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Variational method for solving non-linear problems of unsteady-state heat conduction

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Abstract—A variational formulation of the problem of unsteady-state heat conduction is presented. A non-linear functional obtained as a result of a thermodynamic analysis of the processes of heat transfer in unsteady-state systems is suggested. The variational calculational method can be used for solving problems with a strong non-linearity for which finite-difference schemes do not allow one to obtain satisfactory results. To simplify the presentation, a non-linear one-dimensional problem is considered as an example. The functional can be generalized to the case of three-dimensional problems, as well as transformed for other coordinate systems. A technique for calculating the approximation error in variational calculus is suggested that makes it possible to determine approximations to the solution from below and from above.

INTRODUCTION

Calculations show that variational methods show promise for solving complex non-linear problems of unsteady-state heat conduction in which the thermophysical properties of substance or heat sources depend greatly on temperature. Application of variational schemes in these problems makes it possible to considerably improve solution approximations [1, 2]. The methods of variational calculus usually used do not allow one to determine the functional which has an extremum at the solution of non-linear non-stationary heat conduction problems. Therefore, the present paper suggests a new principle for constructing such a functional based on the thermodynamic analysis of arbitrary variations of the solution.

In this paper a method for approximating solutions is presented that enables one to take into account all the possible errors of a variational calculating scheme. Residuals of a differential heat conduction equation and boundary conditions are considered as fictitious heat sources in a thermodynamic system. In this case variations of the solution are the result of the effect of all the fictitious sources, and the approximating functions will be the solutions of the problem with fictitious sources that is physically meaningful. Under these conditions, based on the first law of thermodynamics, the heat balance equation for fictitious sources can be constructed. In view of the fact that at present the methods for estimating an error in discrete approximations of solutions are absent, a method is suggested for determining approximations to the problem solution from below and from above. These approximations are calculated on the basis of the first law of thermodynamics using the heat balance equation for fictitious sources. Variational calculus shows that approximation errors in this case can be diminished by an order of magnitude or more as compared to finite-difference schemes.

It should be noted that frequently, when finite-difference schemes are used in non-linear non-stationary heat conduction problems, all the attempts to estimate the obtained results by studying the convergence of approximations to the solution turn out to be ineffective. One succeeds in proving the convergence of discrete approximations only for simple physical conditions and under substantial restrictions on the choice of approximating functions. Moreover, some restrictions, in particular the requirement of continuity of derivatives in the region, cannot often be fulfilled, thus leading to great approximation errors not amenable to quantitative estimation.

The variational method presented makes it possible to solve problems with a strong non-linearity inside the region and at the boundaries for the conditions under which other methods do not allow one to obtain satisfactory results, e.g. the action of powerful sources or explosion on a surface, change of a phase state, non-linear problems under non-symmetric conditions of heat transfer at the boundaries. Multidimensional problems can also be solved by the corresponding functional obtained for these conditions [1]. The solution of a system of equations for calculating unknown coefficients is always stable. The solution is approximated by broken curves, which are formed by piecewise-smooth elements in spatial and temporal regions, similarly to spline approximation.

THERMODYNAMIC JUSTIFICATION OF THE VARIATIONAL METHOD

A thermodynamic analysis shows that the directivity of any spontaneous processes of heat transfer in

NOMENCLATURE

a	thermal diffusivity [$m^2 s^{-1}$]
$c(\vartheta)$	heat capacity [$J kg^{-1} K^{-1}$]
C	coefficient of radiation [$W m^{-2} K^{-4}$]
E	residual of a boundary condition [$W m^{-2}$]
f	solution variation
h	relative coefficient of heat transfer
$I(\theta)$	functional [$W m^{-2} K$], [$J m^{-2} K$]
i	number of a spatial step
j	number of a time step
k	coefficient determining the function $\lambda(\vartheta)$
q	specific heat flux [$W m^{-2}$]
Δq_s	fictitious heat flux [$W m^{-2}$]
T	absolute temperature [K]
T_m	medium temperature [K]
x	spatial coordinate [m].

Greek symbols

α_c	coefficient of convective heat transfer [$W m^{-2} K^{-1}$]
β	coefficient determining the function $\lambda(\vartheta)$ [K^{-1}]
$1-\gamma$	relative initial temperature
δI	first variation of the functional [$W m^{-2} K$]
$\delta^2 I$	second variation of the functional [$W m^{-2} K$]
ε	residual of heat conduction equation [$W m^{-3}$]
θ	approximating function
θ_a	approximation to ϑ from below
θ_b	approximation to ϑ from above
ϑ	solution of problem
$\lambda(\vartheta)$	thermal conductivity [$W m^{-1} K^{-1}$]
λ_0	initial value of $\lambda(\vartheta)$ [$W m^{-1} K^{-1}$]
μ	determined coefficient
ν	determined coefficient
ρ	density [$kg m^{-3}$]
τ	time [s]
φ	determined coefficient
Ψ	new thermodynamic function [$J m^{-3} K$].

a closed thermodynamic system towards equilibrium with the environment, can be used as a principle for constructing the functional of the problem of unsteady-state heat conduction. In accordance with the second law of thermodynamics, only spontaneous processes bringing the system closer to thermal equilibrium with the environment are possible in a nonstationary thermodynamic system. Therefore, the system will approach the state of equilibrium with a certain speed that is maximum for the assigned initial and boundary conditions.

The solution will be varied so that during the preceding time instants fictitious sources could exist that would increase the non-equilibrium condition in the system and at the boundaries relative to real processes. Then, under the assigned initial and boundary conditions, as a result of the action of such sources, the speed of the approach of the system to the equilibrium state will decrease. In a system involving sources, the time corresponding to the fixed temperature at some space points, will be greater than the time corresponding to the same temperature in a real system without fictitious sources. This means that in a certain class of approximating functions a variational functional can be determined so that at the extremal point of the functional corresponding to the solution the system approaching the equilibrium state will have the highest speed relative to the system with fictitious sources. If a variational problem has a solution, then the existence of a class of functions is always possible in which the maximum speed of the approach to the equilibrium state will correspond to the solution, since, according to the second law of thermodynamics, a real system only has the processes that bring the system to equilibrium.

The variational calculus shows that in problems of cooling the speed of the system approaching equilibrium with the environment, determined from the conditions of the existence of extremum, can be maximum at some points for the solution of the problem relative to the same speed for a problem with fictitious sources. The same extremum will also be present in problems of heating, if transformation of the coordinate system is made. The origin of the heat source should be shifted so that the problem of heating can be reduced to the problem of cooling [3]. For non-linear conditions the moduli of heat fluxes in the problem of cooling should be kept the same as the moduli of heat fluxes in the problem of heating prior to the transformation of coordinates. Hence, the speed of the approach to equilibrium, calculated from the conditions of the existence of the extremum and determined by the value of the derivatives ϑ'_τ, can also be maximum for the solution. This suggests that the functional expresses a physically existing directivity of spontaneous processes to equilibrium and also testifies to the adequacy of physical and mathematical models from the viewpoint of the second law of thermodynamics.

Allowing for the statistical character of heat transfer in macrosystems, the existence of the maximum speed of the approach of the system to equilibrium in a certain class of functions could be checked, if it could be found that under steady-state conditions the temperature distribution corresponding to the problem solution would be the most probable with respect to arbitrary approximations to the solution from below and from above. Since such a verification cannot be made, there is good reason to assume that the existence of the extremum following from the second law of thermodynamics, to which a certain maximum speed of the approach to equilibrium corresponds, cannot be determined with the aid of any theoretical propositions or formal arguments and, just as the second law, should be justified as a result of observations of physical objects. Therefore, for the problem considered the verification of the existence of the extremum in a certain class of functions should be performed by calculations during the minimization of arbitrary small variations of the solution.

In the case of discrete approximations large errors appear in non-linear problems due to the fact that at the nodal points of the system one can use only numerical values of the thermal conductivity λ and heat capacity c, that are to be averaged in a certain arbitrary manner which prevents one from taking into account the effect of the functions $\lambda(\vartheta)$ and $c(\vartheta)$ in the region. In variational calculus these functions are used directly in the functional, and their effect is determined by integration, i.e. not only at the nodal points, but also over the region, considerably improving the solution approximations as shown by calculations.

The approximating functions are selected so that not only fictitious sources can be minimized, but that their mutual effect can be compensated. When using a variational method, all the possible fictitious heat sources in the system are taken into account, and therefore the problem with fictitious sources is solved correctly. This enables us to use the first law of thermodynamics in the analysis of the variational solution and thus to determine the range of approximations within which the solution exists. The calculations show that in the case of an insufficiently good minimization of errors the functional extremum can exist on the solution of another problem with fictitious sources which differs from the problem being solved without such sources. Therefore, it is expedient to check the existence of the extremum after the minimization of errors. This can be used as an additional means for controlling the results obtained.

VARIATIONAL FUNCTIONAL FOR NON-LINEAR PROBLEMS OF HEAT CONDUCTION

The solution of the non-linear problem ϑ for unsteady-state conditions is approximated with the aid of the functions θ:

$$\theta = \vartheta + f \quad \vartheta = T/T_{\text{m}} \quad \theta \in C^2 \tag{1}$$

that are selected so that the corresponding variations of the solution f would be arbitrarily small. To minimize the errors that can occur when using the approximations in equation (1), determine the functional for a non-linear nonstationary heat conduction problem. The existence of the functional extremum on the solution ϑ will be considered allowing for the above-stated thermodynamic conditions. The studies show that to construct the variational functional of the problem in question, it is expedient to use the following thermodynamic function whose variation is determined as follows [1]:

$$\Delta\Psi = -T_{\text{m}}^2 \int_0^{\tau_a} \vartheta q(\vartheta)\, d\tau. \tag{2}$$

In the case of heat conduction in a solid body, the heat flux $q(\vartheta)$, determined by the Fourier law of heat conduction $q(\vartheta) = -\lambda(\vartheta)\vartheta'_x$, and the quantity Ψ depend only on temperature. Under these conditions Ψ is a function of state, and therefore the change in Ψ within the range (x_0, x_n) is equal to its variation at the boundaries $x = x_0$ and $x = x_n$:

$$T_{\text{m}}^{-2}\Delta\Psi = -\int_0^{\tau_a}\left\{\int_{x_0}^{x_n}(q(\vartheta)\vartheta'_x + \vartheta q'_x(\vartheta))\, dx - \vartheta q(\vartheta)\big|_{x_0}^{x_n}\right\} d\tau = 0. \tag{3}$$

Using the differential heat conduction equation with a negative source $q_{\text{v}}(\vartheta)$

$$\varepsilon(\vartheta) = c(\vartheta)\rho\vartheta'_\tau - (\lambda(\vartheta)\vartheta'_x)'_x + q_{\text{v}}(\vartheta) = 0 \tag{4}$$

find $q'_x(\vartheta) = -(\lambda(\vartheta)\vartheta'_x)'_x$ and from equation (3) determine the functional

$$I(\vartheta) = T_{\text{m}}^2 \int_0^{\tau_a}\left\{\int_{x_0}^{x_n}(c(\vartheta)\rho\vartheta\vartheta'_\tau + \lambda(\vartheta)\vartheta'^2_x + \vartheta q_{\text{v}}(\vartheta))\, dx - \vartheta\lambda(\vartheta)\vartheta'_x\big|_{x_0}^{x_n}\right\} d\tau = 0. \tag{5}$$

The problem will be considered at the boundary conditions

$$T_{\text{m}}^{-1}E(\vartheta) = q(x_0,\tau) - \lambda(\vartheta(x_0,\tau))\vartheta'_x(x_0,\tau) = 0$$
$$\vartheta'_x(x_n,\tau) = 0. \tag{6}$$

After the substitution of approximations of equation (1) into equation (5) it is easy to check that in the class of functions of equation (1) either the obligatory condition $\delta I = 0$ at the sufficient condition $\delta^2 I < 0$ or $\delta^2 I > 0$ for the existence of the extremum of functional (5) on the solution ϑ are not satisfied, if the variations δI and $\delta^2 I$ are calculated in accordance with the requirement of the classical variational calculus that a differential equation should be an Euler equation for the functional. Therefore the existence of the extremum will be determined from the thermodynamic conditions by considering the residuals of the differential equation (4) and of the boundary conditions (6) as fictitious heat sources. Then the functions of equation (1) will be the solutions of the problem with fictitious sources $\varepsilon(\theta)$ and $E(\theta)$, that is physically meaningful, and the variations of the solution $f = \theta - \vartheta$ can be considered as a result of the effect of these sources.

The solution ϑ will be varied so that fictitious sources ε and E could increase the non-equilibrium state of the thermodynamic system (4), (5) and (6) for all the preceding values of τ. In this case, with allowance for the above-considered thermodynamic conditions at the given initial temperature distribution $\vartheta(x, 0)$ and heat transfer at the boundaries (6), the existence of the extremum of functional (5) on the solution ϑ is possible.

To determine the conditions of the existence of this extremum, integrate (5) by parts, and allowing for $\varepsilon(\vartheta) = 0$ in equation (4) find that the functional on the solution always vanishes:

$$I(\vartheta) = \int_0^{\tau_a} \int_{x_0}^{x_n} \vartheta \varepsilon(\vartheta)\, \mathrm{d}x\, \mathrm{d}\tau = 0. \quad (7)$$

In accordance with this expression the existence of the extremum of functional (5) can be found by determining the signs of its increment ΔI, which is equal to the value of the functional $\Delta I(\theta) \equiv I(\theta)$. In this case, the sufficient conditions of the existence of the extremum on the solution ϑ are determined by the inequalities

$$I(\theta_a) < 0 \quad \text{and} \quad I(\theta_b) < 0 \quad \text{or}$$
$$I(\theta_a) > 0 \quad \text{and} \quad I(\theta_b) > 0 \quad (8)$$

that should be fulfilled uniquely for approximations to the solution ϑ from below θ_a and from above θ_b. According to the aforementioned it is supposed that in a certain class of functions the maximum speed of the approach of the system to equilibrium corresponds to the solution ϑ, and for the approximations θ the time for attaining the assigned values of temperature will be larger than for the solution of the problem ϑ. In view of the above, the verification of the existence of the extremum of the functional (5) on the solution ϑ in the class of functions (8) will be calculated during minimization of fictitious sources ε and E.

It follows from equation (7) that the functional (5) at $E(\theta) = 0$ expresses the orthogonality of the residual $\varepsilon(\theta)$ of equation (4) and approximations θ, thus supposing minimization of $\varepsilon(\theta)$. With the use of the function Ψ, the orthogonality of $\varepsilon(\theta)$ and θ in equation (7) is established not formally, but as a consequence of the physical condition equation (3). After the substitution of equation (6) into equation (5) the functional will take into account the boundary conditions, as well as the effect of the fictitious source $E(\theta)$ for any values of τ. As a result of integration over x and τ the effect of the functions $\lambda(\theta)$ and $c(\theta)$ in equation (5) will be allowed for not only at the nodal points, but also inside the ranges (τ_j, τ_{j+1}) and (x_i, x_{x+1}) as variational calculus shows, this considerably improves approximation of the solution of the problem. It should be borne in mind that in the case of finite-difference approximations the effect of $\lambda(\theta)$ and $c(\theta)$ can be taken into account only at the nodal points by substituting arbitrarily averaged numerical values of λ and c into difference equations. Inside the approximating elements the functions $\lambda(\vartheta)$ and $c(\vartheta)$ are approximated with substantial errors. This leads to the violation of the energy conservation law to which there corresponds an increase in fictitious heat sources and the solution variations associating with these sources. A specific feature of the functional (5) is the fact that the coefficients determined by it are independent of the start of temperature reading in the region.

APPROXIMATION OF SOLUTIONS

The errors of the variational solution approximation that depend on the residuals of equations (4) and (6) can be reduced if an approximate solution is presented in the form of broken curves composed of piecewise-smooth elements (1) in space and time regions. In this case we shall also minimize the approximation errors at the discontinuity points of the gradients $(\theta'_x(x_i))_i$ and $(\theta'_x(x_i))_{i+1}$. It is obvious that with a certain choice of approximations it is possible not only to reduce the value of fictitious sources $\varepsilon(\theta)$ and $E(\theta)$, but also to compensate their mutual effect in a certain manner. The action of fictitious sources involves the origination of fictitious heat fluxes in the system that causes the corresponding variations of f.

The residuals of equation (4) at the points of conjugation of the elements $\theta_{i,j}$ are considered as a result of the action of surface fictitious sources at these points that cause the fluxes q_i

$$T_m^{-1} q_i(\theta) = \lambda(\theta_i)\{(\theta'_x(x_i))_i - (\theta'_x(x_i))_{i+1}\} \quad (9)$$

to which there corresponds the variation of the function $\Delta\Psi$

$$T_m^{-2} \Delta\Psi_i = -q_i(\theta)\theta_i. \quad (10)$$

Divide the section $x_n - x_0$ into m intervals (x_i, x_{i+1}) and, integrating into equation (5) over x at fixed τ_j, find $I(\theta)$ for each interval. Then sum all $I(\theta)$ and, with allowance for equations (6) and (10), determine the functional

$$T_m^{-2} I(\theta_j) = q(x_0, \tau_j)\theta(x_0, \tau_j) + \sum_{i=1}^{m-1} q_i \theta_i$$
$$- \sum_{i=1}^{m} \int_{x_i}^{x_{i+1}} (c(\theta)\rho\theta\theta'_\tau + \theta q_v(\theta) + \lambda(\theta)\theta'^2_x)\, \mathrm{d}x = 0. \quad (11)$$

For the conditions adopted in equation (11) $I(\theta_j) = 0$ and $E(\theta_j) = 0$, the sources $\varepsilon(\theta_j)$ and $q_i(\theta_j)$, acting at $\tau = \tau_j$, are mutually compensated in the region $x_0 < x < x_n$. Therefore the functional (11) will also be used as an equation for determining unknown coefficients. The values of $I(\theta)$ can also be calculated for the subregion $x_0 < x_k$ $(x_k < x_n)$.

Determine the approximating functions so that the fictitious source E in equation (6) on the surface $x = x_0$ at time instants τ_j would be equal to the heat flux caused on the surface by the sources $\varepsilon(\theta_j)$ and $q_i(\theta_j)$ with opposite signs and formulate the balance equation for fictitious heat sources [1]:

$$T_m^{-1}\Delta q_s(\theta) = E(\theta) - \sum_{i=1}^{m}\int_{x_i}^{x_{i+1}} \varepsilon(\theta)\,dx = 0$$

$$\tau = \tau_j. \quad (12)$$

The quantity $\Delta q_s(\theta)$ is a fictitious heat flux on the surface x at $\tau \neq \tau_j$. Regardless of the signs of the terms in equation (6), the source E in equation (12) should be equal to the difference of the moduli of heat fluxes behind and in front of the source E to which the quantities $E = |q| - |\lambda\theta'_x|$ and $E = |\lambda\theta'_x| - |q|$ correspond to cooling and heating, respectively.

To determine the values of Δq_s for the ranges $\tau_{j+1} - \tau_j$ we find from equations (4), (6), (9) and (12) at $q_v = 0$ and $c = \text{constant}$ after integrating with respect to x and τ

$$T_m^{-1}\Delta q_{sm} = \int_{\tau_j}^{\tau_{j+1}}\left(q(x_0,\tau) + \sum_{i=1}^{m-1} q_i\right)d\tau - \sum_{i=1}^{m}\int_{x_i}^{x_{i+1}} c\rho(\theta(x,\tau_{j+1}) - \theta(x,\tau_j))\,dx = 0. \quad (13)$$

As a result of the action of fictitious sources ε, q_i and E, the value of Δq_{sm} is equal to the change in the internal energy of a unit area within the range (τ_j, τ_{j+1}).

An analysis shows that, with a certain choice of approximations (1) and arbitrary small variations, and with an increase in the number of steps, $i \to \infty$ and $j \to \infty$, the residuals of equations (4), (6), (11), (12) and (13) can approach zero as a result of which $\theta_{i,j}$ will approach the solution. This means that the variational scheme is adequate to a physical model of the heat conduction process within the residual of the equations used in calculations.

ESTIMATION OF AN ERROR

For the initial range $(0, \tau_1)$, select the approximations $\theta_{a1}(0, \tau_1)$ and $\theta_{b1}(0, \tau_1)$ that would satisfy the conditions

$$E(\theta_{a1}) \leqslant 0 \quad \varepsilon(\theta_{a1}) > 0$$

$$q_i(\theta_{a1}) > 0 \quad \Delta q_s(\theta_{a1}) < 0 \quad (14)$$

$$E(\theta_{b1}) \geqslant 0 \quad \varepsilon(\theta_{b1}) < 0$$

$$q_i(\theta_{b1}) < 0 \quad \Delta q_s(\theta_{b1}) > 0 \quad (15)$$

at all $\tau \in (0, \tau_1)$, and also the initial condition $\vartheta(x, 0)$. Allowing for the fact that for the solution ϑ, being unique from physical considerations, the following relations are satisfied:

$$E(\vartheta) = 0 \quad \varepsilon(\vartheta) = 0 \quad q_i(\vartheta) = 0 \quad \Delta q_s(\vartheta) = 0 \quad (16)$$

find that the solution ϑ lies within the region which is bounded by the conditions of equations (14) and (15) and in which the residuals E, ε and q_i change their signs for the opposite ones. From the relation of equation (12) it follows that at the boundary $x = x_0$ the thermal balance for the fictitious sources E, ε and q_i will be negative in the case of $\Delta q_s < 0$, $\tau \in (0, \tau)$ in equation (14) and positive in the case of the inequality of the opposite sense in equation (15). Then, according to the energy conservation law, θ_{a1} and θ_{b1} ($\theta_{a1} < \theta_{b1}$) will be the approximations to the solution ϑ from below and from above, respectively.

Similarly find the approximations to θ_{a1} from below θ_{a2} and to θ_{b1} from above θ_{b2}. If it is necessary to estimate an error at the points x_i inside the region (x_0, x_n), the conditions of equations (14) and (15) are written for each subregion $x_0 < x_i$ and $x_i < x_n$. In some cases approximations for large values of τ can be reckoned from the values $\vartheta(x, \infty)$, which usually simplifies the estimation of an error [1, 2].

The conditions of equations (14) and (15) can be satisfied for all $\tau \in (0, \tau_1)$ with rather a good choice of the functions θ or with an increase in the number of steps j. It may happen that approximations of θ will not satisfy the inequality $\Delta q_s < 0$, $\tau \in (0, \tau_1)$. In this case we determine θ so that at a certain time instant τ^* within the range $(0, \tau_1)$ the function Δq_s can change its positive sign once $\Delta q_s > \theta$, $\tau \in (0, \tau^*)$ for negative $\Delta q_s < 0, \tau \in (\tau^*, \tau_1)$ and, moreover, the quantity of heat that passed through the boundary $x = x_0$ within the range $(0, \tau_1)$ was the same as for the solution. The equality $\Delta q_{sm} = 0$ corresponds to the latter condition. Then for the entire region $x_n - x_0$ an increase in the internal energy Δq_{sm1} within the range $(0, \tau^*)$ due to the action of the flow $\Delta q_s > 0$ will be equal to the reduction of the internal energy Δq_{sm2} within the range (τ^*, τ_1), which is caused by the flux $\Delta q_s < 0$: $\Delta q_{sm} = |\Delta q_{sm1}| - |\Delta q_{sm2}| = 0$.

The action of the fictitious fluxes $\Delta q_s > 0$ and $\Delta q_s < 0$ is shifted in time. Therefore, in the region at some distance from the boundary $x = x_0$ by the time instant τ_1 an increase in the internal energy, caused first by the flux $\Delta q_s > 0$, will exceed the decrease in the internal energy caused by the flux $\Delta q_s < 0$. Consequently, in this portion of the region fictitious fluxes will increase internal energy. Then, paying attention to the fact that by the time instant τ the fictitious fluxes Δq_s do not change the internal energy of the entire region $x_n - x_0$, we determine that a smaller amount of heat will be accumulated in the vicinity of the boundary $x = x_0$, to which there corresponds the approximation to the solution $\theta_{a1} < \vartheta_1$ ($f_{a1} < 0$) from below. Similarly we find an approximation from above $\theta_{b1} > \vartheta_1$ ($f_{b1} > 0$).

The residual $\varepsilon(\theta)$ of equation (4) can change sign within the range $(0, \tau_1)$. Then the functions θ are selected so that at the boundary $x = x_0$ the inequality $\Delta q_s < 0$ would be satisfied for $\tau \in (0, \tau_1)$. As a result, at the boundary $x = x_0$ within the range $(0, \tau_1)$ the negative thermal balance will be retained for fictitious heat sources and the value of θ_{a1} will be an approximation to the solution ϑ_1, $\theta_{a1} < \vartheta_1$ from below. Other approximations θ_a and θ_b are determined similarly.

In the case of $f(x_0, \tau) = 0$ and $\Delta q_s(\theta_{a1}) = 0$ at the boundary $x = x_0$ the variation of the gradient $f'_x(x_0, \tau) = -E/\lambda(x_0, \tau_1)$ that corresponds to the fictitious flux E takes place, which compensates the action of the fictitious sources ε and q_i within the range $(0, \tau_1)$. Therefore, even at $f(x_0, \tau_1) = 0$ the order of the approximation of the gradient ϑ'_x by integral expressions (12) and (13) will be lower than the order of the approximation of ϑ.

CHOICE OF APPROXIMATING FUNCTIONS

An analysis shows that just as for the case of a steady-state regime, when $\theta'_\tau = 0$, the condition $\Delta\Psi(0) = 0$ in equation (3) can be satisfied for rather a wide class of functions $\theta \in c^2$ that satisfy the boundary conditions. The residuals of the functional in equation (5) appear only after the substitution of the derivative θ'_τ from equation (4) into equation (3) and therefore the error of calculations with the aid of the functional in equation (5) depends mainly on the choice of the approximation of the derivative θ'_τ that determines the change of the residual $\varepsilon(\theta)$ in equation (4) under unsteady-state conditions. The studies of analytical solutions of certain linear problems for small values of τ show that with an increase in τ the maximum of the derivative $(\theta'_\tau)_{\max}$ is usually shifted from the surface into the interior of the body [3]. At large values of τ the maximum of $(\theta'_\tau)_{\max}$ for bodies of finite dimensions and symmetric conditions of heat transfer at the boundaries (a plate, a cylinder) occurs in the center.

It follows from the calculations that by using the approximations $\theta_{i,j}$, that allow for the shift of $(\theta'_\tau)_{\max}$ from the surface with an increase of τ, the number of steps i and j can be substantially decreased [2]. If for small values of τ the approximations $\theta_{i,j}$, to which there corresponds the position of $(\theta'_\tau)_{\max}$ in the region for large τ, for example $\theta_{i,j} = N(\tau)\cos(\mu_i x)$, are used, then this variation of θ'_τ can result in an increase of the source $\varepsilon(\theta)$ in each piecewise-smooth element $\theta_{i,j}$. As a result, the errors caused by the source $\varepsilon(\theta)$ can be rather large. Approximations for small values of τ can be selected by analogy with the solutions of the similar linear problems, assuming that after the introduction of the corresponding coefficients these functions can, to a certain degree, express the above-mentioned character of the shift of $(\theta'_\tau)_{\max}$ for non-linear conditions.

Calculations of equations (11)–(13) also show that for a semi-bounded space, as well as for small values of τ the approximating functions θ are to be selected so that they can always enable the provision of continuity of the derivatives within the entire region of integration, which corresponds to the physical model of the process. In some schemes of approximations during the calculation of the heating processes one uses the depth of the heated layer $x_a(\tau)$ that is determined by a corresponding selection of the functions θ. Beyond the limits of this layer the derivatives θ'_x and θ'_τ are taken to be equal to zero, which leads to the violation of the continuity of the derivatives and, as follows from the calculations, causes considerable errors. It should be noted that in finite-difference non-linear schemes the continuity of derivatives is usually one of the conditions in proving the convergence. However, in these schemes for small values of τ one has to calculate some conditional depth of a heated layer, which is one of the reasons for large and difficult-to-eliminate errors that cannot be estimated quantitatively [4].

CALCULATION OF APPROXIMATIONS

As an example, consider a problem of heating a semi-infinite space by a radiative-convective heat flux

$$q(0,\tau) = cT_m^4(1-\vartheta^4(0,\tau)) + \alpha_c T_m(1-\vartheta(0,\tau)) \quad (17)$$

at the medium temperature T_m = constant and initial condition $T(x, 0)$ = constant. Assume that c = constant and the coefficient λ depends on temperature:

$$\lambda(\theta) = \lambda_0\{1+\beta(\theta(x,\tau)) - (\theta(x,0))^k\} \quad \lambda_0 = \lambda(x,0). \quad (18)$$

The solution is approximated by piecewise-smooth elements:

$$\theta_{i,j} = 1-\gamma(1-F_1(x,\tau)) \quad \gamma = 1-T(x,0)/T_m. \quad (19)$$

With allowance for the above stated, in order to determine the functions $F_1(x, \tau)$, to which the shift inside the region $(\theta'_\tau)_{\max}$ corresponds, we shall use the solution for a semi-infinite body at λ = constant and $c = 0$ [3]:

$$F_1(x,\tau) = \operatorname{erfc} z_1 - v\exp(\mu h_j x + z_2^2)\operatorname{erfc}(\varphi_1 z_2 + \varphi_2 z_1 + \varphi_3 z_3) \quad (20)$$

and introduce the following parameters and notation

$$z_1 = 0.5x/\sqrt{(a\tau)} \quad z_2 = h_j\sqrt{(a\tau)}$$

$$z_3 = \{h_j^2 a(\tau_j - \tau)\}^{1.1}$$

$$a = \lambda/(c\rho) \quad h_j = \alpha(\theta_j)/\lambda(0,\tau_j)$$

$$\alpha(\theta_j) = T_m^{-1} q(\theta(0,\tau_j))/(1-\theta(0,\tau_j)).$$

The coefficients μ, v and φ, as well as the quantity $\vartheta_3 z_3$ allow for the non-linearity in the problem with conditions of equations (11) and (17). For small values of u calculate $\operatorname{erfc} u = 1 - \operatorname{erf} u$ by an asymptotic expansion [5]:

$$\operatorname{erf} u = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{u^{2n+1}}{n!(2n+1)}, \quad u \leqslant 0.9.$$

When $u > 0.9$, we find $\operatorname{erfc} u$ using the approximations [5]:

Table 1. The values of the temperature θ in a semi-bounded space under non-linear conditions of heat transfer

	τ [s]					
$\times 10^3$ [m]	5	10	15	20	25	30
0	0.2689	0.2759	0.2811	0.2854	0.2851	0.2925
50	0.2600	0.2671	0.2723	0.2767	0.2805	0.2839
100	0.2544	0.2602	0.2649	0.2690	0.2727	0.2761

$$\operatorname{erfc} u = (1+0.2784u+0.2304u^2 +0.001u^3+0.0781u^4)^{-4}.$$

The derivatives of the probability integral are determined in an ordinary way $(\operatorname{erf} u)'_u = 2\exp(-u^2)/\sqrt{\pi}$. The coefficient μ is calculated from the boundary condition of equation (5). Successively applying linear interpolation, we find from equations (11) and (13) the values of φ_1 and φ_2, respectively. The coefficient v_j is determined accounting for the conjugation of the elements $\theta_{i,j}$ with iterations $j-1$ and j: $\theta(x_i, \tau_j, v_{j-1}) = \theta(x_i, \tau_j, v_j)$. The value of φ_3 is found from the condition $\Delta q_{sm} = 0$. In the course of calculations we verify the minimization of the functional $I(\theta) \leqslant 3\times 10^{-4}$.

Table 1 presents some results of calculations for the following conditions: $T_m = 1200$ K, $T(x, 0) = 300$ K, $C = 4\times 10^{-8}$ W m^{-2} K^{-4}, $\lambda_0 = 40$ W m^{-1} K^{-1}, $\beta = 2$, $k = 0.5$, $\alpha_c = 50$ W m^{-2} K^{-1}, $c\rho = 4\times 10^6$ J m^{-3} K^{-1}, $q_v = 0$. At $\tau = 10$ s and $x = 0$ the coefficients are: $\mu = 1.0192$, $v = 1.005$, $\varphi_1 = 1.2455$, $\varphi_2 = 0.9961$, $\varphi_3 = 15.93$. The error of calculations for the given values of $\theta(0, \tau)$ does not exceed 0.5%.

In accordance with conditions of equations (7) and (8) the existence of the extremum of the functional of equation (11) is checked at some points by shifting the start of the reading of the values of $I(\theta)$ by ξ_1:

$$I(\theta)+\xi_1 = 0. \tag{21}$$

Until now one has failed to study sufficient conditions for the existence of extrema for variational functionals in many of the problems of mathematical physics. Therefore, some authors suggest seeking extremal points only by the necessary condition from the system of equations of the form $I'_\mu = 0$, $I'_v = 0$, etc. It follows from the calculations that for the functional of equation (5) this method turns out to be ineffective, since in this case it is necessary to perform numerical differentiation. Moreover, the equations obtained can correspond to the inflection points, as a result of which the search for the extremum can turn out to be impossible, and the sense of the variational formulation is lost.

ANALYSIS OF THE RESULTS

The calculations show that the suggested variational method enables us to considerably improve approximation of the solutions of non-linear problems if approximating functions allow the minimization of the residuals and equations (4), (6), (11) and (12). Expressions (11) and (12) are the integral equations of heat balance and therefore the coefficients determined from these equations correspond to the conditions, when the effect of fictitious sources is compensated both at separate points and on average, over the region $0 < x < \infty$. An error of variational calculations with the aid of the functional of equation (5) diminishes by an order or more compared to the results obtained by the finite-difference method. With finite-difference approximations the values of temperature for small values of τ can differ by 50–100% only, due to choice in the way of averaging the coefficient $\lambda(\theta)$ [4]. In this case fluctuations of the approximations θ in the spatial region often take place which contradict the physical sense of the problem.

Minimization of errors in approximation of solutions greatly depends on the choice of approximating functions which, as known, is typical of the variational methods. Piecewise-smooth elements, that allow for the shift of the maximum of the derivative $(\theta'_\tau)_{max}$ in the spatial region with time, approximate the solution of the considered problem much better than other known approximating functions e.g. cubic splines. On using the above-presented variational method, the efficiency of the choice of the approximations $\theta_{i,j}$ can be verified at first steps i and j; in the case of a satisfactory choice of $\theta_{i,j}$ the initial values of the calculated coefficients turn out to be close to their finite values, which considerably reduces computer time expenditures for testing the functions and calculating the first approximations of $\theta_{i,j}$. The obtained solutions can, in fact, represent analytical expressions for some piecewise-smooth elements, and this can simplify the subsequent analysis and the use of the obtained results. On applying the familiar approximate methods (cubic splines and finite-difference elements), the problem of choosing approximating functions does not arise. However, in this case in problems with a strong non-linearity it appears impossible to take into account all the fictitious sources and variations of the solution which can be rather large. Calculations show that in the case of an unsatisfactory choice of the approximations $\theta_{i,j}$, the residuals of the above-presented equations cannot be minimized. Therefore, when using other approximate methods, which, in accordance with the above, usually do not approximate the solutions of non-linear problems so well, the minimization of errors can become considerably more complicated.

During approximation of solutions, all the possible errors are considered that are taken into account by fictitious heat sources $\varepsilon(q)$ and $E(q)$ in equations (4) and (6). In this case, using the first law of thermodynamics, it is possible, during calculations, to estimate the signs of fictitious sources. This enables one to suggest a reliable and thermodynamically justified method of estimating errors for variational approximations of a solution and to find approximations to the solution from below and from above.

When the boundary condition of equation (6) is satisfied allowing for expression (7), functional (11) determines the orthogonality of the residual $\varepsilon(\theta)$ of equation (4) and of the approximations θ, thus making it possible to minimize $\varepsilon(\theta)$. In contrast to projective methods with the use of orthogonalization, for example, of the Galerkin method, the conditions of orthogonality of equations (7) and (11) are found from the physical condition of equation (3) and are written for the approximations θ as a whole but not with respect to separate elements of the series expansions of θ, thus expanding the class of possible approximations. If, while performing iterations by projective schemes, the functions satisfy conditions of equations (8), (14) and (15), then these solutions can be considered variational. The fictitious sources of equation (9) can be eliminated by determining some of the coefficients in equation (20) from the condition of the equality of the gradients at the points of the conjugation of the elements $\theta_{i,j}$ by analogy with splines. For the problem considered, the action of sources in equations (9)–(12) are used to additionally compensate the residual $\varepsilon(\theta)$.

It should be noted that prior to the development of numerical methods similar constructions of approximations were used by solving physically close problems. For example, for approximate calculations of the solidification of metals, the problems of the change of physical state in a semi-infinite space, obtained by Stefan and Lightfoot [3], were successfully used for constructing heat balance equations. The efficiency of these kind of approximations confirms the expediency of the choice of the approximations θ by analogy with the well-known solutions of linear problems. Calculations show that with such a choice it is possible not only to improve approximations, but also to considerably simplify the determination of approximating functions, which can turn to be very laborious for non-linear variational problems.

CONCLUSION

The variational method suggested for the non-stationary heat conduction problems is based on a thermodynamic analysis of arbitrary variations of the solution of non-linear problems with allowance for the directivity of the processes of heat transfer in a closed system, which distinguishes this approach from the classical variational calculus. Earlier attempts to obtain a variational functional for the problem in question by the existing methods of variational calculus turned out to be unsuccessful due to specific features of a non-linear heat conduction equation. In the present paper the functional for unsteady-state heat conduction is determined that allows one to solve the problems with a strong non-linearity simultaneously both in the region and at the boundaries, including semi-bounded regions and small values of τ. Finite-difference schemes do not make it possible to obtain satisfactory results and correctly estimate their authenticity for these problems. The functional in equation (5) can be generalized to a three-dimensional space and also transformed for other coordinate systems [1, 2].

In accordance with the second law of thermodynamics the extremum of the functional in equation (5) realized in a certain class of approximating functions θ should exist on the problem solution ϑ. Here it is supposed that at the extremal point for the solution ϑ there exists the maximum speed of the approach of the system to an equilibrium state ϑ'_τ relative to the same speed for arbitrary approximations θ_a and θ_b. Variational calculus performed for various conditions of the problem show that in the case of the choice of functions, to which there correspond the maximum values of the derivatives θ'_τ at some points, the approximation of the solution is substantially improved. Thus, with a certain choice of approximations θ functional (5) allows for a thermodynamic regularity determining the directivity of real non-equilibrium processes towards equilibrium with the environment. This result indicates the adequacy of physical and mathematical models for the considered problem from the viewpoint of the second law of thermodynamics.

The above implies that with a corresponding choice of approximations θ the proposed functional of equation (5) will minimize the errors of the approximation in the problems of unsteady-state heat conduction rather well, which is confirmed by variational calculations. In particular, the coefficients determined from the conditions of the existence of the extremum of the functional of equation (5) can coincide, up to the fourth sign, with the corresponding coefficients for exact solutions. It should be noted that the functional of equation (5) is one of the possible applications of the second law of thermodynamics for studying irreversible processes. As is known, for these conditions the second law of thermodynamics can be presented in the form of inequalities that substantially limits its use.

Calculations show that the use of variational methods appears to be effective if sufficient conditions for the extremum existence on the solution are found and arbitrary small variations are studied near extremal points corresponding to the solution and a theoretically substantiated estimation of an error is possible. Under these conditions the verification of the existence of the extremum on the solution can also be used as an additional means for controlling the results obtained. Since, during minimization of variations all the possible errors are taken into account, this allows one, based on the first law of thermodynamics, to suggest the method for estimating approximation errors in variational calculations; this could not be accomplished until now.

The approximation to ϑ by the solutions of the problem with fictitious sources $\theta_{i,j}$ should be performed correctly in a thermodynamic sense. If in this case some residuals of equations or really existing variations of the solution $f = \theta - \vartheta$ are not taken into account, then due to the violation of the energy conservation law, an error will be accumulated. Then the extremum will exist on the solution of another problem with fictitious sources that differs from the studied one in which fictitious sources are absent. Therefore, before calculating the coefficients it is necessary to analyze the variational problem and to estimate all the possible heat sources that after the choice of approximating functions $\theta_{i,j}$ will be determined. The described variational principle based on minimization of fictitious sources can similarly be used in a variational analysis of other problems of mathematical physics, if in their formulation certain conservation laws are used.

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