Journal of Engineering Physics and Thermophysics, Vol. 69, No. 2, 1996

THERMODYNAMIC SUBSTANTIATION OF THE VARIATIONAL PRINCIPLE FOR NONLINEAR PROBLEMS OF UNSTEADY-STATE HEAT CONDUCTION

V. A. Bondarev

UDC 536.2:517.9

A variational formulation of the problem of unsteady-state heat conduction is presented. A nonlinear functional obtained as a result of an analysis of unsteady-state heat transfer is suggested. The variational method can be used for solving problems with a strong nonlinearity for which finite-difference approximations do not enable one to obtain sutisfactory results. A technique for calculating the approximation error in variational problems is considered.

The methods of variational calculus usually used do not enable one to determine the functional that has an extremum at the solution of nonlinear problems of unsteady-state heat conduction under the condition that the differential equation of heat conduction will be the Euler equation for the functional studied. The present paper suggests a new principle for constructing such a functional based on thermodynamic analysis of variations of the solution. Here residuals of the heat conduction equation and the boundary conditions are considered as fictitious heat sources that depend on time and the spatial coordinates. For these conditions approximating functions are solutions of a problem with fictitious source, that has a physical meaning, and arbitrary variations of the solution will be the result of the action of these sources [1, 2].

The suggested method for approximating solutions of unsteady-state heat conduction problems enables one to take into account all possible errors of the variational scheme and the corresponding fictitious heat sources. As a result the problem with fictitious sources is always solved correctly. For this problem, on the basis of the first law of thermodynamics, the heat balance equation for fictitious sources can be constructed and the signs of these sources as well as the signs of the corresponding variations of the solution can be determined. This makes it possible to suggest a method for estimating the absolute error that is thermodynamically substantiated. The performed analysis shows that with allowance for the signs of the fictitious sources approximations to the solution of the problem from below and from above can be found. In using the variational scheme considered one can diminish calculation errors by an order of magnitude or more as compared to other approximate methods.

As follows from a thermodynamic analysis, the directivity of all spontaneous processes of heat transfer in a closed thermodynamic system toward equilibrium with the environment can be used as a principle for constructing a functional in problems of unsteady-state heat condution. 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 equilibrium state with a certain speed that is maximum for the assigned initial and boundary conditions.

The solution will be varied so that at the preceding instants of time fictitious sources could exist that would increase the nonequilibrium condition in the system and between the system and the environment. Then in the problem involving sources the time corresponding to specified temperatures at some points will be greater than the time corresponding to the same temperatures for the solution. With such a choice of approximating functions a variational functional can be determined so that at the extremal point of the functional corresponding to the solution, the highest rate of temperature variation relative to some approximations will occur. If the variational problem has a solution, then the existence of a class of functions is always possible in which the maximum rate of temperature

Belarusian State Polytechnic Academy, Minsk, Belarus. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 69, No. 2, pp. 313-323, March-April, 1996. Original article submitted March 29, 1994.

variation corresponds to the solution, since, according to the second law of thermodynamics, in a real closed system, processes are possible that only bring the system to equilibrium.

Use of the suggested functional in calculations is possible under the condition that the approximating functions enable one to realize the above-determined conditions for the existence of a functional extremum for the considered problem. One does not succeed in proving by any theoretical assumptions or formal arguments that in the selected class of functions an extremum can be realized to which the maximum rate of approach of the system to equilibrium corresponds. With allowance for this fact there are reasons to assume that the extremum following from the second law of thermodynamics is a thermodynamic regularity that, just like the second law of thermodynamics, cannot be substantiated theoretically and should be justified as a result of observations of physical objects. Therefore, for the problem considered the existence of an extremum should be checked by calculations.

The minimization of errors in nonlinear variational problems depends strongly on the choice of approximating functions, which, as is known, is typical for variational methods. In linear discrete schemes the approximation to the solution can be improved by increasing the number of steps, whereas in some nonlinear problems an increase in the number of steps does not provide the necessary minimization of errors. Therefore, in nonlinear variational problems minimization of errors should be performed by means of the corresponding choice of approximations.

Approximating functions in nonlinear problems should allow for the character of the distribution of the derivatives Θ_x', Θ_{xx}'', and Θ_τ' in the spatial region and also satisfy conditions of continuity of derivatives in all the cases where continuity occurs in the physical problem. One should take into account the fact that some approximation techniques do not make it possible to realize the existing continuity of derivatives and this can increase considerably the effect of fictitious sources. For example, in calculations of heating processes one can use the depth of the heated layer $x_a(\tau)$, which is determined by means of the corresponding choice of approximating functions Θ. Beyond the limits of this layer the derivatives Θ_x' and Θ_τ' are taken to be equal to zero. In this case in the vicinity of the point $x_a(\tau)$ the derivatives Θ_x' and Θ_{xx}'' can be rather large, whereas the derivative Θ_τ' is close to zero. This results in the appearance of considerable residuals of the heat conduction equation, which in the case of strong nonlinearity cannot be minimized by increasing the number of steps.

In nonlinear finite-difference schemes the continuity of derivatives is one of the conditions for proving the convergence of nonlinear approximations to the solution. One succeeds in proving convergence only for simple physical conditions. However, in finite-difference schemes, for small times or in the case of a semi-infinite space one should also calculate some conventional thickness of the heated layer. With such an approximation it is impossible to provide continuity of derivatives, which, in accordance with the aforesaid, is one of the reasons for large and difficult-to-eliminate errors that cannot be estimated quantitatively [3]. In finite-difference approximations in nonlinear problems one tries to minimize these errors by different artificial techniques that have no theoretical substantiation and are based on the personal experience of the programmer. This makes the creation of unified approaches to the development of standard calculational programs quite difficult. With allowance for the aforesaid, one should assume that in solving nonlinear problems variational schemes may prove to be promising.

Studies show that approximating functions for nonlinear problems can be selected by analogy with solutions of linear problems that are close in meaning, assuming that after the introduction of the corresponding coefficients and some terms allowing for nonlinearity these functions can, to a certain degree, determine the real distribution of derivatives on the region and also take into account continuity of derivatives. Other known approximations in the class of functions $\Theta \in C^2$ can be used; however, as calculations show, this may require a considerable increase in the time for testing and correcting the approximating functions.

Errors of temperature calculation in nonlinear unsteady-state problems can be reduced substantially if the solution of the problem ϑ is approximated by broken curves composed of piecewise-smooth elements in the spatial and time regions. As these elements we use functions Θ,

$$\Theta = \vartheta + f, \quad \vartheta = T/T_m, \quad \Theta \in C^2, \tag{1}$$

that are selected so that the variations f of the solution ϑ are arbitrarily small. It is evident that with some choice of the coefficients functions (1) allow not only minimization of fictitious sources but also compensation of their mutual effect to a certain extent.

Studies show that to construct the corresponding functional in a variational formulation of a nonlinear problem of unsteady-state heat conduction it is expedient to introduce a new thermodynamic function Ψ whose variation is determined as follows [1]:

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

We find the heat flux $q(\vartheta)$ in (2) by the Fourier law of heat conduction $q(\vartheta) = -\lambda(\vartheta)\vartheta'_x$. In view of the fact that the flux $q(\vartheta)$ depends only on the temperature ϑ we determine that in the case of heat conduction in a solid body the quantity Ψ is a function of state. We find $\Delta\Psi$ for an element of unit area with a length $x_n - x_0$:

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

We find the derivative of the heat flux $q'_x(\vartheta) = -(\lambda(\vartheta)\vartheta'_x)'_x$ from the nonlinear differential equation of heat conduction with a negative volumetric heat source $q_v(\vartheta)$:

$$\varepsilon(\vartheta) = c(\vartheta)\rho\vartheta'_\tau - (\lambda(\vartheta)\,\vartheta'_x)'_x + q_v(\vartheta) = 0 . \tag{4}$$

Substituting $q(\vartheta)$ and $q'_x(\vartheta)$ into (3), we determine a functional for one-dimensional conditions:

$$I(\vartheta) = T_m^2 \int_0^{\tau_a} \left\{ \int_{x_0}^{x_n} c(\vartheta)\rho\vartheta\vartheta'_\tau + \lambda(\vartheta)\,\vartheta'^2_x + \vartheta q_v(\vartheta))\, dx - \vartheta\lambda(\vartheta)\,\vartheta'_x \Big|_{x_0}^{x_n} \right\} d\tau = 0 . \tag{5}$$

We assume that an initial temperature distribution is assigned:

$$\vartheta_0 = \vartheta(x, 0) . \tag{6}$$

Moreover, for the boundary surface S_1 the value of the heat flux q_1 is assigned as a function of the temperature ϑ_{s1}, and at the boundary $S_2 = S - S_1$ the temperature distribution $\vartheta_{s2}(x, \tau)$ is known:

$$E_1 = q(\Theta_{s1}) - \lambda(\Theta_{s1})\,(\Theta_{s1})'_n = 0 ; \quad E_2 = \vartheta_{s2} - \Theta_{s2}(x, \tau) . \tag{7}$$

The residuals E_1 are fictitious sources that depend on the temperature of the surface S_1, and E_2 is equal to the change in the temperature of the surface S_2 resulting from the action of fictitious sources on this surface.

Generalizing $I(\vartheta)$ to the spatial region Ω bounded by the surface S, we determine, using (5)-(7), a functional whose extremal properties will be studied:

$$I(\vartheta) = \int_0^{\tau_a} \left\{ \int_\Omega (\lambda(\vartheta)\,\vartheta'^2_k + c(\vartheta)\rho\vartheta\vartheta'_\tau + \vartheta q_v(\vartheta))\, d\Omega - \int_{S_1} \vartheta_{s1} q(\vartheta_{s1})\, dS - \right.$$

$$\left. - \int_{S_2} \lambda(\vartheta_{s2})\,(\vartheta'_{s2})'_n\, \vartheta_{s2}\, dS \right\} d\tau = 0 , \quad \vartheta'_k = \partial\vartheta/\partial x_k , \quad k = 1, 2, 3 . \tag{8}$$

Having substituted approximations (1) into (3), we find that for functional (8) both the necessary condition $\delta I = 0$ and the sufficient condition $\delta^2 I < 0$ or $\delta^2 I > 0$ for the existence of an extremum on the solution ϑ do not hold. Thus, one does not succeed in determining an extremum of the functional for the considered problem by the methods of classical variational calculus. Therefore, the existence of an extremum will be checked with allowance for the thermodynamic analysis presented above, considering residuals of the heat conduction equation (4) and the boundary conditions (7) as fictitious heat sources. With the known initial temperature distribution (6) and the prescribed boundary conditions (7) we find that the approximating functions (1) will be solutions of the physically meaningful problem (4), (6), and (7) with the fictitious sources $\varepsilon(\Theta)$, E_1, and E_2, and variations of the solution f can be considered as resulting from the action of these sources.

We vary the solution ϑ so that the variations f are arbitrarily small and fictitious sources increase nonequilibrium nature of the thermodynamic system (4), (6), and (7) for all preceding τ. Then, in accordance with the thermodynamic conditions, considered above the existence of an extremum of functional (8) on the solution ϑ is possible.

To determine conditions for the existence of a functional extremum in the class of functions (1) by the Ostrogradskii–Gauss formula, we find from (7) and (8)

$$I(\vartheta) = \int_0^{\tau_a} \varepsilon(x_k, \tau)\, \vartheta d\Omega d\tau \,, \tag{9}$$

where

$$\varepsilon(x_k, \tau) = c(\vartheta)\rho\vartheta'_\tau - (\lambda(\vartheta)\vartheta'_k)'_k + q_v(\vartheta) = 0 \,, \quad k = 1, 2, 3 \,. \tag{10}$$

The presence of the operator $\varepsilon(x_k, \tau)$ of Eq. (10) in (9) for three-dimensional conditions is a result of generalization of Eqs. (4) and (5) to the region Ω.

In accordance with (9) and (10) the functional $I(\Theta)$ always vanishes on the solution ϑ. Therefore, the existence of an extremum of the functional $I(\Theta)$ can be established by determining the signs of its increment ΔI, which is equal to the value of the functional $\Delta I(\Theta) \equiv I(\Theta)$. Sufficient conditions for the existence of a functional extremum on the solution ϑ are determined by the inequalities

$$I(\Theta_a) < 0 \text{ and } I(\Theta_b) < 0 \text{ or } I(\Theta_a) > 0 \text{ and } I(\Theta_b) > 0 \,, \tag{11}$$

which should be fulfilled uniquely for approximations to the solution ϑ from below Θ_a and from above Θ_b.

Functional (9) involves the operator of the differential equation of heat conduction (10), which also occurs in the case of a functional for which the equation of heat conduction (10) is the Euler equation. In view of the fact that Eq. (10) is the expression for the first law of thermodynamics in the problem considered, functional (10) and the classical variational functional can be considered thermodynamically equivalent. With allowance for the fact that the problem with fictitious sources is solved correctly, the functional also satisfies the first law of thermodynamics for the problem with fictitious sources.

According to expression (9), the functional $I(\Theta)$ determines the orthogonality of the residual ε of Eq. (4) and the approximations Θ, which assumes minimization of ε. In contrast to projection methods using orthogonalization, for example, the Galerkin method, orthogonality is established not formally, but as a consequence of the physical condition (3) for the function of state Ψ. By integration with respect to x_k and τ in (8) the effect of $\lambda(\Theta)$ and $c(\Theta)$ will be taken into account not only at the nodal points x_i and τ_j but also inside the corresponding ranges; as calculations show this improves considerably the approximation of the solution of the problem. It is well to bear 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 grid equations. Inside the approximating elements λ and c are approximated with substantial errors. This leads to violation of the energy conservation law and to an increase in the fictitious heat sources and in the corresponding variations f.

If functions (1) afford rather good approximations, then it is expeditious to use a functional constructed for the entropy flow dq/T. Calculations show that this functional can have an extremum on the solution ϑ in cases

x_0 than for the solution ϑ, and Θ_{a1} will be the approximation to ϑ from below. Similarly we find that if at the time τ^* the function Δq_s changes sign from "minus" to "plus" once, then for $\Delta q_s(\tau_1) = 0$ the value of Θ_{b1} will be the approximation to ϑ from above. In the same manner other approximations Θ_{aj} and Θ_{bj} are determined, including at points x_l inside the interval $x_n - x_0$.

As an example we consider a nonlinear problem of heating a semibounded space in the case of a nonlinear heat flux on the surface. A specific feature of this example is that the use of discrete approximations for such problems does not make it possible to provide continuity of the derivatives in the region and, as was noted above, to approximate with sufficient accuracy the change in the derivatives of the solution ϑ in space.

We consider heating of the semi-infinite space by a radiative-convective heat flux

$$q(0, \tau) = CT_m^4 (1 - \vartheta^4 (0, \tau)) + \alpha_c T_m ((1 - \vartheta (0, \tau)) \tag{22}$$

with the initial condition $T(x, 0) = \text{const}$ and the medium temperature $T_m = \text{const}$ for the case where the thermal conductivity λ depends on temperature:

$$\lambda (\Theta) = \lambda_0 \left\{1 + \beta (\Theta (x, \tau) - \Theta (x, 0))^{\psi}\right\}; \ \lambda_0 = \lambda (x, 0). \tag{23}$$

We assume that $c = \text{const}$ and $q_v = 0$.

The solution is approximated by piecewise-smooth elements:

$$\Theta_{i,j} = 1 - \gamma (1 - F_1 (x, \tau); \ \gamma = 1 - T (x, 0)/T_m. \tag{24}$$

The functions $F_1(x, \tau)$ are selected so that they take into account the real shift in the maximum of the derivative $(\Theta_\tau')_{\max}$ with increase in τ within the region from the boundary surface $x = 0$. With allowance for the aforesaid, to determine these functions, we use the exact solution [4] for a semibounded space for $C = 0$ and $\lambda = \text{const}$

$$F_1 (x, \tau) = \text{erfc}\, z_1 - \nu \exp (\mu h_j x + z_2^2) \,\text{erfc}\, (\varphi_1 z_2 + \varphi_2 z_1 + \varphi_3 z_3). \tag{25}$$

Here we introduce the following parameters and notation:

$$z_1 = 0.5\, x/\sqrt{a\tau}; \quad z_2 = h_j \sqrt{a\tau}; \quad z_3 = \left\{h_j^2 a (\tau_j - \tau)\right\}^{j,1}; \quad a = \lambda / c\rho;$$

$$h_j = \alpha (\Theta_j)/\lambda (0, \tau_j); \quad \alpha (\Theta_j) = T_m^{-1} q (\Theta (0, \tau_j))/(1 - \Theta (0, \tau_j)).$$

The coefficients μ, ν, and φ and the product $\varphi_3 z_3$ allow for the nonlinearity in the problem with conditions (16), (22), and (23). For small values of u we calculate $\text{erfc}\, u = 1 - \text{erf}\, u$ by the asymptotic expansion [5]

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

When $u > 0.9$, we find $\text{erfc}\, u$ using the approximation [5]

$$\text{erfc}\, u = (1 + 0.2784u + 0.2304u^2 + 0.0010u^3 + 0.0781u^4)^{-4}.$$

The derivatives of the probability integral are determined by the exact formula $(\text{erf}\, u)_u' = 2 \exp(-u^2)/\sqrt{\pi}$. The function $z_3 = \{h_j^2 a(\tau_j - \tau)\}^{1.1}$ is selected so that at the point τ_j the conditions $z_3 = 0$ and $(z_3)_\tau' = 0$ are satisfied, under which z_3 does not affect the values of Θ and Θ_τ' at this point but allows one to change considerably Θ and Θ_τ' within the intervals (τ_j, τ_{j+1}). Approximating functions with these properties are also used in the method of finite elements. Calculations show that by means of the function z_3 it is possible to improve substantially the approximation of the solution in the presence of a pronounced nonlinearity in the region.

TABLE 1. Relative Temperature in a Semibounded Space for Small Times in Heating under Nonlinear Conditions of Heat Transfer

$x \cdot 10^3$, m	τ, sec					
	5	10	15	20	25	30
0	0.2689	0.2759	0.2811	0.2854	0.2891	0.2925
50	0.2600	0.2671	0.2723	0.2767	0.2805	0.2823
100	0.2544	0.2602	0.2649	0.2690	0.2727	0.2761

The values of ν are found from the condition of conjugation of the elements Θ in time for iterations j and $j+1$: $\Theta(x_i, \tau_j, \nu_{j-1}) = \Theta(x_i, \tau_j, \nu_j)$. The coefficient μ is calculated from the boundary condition (15). The values of φ_1 and φ_2 are found from Eqs. (16) and (17) using linear interpolation. The coefficient φ_3 is determined from Eq. (18). In the course of the calculations we check the minimization of the functional $I(\Theta) < 3 \cdot 10^{-4}$.

Table 1 presents some results of calculations for the following conditions: $T_m = 1200$ K, $T(x, 0) = 300$ K, $C = 4 \cdot 10^{-8}$ W/(m$^2 \cdot$K^4), $\lambda_0 = 40$ W/(m·K), $\beta = 2$, $\Psi = 0.5$, $\alpha_c = 50$ W/(m$^2\cdot$K), $c\rho = 4 \cdot 10^6$ J/(m·K). For $\tau = 10$ sec and $x = 0$ the values of the coefficients are $\mu = 1.0192$, $\nu = 1.0050$, $\varphi_1 = 1.2455$, $\varphi_2 = 0.9961$, $\varphi_3 = 15.93$. The error for the given values of $\Theta(0, \tau)$ does not exceed 0.5%.

Variational calculations with the aid of functional (16) show that the error of calculations in this case decreases by an order or more as 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% due only to the choice of the way of averaging of the thermal conductivity $\lambda(\Theta)$ [3]. In this case fluctuations of the approximations in the spatial region that contradict the physical meaning of ten occur. These errors do not appear when the suggested variational scheme is used.

It follows from the calculations that minimization of errors is to a great extent determined by the extremal properties of functional (16). The residuals of the equations can be minimized at certain points by the methods of polydimensional optimization, but if the functional has no extremum or the residual of Eq. (16) is substantial, then minimization of the errors of temperature calculations will, as a rule, be unsatisfactory. Calculations performed for different problems show that if functional (16) has an extremum, then at certain points x_i the maximum rate of approach to equilibrium Θ'_τ can occur. This suggests that functional (16) expresses a physically existing directivity of spontaneous processes to equilibrium, which makes it possible to select approximating functions in an optimum way. In some problems time-dependent coefficients that are found from the condition of the existence of an extremum can coincide up to the fourth sign with the corresponding values of the coefficients for the exact solutions; this also confirms the efficiency of using the extremal properties of functional (16).

Minimization of the error of calculations depends strongly on the choice of approximating functions Θ, which should approximate the change in the derivatives Θ'_x, Θ''_{xx}, and Θ'_τ in space and time with certain reliability. If other approximations are used in the example given above, in particular, the functions $\Theta_{i,j} = N(\tau) \cos(\mu_i x)$ which determine the character of the change in the derivatives only for large values of τ rather well [2], then the errors of calculations grow considerably. With such an unsatisfactory choice of approximations Θ it is often impossible to minimize the errors. Use of Eq. (17), which is obtained by the first law of thermodynamics, improves considerably the process of calculation error minimization.

NOTATION

$\vartheta = T/T_m$, temperature; Ψ, new thermodynamic function; T, absolute temperature; T_m, medium temperature; x, x_i, coordinates; τ, time; q, heat flux; Δq_s, fictitious heat flux; λ, thermal conductivity; c, heat capacity; ρ, density; Θ, approximating functions; $\Theta_{i,j}$, piecewise-smooth elements of the functions Θ; f, arbitrarily small variations of the solution of the problem ϑ; Θ_a, Θ_b, approximations to the solution from below and from above; I, functional; δI, first variation of the functional; $\delta^2 I$, second variation; ε, residual of the heat conduction equation;

E, residual of the boundary condition; i, number of a spatial step; j, number of a time step; $1 - \gamma$, relative initial temperature; a, thermal diffusivity; C, coefficient of radiation; α_c, coefficient of convective heat transfer; β and Ψ, coefficients determining the function $\lambda(\Theta)$; μ, ν, φ, unknown coefficients.

REFERENCES

1. V. A. Bondarev, Inzh.-Fiz. Zh., **62**, No. 1, 130-139 (1992).
2. V. A. Bondarev, Inzh.-Fiz. Zh., **65**, No. 3, 341-349 (1993).
3. N. M. Belyaev and A. A. Ryadno, Methods of Heat Conduction Theory [in Russian], Pt. 2, Moscow (1982).
4 H. S. Carslaw and J. C. Jaeger, Conduction of Heat in Solids [Russian translation], Moscow (1964).
5 M. Abramowitz and I. A. Stegun (eds.), Handbook of Mathematical Functions [Russian translation], Moscow (1979).