_k^3 \left(\frac{\partial^5 T\left(t_n, x_k\right)}{\partial x^5} \beta_k^n - \frac{\partial^5 T\left(t_n, x_k\right)}{\partial x^5} \gamma_k^n\right) \Psi_k^n h_k \tau \,. \tag{15}$$

The first part has the second order over h; it can be calculated and used to verify the functional

$$\Delta T_x^{\text{corr}} = \Delta \varepsilon \ (\delta T) = -\frac{\lambda}{12} \sum_{k=1,i=1}^{N_x,N_t} h_k^3 \frac{\partial^4 T(x_k)}{\partial x^4} \Psi_k^n \tau \ ; \tag{16}$$

a noncontrollable error is produced by the second part of (15) (the third order over *h*). We can obtain an upper estimate of the second term of the functional error (assuming  $\beta_k^n - \gamma_k^n = 1$ ):

$$\frac{\lambda}{24}\sum_{k=1,n=1}^{N_x,N_t} h_k^3 \left( \frac{\partial^5 T(t_n, x_k)}{\partial x^5} \beta_k^n - \frac{\partial^5 T(t_n, x_k)}{\partial x^5} \gamma_k^n \right) \Psi_k^n h_k \tau < \frac{\lambda}{24}\sum_{k=1,n=1}^{N_x,N_t} h_k^4 \left| \frac{\partial^5 T(t_n, x_k)}{\partial x^5} \Psi_k^n \right| \tau.$$

$$\tag{17}$$

Here we consider it as an upper estimate of the error of approximation of the spatial derivative

$$\Delta T_x^{\text{sup}} = \frac{\lambda}{24} \sum_{k=1,n=1}^{N_x \cdot N_t} h_k^4 \left| \frac{\partial^5 T(t_n, x_k)}{\partial x^5} \Psi_k^n \right| \tau .$$
(18)

Strictly speaking, we can retain a larger number of terms of the Taylor series; in the subsequent, second order of accuracy the upper estimate  $T_{x,2}^{sup}$  has the form

$$\delta\varepsilon_{2} = \frac{\lambda}{48} \sum_{k=1,n=1}^{N_{x},N_{t}} h_{k}^{5} \left( \frac{\partial^{6}T(t_{n},x_{k})}{\partial x^{6}} \beta_{k}^{n} + \frac{\partial^{6}T(t_{n},x_{k})}{\partial x^{6}} \gamma_{k}^{n} \right) \Psi_{k}^{n} \tau < \frac{\lambda}{24} \sum_{k=1,n=1}^{N_{x},N_{t}} \left| \frac{\partial^{6}T}{\partial x^{6}} \Psi_{k}^{n} \right| \tau h_{k}^{5} = \Delta T_{x,2}^{\sup} .$$

$$\tag{19}$$

179

As a result, we can obtain the estimate of the error of the verified solution  $|T - \Delta T_x^{\text{corr}} - T_{\text{exact}}| < \Delta T_x^{\text{sup}} + \Delta T_{x,2}^{\text{sup}}$ . However, the numerical experiments conducted show that the first-order estimate would suffice.

Estimation of the Error of Approximation of the Time Variable. A similar approach for the error of approximation of the time variable yields an eliminable error

$$\Delta T_t^{\text{corr}} = \Delta \varepsilon \left(\delta T\right) = -\frac{C\rho}{12} \sum_{k=1,n=2}^{N_x,N_t} \frac{\partial^3 T\left(t_n, x_k\right)}{\partial t^3} \Psi_k^n h_k \tau^3$$
(20)

and the maximum estimate of an uneliminable error

$$\Delta T_t^{\sup} = \Delta \varepsilon \left(\delta T\right) = \frac{C\rho}{4} \sum_{k=1,n=2}^{N_x N_t} \frac{\partial^4 T\left(t_n, x_k\right)}{\partial t^4} \Psi_k^n h_k \tau^4.$$
<sup>(21)</sup>

Variable Grid Meshes and Thermal Conductivity. Variability of the spatial grid and thermal conductivity over a space is the source of an additional error. For the sake of analysis, we turn back from the simplified form of presentation of finite-difference equations (4) to the complete form of writing of the integro-interpolation method [6]:

the first step

$$C_k \rho_k \frac{T_k^{n+1/2} - T_k^n}{\tau} = Z_{k+1/2} \left( T_k^n - T_{k+1}^n \right) + Z_{k-1/2} \left( T_k^n - T_{k-1}^n \right),$$
(22a)

the second step

$$C_k \rho_k \frac{T_k^{n+1} - T_k^{n+1/2}}{\tau} = Z_{k+1/2} \left( T_k^{n+1} - T_{k+1}^{n+1} \right) + Z_{k-1/2} \left( T_k^{n+1} - T_{k-1}^{n+1} \right),$$
(22b)

where

$$Z_{k+1/2} = \frac{2}{hx_k \left(\frac{hx_k}{\lambda_k} + \frac{hx_{k+1}}{\lambda_{k+1}}\right)}; \quad Z_{k-1/2} = \frac{2}{hx_k \left(\frac{hx_k}{\lambda_k} + \frac{hx_{k-1}}{\lambda_{k-1}}\right)}.$$

Approximation of the second derivative on a nonuniform grid with a variable coefficient of heat conduction generates the following expansion terms:

$$z_{1} \frac{\partial T}{\partial x}, \quad z_{1} = \left[\frac{h_{k+1} + h_{k}}{h_{k+1}/\lambda_{k+1} + h_{k}/\lambda_{k}} - \frac{h_{k} + h_{k-1}}{h_{k}/\lambda_{k} + h_{k-1}/\lambda_{k-1}}\right] \frac{1}{h_{k}}, \quad (23c)$$

$$(z_2 - \lambda) \frac{\partial^2 T}{\partial x^2}, \quad z_2 = \left[ \frac{1}{2} \frac{(0.5 (h_{k+1} + h_k))^2}{0.5 (h_{k+1}/\lambda_{k+1} + h_k/\lambda_k)} + \frac{1}{2} \frac{(0.5 (h_k + h_{k-1}))^2}{0.5 (h_k/\lambda_k + h_{k-1}/\lambda_{k-1})} \right] \frac{1}{h_k}, \quad (23d)$$

$$(z_{3} - \lambda) \frac{\partial^{3} T}{\partial x^{3}}, \quad z_{3} = \lambda + \left[ \frac{1}{6} \frac{\left(0.5 \left(h_{k+1} + h_{k}\right)\right)^{3}}{0.5 \left(h_{k+1}/\lambda_{k+1} + h_{k}/\lambda_{k}\right)} - \frac{1}{6} \frac{\left(0.5 \left(h_{k} + h_{k-1}\right)\right)^{3}}{0.5 \left(h_{k}/\lambda_{k} + h_{k-1}/\lambda_{k-1}\right)} \right] \frac{1}{h_{k}}, \quad (23e)$$

$$z_{4,1} \frac{\partial^{4} T \left(t_{n}, x_{k} + 0.5\alpha_{k}^{n} \left(h_{k+1} + h_{k}\right)\right)}{\partial x^{4}} + z_{4,2} \frac{\partial^{4} T \left(t_{n}, x_{k} - 0.5\gamma_{k}^{n} \left(h_{k} + h_{k-1}\right)\right)}{\partial x^{4}},$$

180

$$z_{4,1} = \left[\frac{1}{24} \frac{\left(0.5\left(h_{k+1}+h_{k}\right)\right)^{4}}{0.5\left(h_{k+1}/\lambda_{k+1}+h_{k}/\lambda_{k}\right)}\right] \frac{1}{h_{k}}, \quad z_{4,2} = \left[\frac{1}{24} \frac{\left(0.5\left(h_{k}+h_{k-1}\right)\right)^{4}}{0.5\left(h_{k}/\lambda_{k}+h_{k-1}/\lambda_{k-1}\right)}\right] \frac{1}{h_{k}}.$$
(23f)

The terms of the first, second, and third derivatives (23a)-(23c) are not zero on the nonuniform grid and with a variable coefficient of heat conduction which causes an additional error of calculation. Using these expressions, we can calculate the eliminable error

$$\Delta T_x^{\text{corr}} = -\Sigma \left( z_1 \frac{\partial T}{\partial x} + (z_2 - \lambda) \frac{\partial^2 T}{\partial x^2} + (z_3 - \lambda) \frac{\partial^3 T}{\partial x^3} + (z_{4,1} + z_{4,2}) \frac{\partial^4 T}{\partial x^4} \right) \Psi_k^n \tau h_k .$$
(24)

The estimate of the uneliminable error takes on the form

$$\Delta T_x^{\sup} = \Sigma \left[ (z_{4,1} \alpha_k^n (h_{k+1} + h_k)/2 - z_{4,2} \gamma_k^n (h_k + h_{k-1})/2) \frac{\partial^5 T(t_n, x_k)}{\partial x^5} \right] \Psi_k^n \tau h_k .$$
(25)

On the uniform grid and with a constant coefficient of heat conduction, expression (24) coincides with (16) and (25) coincides with (18).

**Results of Test Calculations.** As an illustration, we calculated the temperature error at a finite instant of time for the solution which describes evolution of the temperature field generalized by a point heat source ( $t_0$  and  $\xi$  are the initial time and the coordinate of the point source):

$$T_{\rm an}(x,t) = Q \sqrt{\frac{C\rho}{4\pi\lambda(t-t_0)}} \exp\left(-\frac{(x-\xi)^2 C\rho}{4\lambda(t-t_0)}\right).$$
(26)

As the initial data  $T_0(x_k)$  for calculation of the heat-conduction equation we used the temperature calculated by expression (26). The size of the field was taken such that the effect of boundary conditions was negligibly small compared with the approximation error of the differential equation. The effect of the computer accuracy on the results was estimated by comparing calculations with single and double precision; the discrepancies are negligible. To calculate the noncontrollable error  $\iint_{\Omega} \delta T \Delta \Psi(x, t) dt dx$ , we used the corresponding equation (the "conjugate second-order

equation" [8])

$$C\rho \frac{\partial \Delta \Psi}{\partial t} - \frac{\partial}{\partial x} \left( \lambda \frac{\partial \Delta \Psi}{\partial x} \right) + \delta \Psi_t(t, x) + \delta \Psi_x(t, x) = 0.$$
<sup>(27)</sup>

All of this made it possible to distinguish the effect of the errors of approximation of the finite-difference scheme against the background of other errors.

To solve the heat-conduction equation and the conjugate equations of both orders we used an implicit integrointerpolation method realized by three-point factorization. The problem had 20-2000 cells over the space and 10-1000 steps over time. The thermal conductivity of the material is  $\lambda = 10^{-4}$  kW/(m·K) and the bulk heat capacity is  $C\rho =$ 500 kJ/(m<sup>3</sup>·K). The initial and final distributions of temperature are given in Fig. 1.

We calculated the error of solution  $T_{est}$  at the central and several peripheral points at a finite instant of time. The estimates of the computational error of temperature  $T_{est}$  as a function of the space step are given in Table 1. The time step is chosen to be rather small (0.1 sec) in order to provide the smallness of the error of time approximation compared with the error of space discretization. The error caused by the time step did not exceed  $2 \cdot 10^{-5}$  and that due to the error of approximation of the conjugate equation  $(\iint \delta T \Delta \Psi(x, t) dt dx)$  was even smaller by several orders.

In Table 1,  $T_x^{\text{corr}} = T - \Delta T_x^{\text{corr}}$  is the numerical solution verified by the conjugate equation. The comparison of the deviation of the calculation  $T - T_{\text{an}}$  and the verified calculation  $T_x^{\text{corr}} - T_{\text{an}}$  from the analytical solution shows



Fig. 1. Initial (1) and final (2) temperature distributions as a function of the number of the node over the coordinate.



Fig. 2. Verified solution and range of errors compared with the result of the numerical calculation and analytical solution: a) zone A of Fig. 1; b) zone B of Fig. 1; 1) analytical solution; 2) numerical solution; 3) verified solution; 4) lower limit; 5) upper limit (k, numbers of the nodes over the coordinate).



Fig. 3. Results of the numerical calculation of temperature, verified solution, and the range of errors normalized to the analytical solution: 1) numerical solution; 2) verified solution; 3) lower limit; 4) upper limit (k, numbers of the nodes over the coordinate).

TABLE 1. Estimates of the Computational Error of Temperature as a Function of the Spatial Grid Mesh

<i>h</i> , m	$T - T_{an}$ , K	$\Delta T_x^{\rm corr}$ (16)	$T_x^{\rm corr} - T_{\rm an}$	$\Delta T_x^{\text{sup}}$ (18)
0.002	3.0607	2.719	0.341	6.3
0.001	0.772345	0.751934	0.0204	1.86
0.0008	0.494818	0.48683	0.0080	1.08
0.0004	0.123853	0.123579	$2.74 \cdot 10^{-4}$	0.163
0.0002	0.030948	0.031011	$6.3 \cdot 10^{-6}$	$2.1 \cdot 10^{-2}$
0.0001	0.007711	0.007760	$4.9 \cdot 10^{-5}$	$2.7 \cdot 10^{-3}$

TABLE 2. Comparison of Errors for Constant and Variable Grid Meshes over the Coordinate

Grid	$T - T_{an}$	$\Delta T_x^{\rm corr}$	$T_x^{\rm corr} - T_{\rm an}$	$\Delta T_x^{sup}$
Uniform, $h = 0.0001$ m	0.00732	0.00735	$3 \cdot 10^{-5}$	$5.33 \cdot 10^{-3}$
Nonuniform	-0.023	-0.00917	0.008	0.456

TABLE 3. Comparison of Errors for Constant and Variable Thermal Conductivities over the Coordinate

Thermal conductivity, $\lambda$	$\Delta T_x^{\text{corr}}, \text{ K}$	$\Delta T_x^{sup}$ , K
Constant	0.00735	0.00533
Variable over the coordinate	1.1	0.0513

that verification of the calculation by  $\Delta T_x^{\text{corr}}$  (16) allows one to eliminate a considerable part of the approximation error. Comparing the remaining error  $T_x^{\text{corr}} - T_{\text{an}}$  and  $T_x^{\text{sup}}$ , we can note a reliable upper estimate (18) and the fact that it is not too overestimated. We should also note the quadratic character of variation of the eliminable error  $\Delta T_x^{\text{corr}}$  and the cubic character of variation of the uneliminable error  $\Delta T_x^{\text{sup}}$  as a function of the grid mesh.

Figure 2 presents a comparison of the analytical, numerical, and corrected solutions and also the range of the error (h = 0.001 m,  $\tau = 0.1$  sec) at different points (Fig. 1, zones A and B). Figure 3 shows the numerical and verified solutions and the upper and lower limits of the verified solution; all parameters are normalized to the analytical solution.

Table 2 gives the results of the estimation of the error caused by a 20% decrease of the grid mesh at 10 central points. The nonuniformity of the grid resulted in an additional error which was partially compensated by the conjugate equations; nevertheless the resultant error increased. The steps of the calculation are h = 0.0001 m and  $\tau = 0.1$  sec.

Thus, the conjugate equations allow one to follow approximation errors on both uniform and nonuniform grids.

Just so is the case with the effect of spatial nonuniformity of the coefficient of heat conduction on the accuracy of the solution. Table 3 gives the error due to variability of the coefficient of heat conduction (20% variation of the coefficient at the center of the grid) compared to the eliminable and uneliminable errors of approximation. It is seen that the effect of the variability of the coefficient of heat conduction on the accuracy of calculation is much higher than the effect of the approximation error caused by the finite grid mesh.

**Discussion.** The analysis and numerical experiments showed that the main part of the computational error due to the finite grid mesh can be compensated by use of the conjugate equations. In this case, the order of the accuracy of calculation on the uniform grid increases by a unity. Numerical experiments indicate that the upper estimate of the error holds, it is rather realistic, and, therefore, can be used in practical calculations.

Thus, this approach is close to a laboratory experiment from the point of view of estimation of systematic and random errors and allows calculation of the error of not only a temperature written in the form of functional (6) but also other functionals of temperature. The differences will be only in the form of the source in the conjugate equation (8).

With the precise conjugate temperature we can obtain an infinitely accurate solution. The limitation of this method is the error of numerical approximation of conjugate temperature and the necessity of calculation of high-order temperature derivatives, the existence of which can be ensured by Eq. (1). However, a wide class of problems (e.g., of those which correspond to initial conditions (26)) admits the existence of a larger number of derivatives; the numerical experiments confirmed the possibility of their use for verification and estimation of the resultant error. With the same order of approximation of direct and conjugate problems the order of the noncontrollable error ( $\iint \delta T \Delta \Psi(x, x)$ )

t) dtdx) is twice as high, which explains the small values obtained for this quantity in the numerical experiments. The simplest way of determination of the latter is calculation of Eq. (27); however, for the schemes of the third and higher orders of accuracy this error has an order higher than the order of estimations (16) and (18); therefore, it is hardly worthwhile to control it.

**Conclusions.** The error of the finite-difference calculation of temperature at a certain coordinate-time point can be decreased by solving the conjugate equation. The remaining error can be estimated from above by the conjugate temperature and the space and time steps of calculation.

# NOTATION

C, heat capacity, kJ/(kg·K); h, spatial step of calculation;  $N_t$ , number of nodes of approximation over time;  $N_x$ , number of nodes over the coordinate; t, time;  $t_f$ , duration of the process; T, temperature, K;  $T_0$ , initial temperature, K; x, coordinate, m; X, specimen thickness, m;  $\alpha$ ,  $\beta$ , and  $\gamma$ , coefficients in the Taylor–Lagrange expansion;  $\delta$ , Dirac delta function;  $\delta T$ , terms of the Taylor series;  $\Delta T$ , temperature increment;  $\Delta T_x^{\text{corr}}$ , eliminable error due to expansion over the coordinate;  $\Delta T_t^{\text{corr}}$ , eliminable error due to expansion over time;  $\Delta T_x^{\text{sup}}$ , upper estimate of the uneliminable error due to expansion over the coordinate;  $\Delta T_t^{\text{sup}}$ , upper estimate of the uneliminable error due to expansion over time;  $\Delta T_{x,2}^{\text{sup}}$ , upper estimate of the uneliminable error due to expansion over time;  $\Delta T_{x,2}^{\text{sup}}$ , upper estimate of the uneliminable error of second order due to expansion over the coordinate;  $\varepsilon$ , functional;  $\lambda$ , thermal conductivity, kW/(m·K);  $\rho$ , density; kg/m<sup>3</sup>;  $\tau$ , step of calculation over time;  $\Omega$ , computational domain;  $\Psi$ , conjugate temperature. Sub- and superscripts: an, analytical solution; corr, eliminable error; est, estimated point; exact, exact solution; k, number of the node over the coordinate; n, number of the node over time; sup, upper estimate of the uneliminable error; x, component of the error due to expansion into the Taylor series in terms of time coordinate; t, component of the error due to expansion into the Taylor series in terms of time.

### REFERENCES

- 1. G. I. Marchuk, Conjugate Equations and Analysis of Complex Systems [in Russian], Nauka, Moscow (1992).
- 2. O. M. Alifanov, Inverse Problems of Heat Transfer [in Russian], Mashinostroenie, Moscow (1988).
- M. B. Giles, On Adjoint Equations for Error Analysis and Optimal Grid Adaptation in CFD, in: M. Hafez and D. A. Caughey (Eds.), *Computing the Future II: Advances and Prospects in Computational Aerodynamics*, Wiley, New York (1998).
- N. A. Pierce and M. B. Giles, Adjoint Recovery of Superconvergent Functionals from PDE Approximations, SIAM Rev., 42, 247–264 (2000).
- 5. D. Venditti and D. Darmofal, Grid Adaptation for Functional Outputs: Application to Two-Dimensional Inviscid Flow, *J. Comput. Phys.*, **176**, 40–69 (2002).
- 6. A. A. Samarskii, The Theory of Difference Schemes [in Russian], Nauka, Moscow (1977).
- 7. A. K. Alekseev, Calculation of a Temperature Error by a Conjugate Equation, *Inzh.-Fiz. Zh.*, **77**, No. 1, 141–145 (2004).
- 8. A. K. Alekseev, Use of the First- and Second-Order Conjugate Equations in Estimation of an Error of Solution of the Heat-Conduction Equation, *Inzh.-Fiz. Zh.*, **75**, No. 2, 143–147 (2002).