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ERROR MINIMIZATION IN NONLINEAR VARIATIONAL UNSTEADY-STATE HEAT CONDUCTION PROBLEMS

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The article considers a variational method of solving unsteady-state heat conduction problems.

Conventional methods used for approximation of solutions, in particular, the finite-difference method, often prove ineffective for nonlinear unsteady-state heat conduction problems in which the thermophysical properties of the material or the heat sources depend on temperature. Calculations show that variational methods are promising for this class of problems.

For error analysis in nonlinear variational problems, we will carry out the calculation of heating of an infinite cylinder of radius R by a radiative and convective heat flux:

$$\frac{1}{2\pi R} q_a(R, \tau) = C(T_m^4 - T^4(R, \tau)) + \alpha_c(T_m - T(R, \tau)) \tag{1}$$

at the medium temperature T_m = const and with the initial condition T(r, 0) = const. The thermal conductivity λ is assumed to depend on temperature: $\lambda = \lambda(\vartheta)$ ($\vartheta = T/T_m$).

The calculation will be done using the functional from [1]. Taking into account the Fourier heat conduction law $q = -2\pi r T_m \lambda(\vartheta)\vartheta_r'$, the change of the function Ψ in an element of unit length $l = 1$ will be found:

$$\frac{1}{2\pi T_m^2} \Delta\Psi = -\int_0^{\tau_1}\left\{\int_0^R \left[\vartheta \frac{\partial}{\partial r}(r\lambda(\vartheta)\vartheta_r') + r\lambda(\vartheta)\vartheta_r'^2\right] dr - - r\lambda(\vartheta)\vartheta\vartheta_r'\Big|_0^R\right\} d\tau = 0. \tag{2}$$

From the heat conduction equation

$$\frac{1}{2\pi T_m} \varepsilon(\vartheta) = c\rho r\vartheta_\tau' - \frac{\partial}{\partial r}(r\lambda(\vartheta)\vartheta_r') = 0 \tag{3}$$

we will find the first term in (2) and determine the functional for the conditions of problem (1) and (3)

$$\frac{1}{2\pi T_m^2} = -\int_0^{\tau_1}\left\{\int_0^R (c\rho\vartheta\vartheta_\tau' + \lambda(\vartheta)\vartheta_r'^2) r dr - r\lambda(\vartheta)\vartheta_r'\vartheta\Big|_0^R\right\} d\tau = 0. \tag{4}$$

The approximation errors in variational heat conduction problems depend on the residuals in differential equation (3) and the boundary condition

$$E_1(\vartheta) = 2\pi R T_m (q_a(\vartheta) - \lambda(\vartheta)\vartheta_r'(R, \tau)). \tag{5}$$

These errors can be diminished if the solution is approximated using piecewise-smooth elements Θ_i ($\Theta_i \in C^2$), expressing the approximate solution as a broken curve. The approximation errors at the discontinuity points of the gradients Θ_r' should be minimized.

In estimating the approximation errors, their effect can be considered to be a result of the action of fictitious heat sources on the boundary R and in the region $0 < r \le R$, including the conjugation points of the elements Θ_i.

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Therefore, an approximation using the functions Θ_i is a solution of a physically meaningful problem with fictitious sources. Some fictitious sources can be estimated, because of which it is possible to specify the approximating functions and the error minimization process is simplified [1]. The effect of fictitious source functions can be included in variational functional (4). Moreover, the heat balance equation for these sources can be constructed.

The approximating functions will be determined so that the net effect of all fictitious sources is minimal at the points at which the approximation is to be found. It should be borne in mind that the indicated errors exist with any approximation methods used. Evidently, by choosing steps along the coordinate i and in time j, it is possible not only to reduce these errors but also to compensate, in a certain way, for their mutual effect.

Since trigonometric functions have good approximating properties [2, 3], the following piecewise-smooth elements will be used for large τ:

$$\Theta_{i,j}(r,\ \tau) = 1 - \gamma \cos(\mu_{i,j} r/R) N_j(\tau);\quad \Theta \in C^2;$$
$$\gamma = 1 - T(r,\ 0)/T_m;\quad N(\infty) = 0;\quad \mu_{i,j} = \mu_j + ih. \tag{6}$$

In order to determine the form of the functions $N_j(\tau)$, (6) will be substituted into Eq. (3). After integration of (3) with respect to r and τ we will find for a linear function $\lambda(\Theta)$:

$$N_j(\mathrm{Fo}) = D_j \exp(-\varphi_j \mathrm{Fo})/(1 + \nu_j \exp(-\varphi_j \mathrm{Fo}));\quad \mathrm{Fo} = a\tau/R^2. \tag{7}$$

Since functions (7) have been determined for the condition $\varepsilon(\Theta) = 0$, assumed in (3), with a particular choice of the coefficients D_j, φ_j, and ν_j, they allow compensation of the mutual effect of the sources $\varepsilon(\Theta)$ in the region $0 < r \le R$. The coefficients Dj are assumed to be constant for every interval $\tau_{j+1} - \tau_j$. In determining the coefficients D_j for large τ, we will use a method used in mathematical physics and assume that the initial temperature distribution $1 - \gamma$ can be expressed using the incomplete Fourier series in the class of functions $\cos(\mu r/R)$, orthogonal with weight r [3]:

$$1 - \gamma = 1 - \gamma \sum_{n=1}^{\infty} D_{j,n} \cos(\mu_{j,n} r/R);\quad \tau = 0. \tag{8}$$

It will be found that

$$D_{j,n} \int_0^R r \cos^2(\mu_{j,n} r/R)\, dr = \int_0^R r \cos(\mu_{j,n} r/R)\, dr; \tag{9}$$

$$D_j = \frac{4\,[\sin\mu_j + (\cos\mu_j - 1)/\mu_j]}{\mu_j + \sin 2\mu_j + 0{,}5\,(\cos 2\mu_j - 1)/\mu_j},\quad n = 1. \tag{10}$$

Functions (6) can be considered as elements of the series expansion of ϑ with Fourier coefficients (10), assuming that the series terms decrease with time. Therefore, it is assumed that the coefficients D_j, calculated with expression (10), allow the best minimization of the mean root square error with weight r.

In what follows, use will be made of the dimensionless parameters

$$X = r/R;\quad \mathrm{Fo} = a_0\tau/R^2;\quad \mathrm{Bi}_{ra} = CT_m^3 R/\lambda_0;$$
$$\mathrm{Bi}_c = \alpha_c R/\lambda_0;\quad \lambda_0 = \lambda(r,\ 0);\quad a_0 = \lambda_0/c\rho.$$

Discontinuities of the gradient Θ_r' at the conjugation points of elements (6) and (7) will be found as a result of the action of the fictitions sources

$$Q_i = 2\pi r_i T_m q_i,\quad q_i = \lambda(\Theta_i)((\Theta_i)_r' - (\Theta_{i+1})_r'). \tag{11}$$

The change of the function Ψ, caused by source (11), will be

$$\Delta\Psi = -2\pi r_i T_m^2 q_i \Theta_i. \tag{12}$$

We will find the change of Ψ in the region $0 < r < R$ by integrating over X in (4) with fixed Fo_j and summing $I(\Theta)$ for m intervals $X_{i+1}-X_i$. Taking into account (5) and (12), the functional is found:

$$\frac{1}{2\pi\lambda_0 T_m^2} I(\Theta) = \frac{R}{\lambda_0}\left(q_a\Theta(R,\ Fo_j) + \sum_{i=1}^{m-1} X_i\Theta_i q_i\right) - \\ - \sum_{i=1}^{m}\int_{X_i}^{X_{i+1}}\left(\Theta\Theta'_{Fo} + \frac{\lambda(\Theta)}{\lambda_0}\Theta_x'^2\right) X dX = 0. \qquad (13)$$

For the conditions $I(\Theta_j) = 0$ and $E_1(\Theta_j) = 0$, adopted in (13), the effects of the sources ε and Q_i are mutually compensated at the moment Fo_j. Therefore, functional (13) will also be used as an equation in determining unknown coefficients. The function $I(\Theta)$ can also be evaluated for the subregion $r_i < r < R$ $(i < m)$.

With the condition $I(\vartheta) = 0$ included, the existence of an extremum of functional (13) in the solution ϑ at some points will be checked by shifting the reference point of $I(\Theta)$ by ξ_1:

$$I(\Theta(R,\ Fo_j)) + \xi_1 = 0 \qquad (14)$$

and considering the thermodynamic conditions [1]

$$\Delta q_s(\Theta_a) < 0;\ \ \Delta q_s(\Theta_b) > 0;\quad \Theta_a < \vartheta < \Theta_b \qquad (15)$$

for approximations to ϑ from below Θ_a and from above Θ_b. The search for the extremum from the set of equations $I'_\mu = 0$, $I'_\varphi = 0$, etc. is unreasonable, since this conventional method requires numerical differentiation and the resultant equations can correspond to inflection points.

The approximations $\Theta_{i,j}$ will be determined in such a way that at times Fo_j fictitious heat source [5] is equal to the heat flux at the surface $r = R$ due to sources (3) and (11) with the opposite signs, and the balance equation will be constructed for the fictitious sources [1]

$$\frac{1}{T_m}\Delta q_s(\Theta) = E_1(\Theta) - \sum_{i=1}^{m}\int_{X_i}^{X_{i+1}}\varepsilon(\Theta)\, dX = 0. \qquad (16)$$

The quantity $\Delta q_s(Q)$ is a fictitious heat flux on the surface. In what follows, the coefficients from (16) will be determined with $E_1(\Theta_j) = 0$. In this case the effects of all sources (3) and (11) acting at the time Fo_j on the surface temperature $\Theta(R,\ Fo_j)$ are mutually compensated.

For evaluation of Δq_s for the intervals $Fo_{j+1}-Fo_j$ we will find from (3), (5), (11), and (16) after integration with respect to Fo:

$$\frac{1}{2\pi c\rho T_m R^2}\Delta q_{sm} = \frac{1}{\lambda_0}\int_{Fo_j}^{Fo_{j+1}}\left(q_a + \sum_{i=1}^{m-1} q_i X_i\right) d\,Fo - \\ - \sum_{i=1}^{m}\int_{X_i}^{X_{i+1}}(\Theta(X,\ Fo_{j+1}) - \Theta(X,\ Fo_j))\, X dX = 0. \qquad (17)$$

When using approximations (6) and (7) for small times τ, the number of steps j should be increased. Investigations of analytic solutions of some linear problems for small τ show that before the regular regime sets in, the maximum of the derivative Θ'_τ is displaced with time from the surface into the interior of the body. If the approximating functions include this displacement of $(\Theta'_\tau)_{max}$, the number of steps j can be decreased substantially. The following functions will be chosen as approximations for small τ:

$$\Theta_{i,j} = 1 - \gamma(1 - f_2(r_1,\ \tau));\quad r_1 = R - r. \qquad (18)$$

The functions $f_2(r_1, \tau)$, which include the displacement of $(\Theta'_\tau)_{max}$ into the interior of the cylinder, will be determined using the solution for a semi-infinite space at $Bi_{ra} = 0$ and $\lambda = const$ [3]:

$$f_2(r_1,\ \tau) = \operatorname{erfc} z_1 - \exp z_2 \operatorname{erfc} z_3; \qquad (19)$$

$$z_1 = \psi_1 \frac{r_1}{2\sqrt{a_0\tau}}; \quad z_2 = \psi_2 (Hr_1 + H^2 a_0 \tau);$$

$$z_3 = \psi_3 (z_1 + H\sqrt{a_0\tau}); \quad H = \alpha_e/\lambda_0.$$

The coefficients ψ_1, ψ_2, and ψ_3, which are unity for a solution of the linear problem, are introduced to take into consideration the nonlinear conditions. In calculating erfc z, use will be made of three terms from the known asymptotic expansion [3]

$$\operatorname{erfc} z = 1 - \frac{2}{\sqrt{\pi}} \left(z - \frac{z^3}{3} + \frac{z^5}{10} \right); \quad z \leqslant 1.$$

Since the approximations $\Theta_{i,j}$ are chosen in the class of the functions $\Theta_{i,j} \in C^2$, with a definite selection of the coefficients and arbitrarily small variations of the solution, the residuals of Eqs. (3), (5), (13), (16), and (17) can approach zero as the number of steps $i \to \infty$ and $j \to \infty$. Under these conditions the functions $\Theta_{i,j}$ will tend to a solution of the problem, and this will be checked by estimating the approximations from below Θ_a and from above Θ_b to the solution ϑ .

After substitution of the arbitrary variations

$$f = \Theta - \vartheta; \quad \Theta \in C^2 \tag{20}$$

into (4), it is easy to see that in the class of functions (20) neither the necessary condition $\delta I = 0$ nor the sufficient condition $\delta^2 I < 0$ (or $\delta^2 I > 0$) for the existence of an extremum of functional (14) in the solution ϑ is satisfied. The sufficient condition can be satisfied in the case of some thermodynamically reasonable restrictions on the choice of approximating functions. In particular, if the fictitious sources ε and E_1 in (3) and (5) are chosen so that they increase the thermal nonequilibrium for all r and all the previous τ, then with a prescribed heat transfer law on the boundaries (5) and the initial condition $\Theta(r, 0) = 1 - \gamma$, the time to attain the specified temperature for the solution will be the smallest. Then, the variational principle can be based on minimization of the fictitious source actions and implemented in a particular class of functions that satisfy the indicated choice of sources $E_1(\Theta)$ and $\varepsilon(\Theta)$ [1]. If the variational problem has a solution, these functions can always exist, since according to the second law of thermodynamics in a closed system only processes that bring the system close to equilibrium can occur.

Integration by parts in (4) and substitution of the solutions into functional (4) make it vanish: $I(\vartheta) = 0$. Consequently, the existence of a functional extremum can be checked by determining its increment signs: $\Delta I(\Theta) = I(\Theta)$. Therefore, the sufficient conditions $I(\Theta_a) < 0$ and $I(\Theta_b) < 0$ for the existence of a maximum in functional (4) in the solution ϑ will be verified by calculations, using approximations to the solution ϑ from below and from above. The existence of a maximum will be also determined with a more severe restriction on the choice of approximating functions, when the time of achieving a best approximation Θ_ν will be minimal relative to the approximations from below and from above.

We choose the functions $\Theta_{a1}(R, Fo)$ and $\Theta_{b1}(R, Fo)$ satisfying the conditions

$$E_1(\Theta_{a1}) \leqslant 0; \quad \varepsilon(\Theta_{a1}) > 0; \quad q_i(\Theta_{a1}) > 0; \quad \Delta q_s(\Theta_{a1}) < 0; \tag{21}$$

$$E_1(\Theta_{b1}) \geqslant 0; \quad \varepsilon(\Theta_{b1}) < 0; \quad q_i(\Theta_{b1}) < 0; \quad \Delta q_s(\Theta_{b1}) > 0, \tag{22}$$

and the initial condition $\Theta(r, 0) = 1 - \gamma$ in the interval $(0, Fo_1)$. In view of the fact that for the solution ϑ, which is unique from physical considerations, the conditions

$$E_1(\vartheta) = 0; \quad \varepsilon(\vartheta) = 0; \quad q_i(\vartheta) = 0; \quad \Delta q_s(\vartheta) = 0, \tag{23}$$

are satisfied, it is found that the solution ϑ is inside the region restricted by conditions (21) and (22), where the residuals E_1, ε, and Δq_s change their signs. Then, bearing in mind the signs at E_1 and Δq_s in (17), (21), and (22), we will find that Θ_{a1} and Θ_{b1} are approximations to the solution from below and from above, respectively.

Conditions (21) and (22) for all Fo in the interval (0, Fo_1) can be satisfied with a sufficiently good choice of the approximating functions $\Theta_{i,j}$. It is assumed that the functions $\Theta_{i,j}$ in (21) and (22) are determined so that integration of E_1 and Δq_m in (5) and (17) with respect to τ between 0 and Fo_1 results in fulfillment of the conditions $\Delta q_s < 0$ and $\Delta q_{sm}(\Theta) < 0$ in the interval (0, Fo_1). Then on the surface r = R the heat balance for fictitious fluxes (16) will be negative at the time Fo_1. Since the approximations $\Theta_{i,j}$ differ from the solution ϑ only by the presence of the fictitious sources E_1, q_i, and ε, in accordance with the energy conservation law Θ_{a1} will approximate ϑ from below. In a similar way it will be found that when reciprocal inequalities in (22) are fulfilled, Θ_{b1} will approximate ϑ from above. In accordance with this reasoning, the approximation Θ_{a2} to Θ_{a1} from below and the approximation Θ_{b2} to Θ_{b1} from above will be found for the subsequent time interval Fo_{j+1}-Fo_j. If it is necessary to determine the errors at the points r_i inside the region $0 < r_i < R$, expressions (3), (16), and (17) are written for each subregion $0 < r_i$ and $r_i < R$ [1]. It is assumed that the approximating functions $\Theta_{i,j}$ will result in arbitrarily small residuals E_1, q_i, and ε, which will be verified in the computations.

At large Fo, $Fo_j < Fo < \infty$ and $\Theta(R, Fo) = 0.9900$ the functions Θ_a and Θ_b will be chosen so that they satisfy inequalities (21) and (22). With relations (23) in view, it will be found that the domain of definition of Θ, restricted by constraints (21) and (22), contains solutions of Eqs. (3) and (5) for various initial conditions, including the condition $\vartheta(r, 0) = 1 - \gamma$. With the signs at E_1 and Δq_s in (21) and (22) taken into consideration, the solutions Θ_a and Θ_b will approximate the final value $\vartheta(r, \infty) = 1$ either only at negative or only at positive fictitious fluxes Δq_s, i.e., either more slowly or more quickly than the solution ϑ will. Therefore, Θ_a and Θ_b will be approximations to the solution ϑ from below or from above, respectively. In a similar way $\Theta_{a,j}$ and $\Theta_{b,j}$ will be found for all previous Fo_j.

In order to determine why these approximations can be realized using functions (6) and (7), it will be assumed that the solution ϑ can be expressed by a series for r in the full orthonormal set of functions (6) with coefficients (7). It is assumed that the coefficients $N_j(\varepsilon)$ decrease with time and that at large Fo only one term in series (8) remains. In this case the solution ϑ for $\vartheta(r, 0) = 1 - \gamma$ and the solution ϑ_1 of another problem with the initial condition $\vartheta_1(r, 0) = 1 - \gamma D\cos(\mu r/R)$, corresponding to one term in (8), will coincide at large Fo within the remainder of the series, which is usually the case in analytical solutions [3].

At present there are no theoretically substantiated methods for error estimation in nonlinear unsteady-state problems. In the case of piecewise-difference approximations the results are sometimes estimated by considering the condition $\Theta_{k+1}(r_i, Fo_j) - \Theta_k(r_i, Fo_j) < \xi_2$, which is not theoretically successive, for two subsequent iterations. It is assumed here that as the number of steps increases, the approximations can tend to the solution, just as in linear problems. As follows from the above analysis, in grid methods the residuals in Eqs. (3) and (5) are uncontrollable sources that, when accumulating, can disturb the balance equations. When results in nonlinear problems are estimated using the above condition, approximations can tend to the solution of another problem with fictitious sources and this can bring about very serious computation errors that cannot be estimated [4].

The unknown coefficients in (6), (7), and (19) will be found from Eqs. (5), (13), (16), and (17). In this case the calculations can be done easily, using the law of variation of the coefficient $\mu_{i,j}$ adopted in (7), followed by determination of the computation error $\delta = (\Theta_b - \Theta_a)/\Theta_a$. The coefficients μ_j are found from boundary condition (5) for the conjugation points of the elements $\Theta_{i,j}$. If inside the elements the approximations do not satisfy Eq. (5), then with condition (16) the source E_1 on the surface r = R will compensate for the action of all the sources inside the cylinder. The coefficients φ_j are found from (16) and $\varphi_{i+1,j}$ are determined from the element conjugation condition

$$\Theta(r_i, Fo_j, \mu_{i+1,j}, \varphi_{i+1,j}) = \Theta(r_i, Fo_j, \mu_{i,j}, \varphi_{i,j}).$$

The values of ν_{j+1} are found with the aid of functional (13). The functional increment $\Delta I = I(\nu_k) - I(\nu_j)$ is calculated here and, using the linear interpolation $I(\nu_k)/\Delta I(\nu) = (\nu_k - \nu_{j+1})/(\nu_k - \nu_j)$, the coefficient ν_{j+1} will be determined and the condition $|I(\Theta)| < 1 \cdot 10^4$ is verified for it.

The coefficient $\mu_{i+j,\ j+1}$ inside the domain is found in accordance with the law of variation of $\mu_{i,j}$ taken in (7). The coefficient μ_{j+1} can be evaluated from the condition of conjugation of $\Theta(r_i, \mu_j)$ and $\Theta(r_i, \mu_{j+1})$ in time. These approximations will be expressed in terms of the coefficients for the two iterations j and j+1:

TABLE 1. Relative Temperature in an Infinite Cylinder Heated under Nonlinear Heat Transfer Conditions

$Bi_{ra} = 0.2$; $Bi_c = 0.25$; $1-\gamma = 0.3$; $\beta = 2$					
Fo	0.2	0.5	1.0	1.5	2.0
$\Theta(0)$	0.4070	0.6263	0.8635	0.9528	0.9831
$\Theta(0.5R)$	0.4312	0.6406	0.8691	0.9548	0.9838
$\Theta(R)$	0.4905	0.6791	0.8847	0.9606	0.9859
$Bi_{ra} = 0.5$; $Bi_c = 0.15$; $1-\gamma = 0.2$; $\beta = 2$					
Fo	0.2	0.5	1.0	1.5	2.0
$\Theta(0)$	0.4157	0.8033	0.9738	0.9960	0.9994
$\Theta(0.5R)$	0.4538	0.8174	0.9759	0.9964	0.9994
$\Theta(R)$	0.5418	0.8543	0.9813	0.9972	0.9996
$Bi_{ra} = 0.5$ and $Bi_c = 0.15$					
μ	0.6524	0.7293	0.7693	0.7744	0.7752
φ	2.1525	3.0660	3.5705	3.6417	3.6505
ν	0.4940	0.1713	0.0143	0	0
h	0.0740	0.0341	0.0237	0.0230	0.0230

$$\Theta(r_i, \mathrm{Fo}_j, \varphi_{j+1}, h_{j+1}, \mu_{j+1}) = \Theta(r_i, \mathrm{Fo}_j, \varphi_j, h_j, \mu_j).$$

We will find μ_{j+1}, using $\Theta(r_i, \mu_j)$, evaluated in the previous iteration j.

In order to find the initial φ and h at large Fo, we will take $\Theta(r, \infty) = 1$ as the reference point for temperature and calculate the coefficients φ and h for the approximation $\Theta(R, \mathrm{Fo}) \approx 0.9995$ at $\nu = 0$. The initial μ will be found from the characteristic equation $\mu \tan \mu = 4\mathrm{Bi}_{ra} + \mathrm{Bi}_c$, which follows from boundary condition (5) at $\mathrm{Fo} = \infty$ [1].

Some results for λ calculated as a function of temperature $\lambda(\Theta) = \lambda(\Theta(r, 0))\{1 + \beta[\Theta(r, \mathrm{Fo}) - \Theta(r, 0)]^{0.4}\}$ are given in Table 1. The computation error of the estimates given in the table does not exceed 1%. The computations have shown that a solution of a variational nonlinear problem can be approximated by choosing the approximating functions so that they allow minimization of the residuals in Eqs. (13) and (16), obtained from analysis of the problem with fictitious heat sources. The coefficients obtained from expressions (13) and (16), which are integral balances, correspond to the conditions where the effects of the fictitious sources $\varepsilon(\Theta)$ and $E_1(\Theta)$ compensate for each other at some points and, on the average, over the integration region, and the computation error is minimized.

The error of the temperature calculated using variational functional (13), which corresponds to nonlinear heat conduction equation (3) and nonlinear boundary heat transfer law (1), can be decreased by an order of magnitude or more compared with that of finite-difference approximations. In finite-difference approximations one can only replace the functions $\lambda(\Theta)$ at the nodes by numerical values of $\lambda(\Theta)$ averaged in a certain arbitrary way. For such approximations the temperatures $\Theta_{i,j}$ can change by 50 to 100% just due to the method used for averaging $\lambda(\Theta)$ [4]. In this case substantial variations of $\Theta_{i,j}$ inconsistent with the physical meaning of the problem can often occur over the spatial region. The variational principle just described practically excludes the effects of this kind of errors, since the function $\lambda(\vartheta)$, consistent with the physical law, is taken into consideration inside every element $\Theta_{i,j}$ and at its boundaries, which improves the solution approximation substantially. In addition, the proposed method for estimating the error from the heat balance equations for fictitious sources (17) makes it possible to determine both the order of magnitude of the error and its absolute value.

Functional (13) and heat balance equation (16) should include the action of fictitious sources (11) and (12) to reduce the accumulation of residuals in the equations during iterations. Errors (11) and (12) can also be eliminated by determining some coefficients from the condition of gradient equality at the conjugation points; however, this constraint restricts the class of approximating functions, because of which it may be required that i and j be increased. For the above problem, computation of sources (11) and (12) in (13) and (16) will provide an additional compensation for the residuals ε.

Minimization of the computation errors depends largely on the choice of approximating functions, which is known to be typical of variational methods. Piecewise-smooth elements (6), (7), and (18) form a sufficiently wide class of approximating functions for a solution of nonlinear heat conduction problems and give approximations with a small number of steps i and j. The use of equations (17), which define the heat balance for fictitious sources, in variational computations improves minimization of the residuals $\varepsilon(\Theta)$ and $E_1(\Theta)$. The condition $\Theta \in C^2$ in (6) is also satisfied by cubic splines, but they approximate the solution of problem (3) and (5) much worse than functions (6), (7), and (18). Cubic splines can be useful in solving linear problems for which there exist proofs of convergence of the approximations to the solution.

If the number of coefficients and equations for determining these coefficients should be increased, the computation can also be done for intermediate Fo in the interval $Fo_{j+1} - Fo_j$. In the computation it is also useful to control the residuals of the equations inside the intervals $Fo_{j+1} - Fo_j$, especially with a small number of steps. In order to reduce the machine time for determination of the initial coefficients, if necessary, use could be made of multidimensional optimization methods or analytic solutions of linear problems with conditions as close as possible to those of the problem to be solved.

It should be noted that for functionals that can be obtained with irreversible thermodynamic methods [5] investigation of a sufficient condition for the existence of an extremum has failed. The search for an extremum just from a necessary condition fails because of inflection points, which is confirmed by computations. Values of the functional are always determined with severe restrictions, in particular, with linear conditions on the boundary and also in the absence of particular variations of q and Θ'_τ and all variations of the boundary conditions. Since without variations of (20) the functions Θ to be determined can only be solutions, the extrema of these functionals can occur in the solution ϑ only when the corresponding values of ϑ are substituted as nonvaried quantities. The solution of the problem is usually unknown and for the approximations Θ and all r and τ there exist residuals E_1 and ε that are arbitrary variations of the solution. Therefore, functionals with the above restrictions could only be of theoretical interest since substitution of the possible approximations into this functional violates the energy conservation law. Evidently, an extremum of this functional can only exist in a solution of another problem with fictitious sources E_1 and ε. Computations confirm that minimization of these sources by a balance equation such as (16) is only possible if the energy conservation law is satisfied.

Since the extrema of such functionals usually cannot be investigated, the functionals are only used as equations for determination of the coefficients, and the meaning of the variational formulation is lost. These equations, which are, however, called variational, are often physically meaningless, which hinders the computation process. In this situation other methods yield results more efficiently. Calculations with the use of a functional show that variational methods are effective if sufficient conditions for the existence of an extremum are found and arbitrarily small variations are investigated near the extremal points and if a theoretically reasonable error estimation is possible. Under these conditions verification of the existence of a variational functional extremum in the solution is a sufficiently effective means for checking the results.

Since functional (13) takes into account nonlinear conditions by means of the substitution of the appropriate functions into it, in particular, the condition $\lambda = \lambda(\Theta)$, the present calculation method can be used for solving problems with strong nonlinearity, for which finite-difference approximations do not provide sufficient computational accuracy, for example, in the case of an active powerful instantaneous source, asymmetrical nonlinear problems, etc. The present analysis shows that this variational principle, based on minimization of the action of fictitious sources, can be used in constructing functionals for other problems of mathematical physics, if their formulations use some conservation laws. The estimation of the approximation to the solution from below and from above, adopted here, can also be done for nonvariational methods in approximation by approximating functions in the class $\Theta \in C^2$.

NOTATION

$\vartheta = T/T_m$, temperature; Ψ, thermodynamic function; T, absolute temperature; T_m, medium temperature; r, r_i, coordinates; R, cylinder radius; τ, time; q, heat flux; λ, thermal conductivity; ρ, density; c, heat capcity; Θ, approximating function; Θ_i, piecewise-smooth elements of the function Θ; $1 - \gamma$, relative initial temperature; a, thermal diffusivity; C, emissivity; I, functional; f, arbitrarily small variations of the problem solution ϑ; α_c, convective heat transfer coefficient; μ, φ, ν, h, D, ψ, β, coefficients; Fo, Fourier number (dimensionless time); Bi_c, Biot number; Bi_{ra}, radiative Biot number; i, coordinate step; j, time step; Θ_a and Θ_b, approximations to the solution from below and from above; $\delta I(\Theta)$, first functional variation; $\delta^2 I(\Theta)$, second functional variation; δ, error; $\lambda_0 = \lambda(r, 0)$, initial thermal conductivity; $\alpha_e = q_a/(T_m - T(R, \tau))$, net heat transfer coefficient.

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