

Electronic Journal of Polish Agricultural Universities is the very first Polish scientific journal published exclusively on the Internet, founded on January 1, 1998 by the following agricultural universities and higher schools of agriculture: University of Technology and Agriculture of Bydgoszcz, Agricultural University of Cracow, Agricultural University of Lublin, Agricultural University of Poznan, University of Podlasie in Siedlce, Agricultural University of Szczecin and Agricultural University of Wrocław.



**ELECTRONIC
JOURNAL
OF POLISH
AGRICULTURAL
UNIVERSITIES**

**2005
Volume 8
Issue 4
Topic
CIVIL
ENGINEERING**

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PODHORECKI A. 2005 GENERALIZATION OF THE EQUATION OF HEAT CONDUCTION IN SOLIDS AND NEW APPROACH OF NUMERICAL SOLUTION Electronic Journal of Polish Agricultural Universities, Civil Engineering, Volume 8, Issue 4.

Available Online <http://www.ejpau.media.pl>

GENERALIZATION OF THE EQUATION OF HEAT CONDUCTION IN SOLIDS AND NEW APPROACH OF NUMERICAL SOLUTION

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ABSTRACT

The problem of non-linear heat flow in solids at large temperature changes and variable material properties is considered in this paper. The equation of heat conduction has been formulated and then – the equations of the finite elements method in the two versions: non-incremental and incremental have been derived.

Key words: initial-boundary problem, generalized equation of heat conduction in solids, large changes of temperature, finite elements method in non-incremental and incremental version.

INTRODUCTION

Heat exchange occurs as a result of differences between temperatures. To analyze such exchange, it is necessary to know a temperature field T , which is described by the correlation between the temperature, space coordinates X and time t .

The physical model of heat conduction in solids is described by the Fourier's law, which includes heat flux density and the condition of the explicitness of the solution of this equation [see e.g. Nowacki 1963, Whitaker 1976, Holman 1992].

The analytic methods of solving the problems of heat exchange for complicated shapes and boundary conditions of a body require far-reaching simplifying assumptions, which make these solutions not very useful. Numerical methods (mainly the finite elements method) allow for relatively easy consideration of complicated shapes, boundary conditions and variable material properties, but in this case it is important to correctly formulate solving equations.

The mathematical foundations of the heat conduction theory originate from the thermodynamics of continuous media, so-called phenomenological thermodynamics [Woźniak 1970, Wilmański 1985]. The issues of heat conduction make an important research problem and are the domain of physics of buildings. The equation of

heat conduction applied there is right at a small temperature increase [Nowacki 1963, Whitaker 1976, Holman 1992]. The cases occur, however, when this increase is high (i.e. during fire) and the classical equation of heat conduction is useless to analyze such problems.

The equation of heat conduction in solids at large temperature changes is generalized in this paper. This generalization consists in taking the non-linear components of temperature increase into account as well as the time-variability of material properties in the equation of heat conduction. Finally, basing on the generalized equation, the following equations will be formulated: in the non-incremental version of the finite elements method in a stationary coordinate system as well as in the incremental version of FEM in an actualized coordinate system.

ASSUMPTIONS

Solid, occupying in natural (initial) configuration an area \mathfrak{R} , which is a subset of the Euclidean space R^3 . \mathfrak{R} is the denotation of the interior of this area and $\partial\mathfrak{R}$ – the area's boundary is considered.

A temperature field T is being investigated within a time range $t \in \langle 0, \infty \rangle$ and described in the Cartesian coordinate system \mathbf{X} . The body in a non-deformed and stress-free state is in constant temperature $T_0 = T(\mathbf{X}, 0) = \text{const}$. Such initial state is called the natural state of the body.

As heat sources work inside the body as well as its surface is heated or cooled, the body deforms itself. It is accompanied by time-variable deformations, stresses and temperature $T(\mathbf{X}, t)$. It may be assumed that the change of temperature $\Theta(\mathbf{X}, t) = T(\mathbf{X}, t) - T_0$ is high and this increasing may evoke the change of material properties. An important simplification is the assumption about the negligible influence of the deformation on the temperature field. In this case one deals with the problem of non-coupled thermoelasticity, what comes down to two-phased calculations. In the first phase, a temperature dispersion as the result of the solution of the problem of heat conduction has been established. In the second phase, knowing the temperature dispersion, by means of the equations of the theory of elasticity, it is possible to establish the fields of displacement, deformation and stress. The topic of this paper is therefore the first phase of the problem of non-coupled thermoelasticity.

It may be assumed that all dynamic variables are continuous and sufficiently smooth functions.

THE EQUATIONS OF HEAT CONDUCTION

The second law of thermodynamics gives so-called the equation of entropy production [Nowacki 1963, Woźniak 1970]:

$$\dot{S} = -\frac{q_{i,i}}{T} + \frac{W}{T} \quad (1)$$

where S denotes entropy, $\dot{S} \equiv \frac{\partial S}{\partial t}$ – an entropy increase in time, q_i describes the components of the vector of

heat flux (density of heat flux), $q_{i,i} \equiv \frac{\partial q_i}{\partial x_i}$, $W = W(\mathbf{X}, t)$ is the volumetric performance of internal heat sources,

that is the velocity of heat generation inside a body related to a volume unit, $T = T(\mathbf{X}, t)$ – absolute temperature.

The equation (1) may be put in another – equivalent – form:

$$\dot{S} = -\left(\frac{q_i}{T}\right)_i - \frac{q_i T_{,i}}{T^2} + \frac{W}{T} \quad (2)$$

After the introduction of a denotation

$$\sigma = -\frac{q_i T_{,i}}{T^2} + \frac{W}{T} \quad (3)$$

it is to obtain

$$\dot{S} = -\left(\frac{q_i}{T}\right)_i + \sigma \quad (4)$$

If integrated the latter expression regarding the volume \mathfrak{R} ,

$$\int_{\mathfrak{R}} \dot{S} d\mathfrak{R} = - \int_{\mathfrak{R}} \left(\frac{q_i}{T} \right)_{,i} d\mathfrak{R} + \int_{\mathfrak{R}} \sigma d\mathfrak{R} \quad (5)$$

may be obtained.

After the application of the Gauss-Ostrogradski transformation, one gets the following integral equation:

$$\int_{\mathfrak{R}} \dot{S} d\mathfrak{R} = - \int_{\partial\mathfrak{R}} \frac{q_i n_i}{T} d\mathfrak{R} + \int_{\mathfrak{R}} \sigma d\mathfrak{R} \quad (6)$$

where n_i is the component of the normal vector \vec{n} to the area $\partial\mathfrak{R}$. The first integral in the right side of the equation (6) describes the decline of entropy in time, evoked by the heat flow through the boundary surface $\partial\mathfrak{R}$. It is the velocity of the entropy exchange with the environment. The second one has the character of an entropy source and describes the velocity of energy formation. Basing on the postulate of the thermodynamics of irreversible processes, it is justified that:

$$\dot{\sigma} = \int_{\mathfrak{R}} \sigma d\mathfrak{R} > 0 \quad (7)$$

what means that the entropy production, evoked by the processes occurring in the body, is non-negative [Woźniak 1970]. The entropy source σ is connected with the reasons of irreversible processes, so-called thermodynamic stimuli F_i . Hence, so it may be written

$$\sigma = q_i F_i + \frac{W}{T} \quad (8)$$

Basing on the equations (8) and (3), it is possible to determine a function F_i :

$$F_i = - \frac{T_{,i}}{T^2} \quad (9)$$

It is visible that a temperature gradient is the sought thermodynamic stimulus.

In the case of laminar flows, the following linear connections, so-called phenomenological equations, are admitted:

$$q_i = L_{ij} F_j \quad (10)$$

where the tensor L_{ij} consists the parameters of heat conduction of anisotropic medium and satisfies the Onsager's rule on symmetry:

$$L_{ij} = L_{ji} \text{ for } i \neq j \quad (11)$$

Connecting (9) and (10), the generalized form of the Fourier's law may be obtained:

$$q_i = - \frac{\lambda_{ij}}{\left(1 + \frac{\Theta}{T_0}\right)^2} T_{,j} \quad (12)$$

where the coefficients

$$\lambda_{ij} = - \frac{L_{ij}}{T_0^2} \quad (13)$$

characterize the heat conduction in the analyzed body.

Substituting (11) with (12), one gets:

$$T_0 \left(1 + \frac{\Theta}{T_0} \right) \dot{S} = \left[\frac{\lambda_{ij}}{\left(1 + \frac{\Theta}{T_0} \right)^2} \Theta_{,j} \right]_{,i} + W \quad (14)$$

Thus, basing on the aforementioned, that entropy as the function of temperature may be stated. Therefore one may expand the function $S = S(T)$ in Taylor's series in the neighborhood of the natural state, in which the body is in non-deformed and non-stress state and the temperature $T = T_0$:

$$S(T) = S(T_0) + \frac{\partial S}{\partial T} \Big|_{T_0} (T - T_0) + \frac{1}{2} \frac{\partial^2 S}{\partial T^2} \Big|_{T_0} (T - T_0)^2 + \frac{1}{6} \frac{\partial^3 S}{\partial T^3} \Big|_{T_0} (T - T_0)^3 + \dots \quad (15)$$

According to the previous assumptions concerning the natural state, it is possible to write:

$$S(T_0) = 0 \quad (16)$$

The denotations of material characteristics:

$$\frac{\partial S}{\partial T} \Big|_{T_0} = m \quad \frac{\partial^2 S}{\partial T^2} \Big|_{T_0} = n \quad \frac{\partial^3 S}{\partial T^3} \Big|_{T_0} = p \quad (17)$$

may be introduced and the following constitutive equation connecting entropy with temperature:

$$S = m\Theta + \frac{1}{2} n\Theta^2 + \frac{1}{6} p\Theta^3 + \dots \quad (18)$$

may be obtained.

$$\Theta = T - T_0$$

Substituting (14) with (18), the equation of heat conduction in the following form:

$$\left(1 + \frac{\Theta}{T_0} \right) \left[\dot{m}\Theta + m\dot{\Theta} + \frac{1}{2} (\dot{n}\Theta + 2n\dot{\Theta})\Theta + \frac{1}{6} (\dot{p}\Theta + 3p\dot{\Theta})\Theta^2 \right] = \left[\frac{\lambda_{ij}}{\left(1 + \frac{\Theta}{T_0} \right)^2} \Theta_{,j} \right]_{,i} + \frac{W}{T_0} \quad (19)$$

is to obtain.

It is the generalized equation of heat conduction at large temperature changes and variable material characteristics.

If temperature increments are moderate, the equation (19) can be linearized, what results in the known equation of non-stationary heat flow in anisotropic continuous medium:

$$c_\varepsilon \dot{\Theta} = (\lambda_{ij} \Theta_{,j})_{,i} + W \quad (20)$$

where c_ε is the specific heat for constant deformation, $\frac{J}{m^3 \cdot K}$.

The equation (19) is supplied by the following boundary conditions:

a) primary conditions:

$$\begin{aligned} \Theta(\mathbf{X}, t) &= \hat{\Theta}(\mathbf{X}, t) \\ (\mathbf{X}, t) &\in \partial \mathfrak{R}_1 \times \langle 0, \infty \rangle \end{aligned} \quad (21)$$

where

$$\hat{\Theta}(\mathbf{X}, t) = \hat{T}(\mathbf{X}, t) - T_0(\mathbf{X}, 0) \quad (22)$$

b) secondary conditions:

$$q_n(\mathbf{X}, t) = \frac{\lambda_{ij}}{\left(1 + \frac{\Theta}{T_0}\right)^2} \Theta_{,j} n_i = \hat{q}_n \quad (23)$$

$$(\mathbf{X}, t) \in \partial\mathfrak{R}_2 \times \langle 0, \infty \rangle$$

where \hat{q}_n is the given distribution of the heat flow density on the surface $\partial\mathfrak{R}_2$ and the initial condition:

$$\Theta(\mathbf{X}, t) = T(\mathbf{X}, t) - T_0 = 0 \quad (24)$$

$$(\mathbf{X}, t) \in \mathfrak{R} \times \{0\}$$

EQUATIONS OF THE NON-INCREMENTAL VERSION OF THE FINITE ELEMENTS METHOD

To formulate the equations in the finite elements method (FEM), the weighted residual method is applied [Zienkiewicz 1972, Kleiber 1995].

The area \mathfrak{R} of a body is divided into finite elements (FE), i.e. subareas \mathfrak{R}_e , $e = 1, 2, \dots, E$. An unknown temperature function $\Theta(\mathbf{X}, t)$ is described as below:

$$\Theta^e(\mathbf{X}, t) = \Phi_\alpha^e(\mathbf{X}) r_\alpha^e(t) \quad (25)$$

$$\alpha = 1, 2, \dots, A, \quad (\mathbf{X}, t) \in \mathfrak{R}_e \times \langle 0, \infty \rangle, \quad e = 1, 2, \dots, E$$

where Φ_α^e are the shape functions depending on \mathbf{X} , whereas $r_\alpha^e = r_\alpha^e(t)$ represents the set of node temperatures (parameters), depending on t .

If the equation (19) is being substituted with the approximation (25), this equation will not be equal to 0 but it will generate the rest Λ^e :

$$\left(m^e \Phi_\beta^e + n^e \Phi_\beta^e \Phi_\gamma^e r_\gamma^e + \frac{1}{2} p^e \Phi_\beta^e \Phi_\gamma^e \Phi_\eta^e r_\gamma^e r_\eta^e \right) r_\beta^e + \left\{ \dot{m}^e \Phi_\beta^e + \frac{1}{2} \dot{n}^e \Phi_\beta^e \Phi_\gamma^e r_\gamma^e + \frac{1}{6} \dot{p}^e \Phi_\beta^e \Phi_\gamma^e \Phi_\eta^e r_\gamma^e r_\eta^e - \right.$$

$$\left. - \frac{1}{T_0 + \Phi_\alpha^e r_\alpha^e} \frac{\Phi_{\beta,j}^e \left[\lambda_{ij}^e (1 + \Phi_\tau^e r_\tau^e) (1 + \Phi_\gamma^e r_\gamma^e) - 2\lambda_{ij}^e \frac{1}{T_0} \Phi_{\tau,i}^e r_\tau^e (1 + \Phi_\gamma^e r_\gamma^e) \right]}{\left(1 + \frac{\Phi_m^e r_m^e}{T_0} \right) \left(1 + \frac{\Phi_n^e r_n^e}{T_0} \right) \left(1 + \frac{\Phi_p^e r_p^e}{T_0} \right) \left(1 + \frac{\Phi_s^e r_s^e}{T_0} \right)} \right\} r_\beta^e - \frac{W}{T_0 + \Phi_\alpha^e r_\alpha^e} = \Lambda_e \quad (26)$$

In this situation, the rest Λ^e must be reduced to the least value in all of the points of the body \mathfrak{R} with a tapering function $W_\alpha = W_\alpha(\mathbf{X})$:

$$\sum_{e=1}^E \iint_{\mathfrak{R}_e} W_\alpha^e \Lambda^e d\mathfrak{R} = 0 \quad (27)$$

where the tapering function W_α^e can be, particularly, equal to the shape function Φ_α^e . Such procedure is called the residual method. Substituting (27) with (26), the system of the ordinary differential equations

$$\sum_{e=1}^E \left(C_{\alpha\beta}^e \dot{r}_\beta^e + K_{\alpha\beta}^e r_\beta^e + R_\alpha^e \right) = 0 \quad (28)$$

may be obtained, where:

$$\begin{aligned} C_{\alpha\beta}^e &= \iint_{\mathfrak{R}_e} W_\alpha^e \left(m^e \Phi_\beta^e + n \Phi_\beta^e \Phi_\gamma^e r_\gamma^e + \frac{1}{2} p^e \Phi_\beta^e \Phi_\gamma^e \Phi_\eta^e r_\gamma^e r_\eta^e \right) d\mathfrak{R} \\ K_{\alpha\beta}^e &= \iint_{\mathfrak{R}_e} W_\alpha^e \left(\dot{m}^e \Phi_\beta^e + \frac{1}{2} \dot{n} \Phi_\beta^e \Phi_\gamma^e r_\gamma^e + \frac{1}{6} \dot{p}^e \Phi_\beta^e \Phi_\gamma^e \Phi_\eta^e r_\gamma^e r_\eta^e \right) d\mathfrak{R} - \\ &\quad - \iint_{\mathfrak{R}_e} \frac{W_\alpha^e}{T_0 + \Phi_\zeta^e r_\zeta^e} \frac{\Phi_{\beta',j}^e \left[\lambda_{ij}^e \left(1 + \Phi_\tau^e r_\tau^e \right) \left(1 + \Phi_\gamma^e r_\gamma^e \right) - 2\lambda_{ij}^e \frac{1}{T_0} \Phi_{\tau,i}^e r_\tau^e \left(1 + \Phi_\gamma^e r_\gamma^e \right) \right]}{\left(1 + \frac{\Phi_m^e r_m^e}{T_0} \right) \left(1 + \frac{\Phi_n^e r_n^e}{T_0} \right) \left(1 + \frac{\Phi_p^e r_p^e}{T_0} \right) \left(1 + \frac{\Phi_s^e r_s^e}{T_0} \right)} d\mathfrak{R} - \\ &\quad - \iint_{\mathfrak{R}_e} \frac{W_\alpha^e}{T_0 + \Phi_\zeta^e r_\zeta^e} \frac{\Phi_{\beta',ji}^e}{\left(1 + \frac{\Phi_m^e r_m^e}{T_0} \right) \left(1 + \frac{\Phi_n^e r_n^e}{T_0} \right)} d\mathfrak{R} \\ R_\alpha^e &= - \iint_{\mathfrak{R}_e} \frac{W_\alpha^e W^e}{T_0 + \Phi_\zeta^e r_\zeta^e} d\mathfrak{R} \end{aligned} \quad (29)$$

After aggregation and introduction of boundary conditions, this system of equations assumes the form:

$$\mathbf{C}(\mathbf{x})\dot{\mathbf{x}} + \mathbf{K}(\mathbf{x})\mathbf{x} + \mathbf{R}(\mathbf{x}) = \mathbf{0} \quad (30)$$

where \mathbf{C} and \mathbf{K} are global square matrices, \mathbf{R} is a column matrix, including thermal impulses causing the heat exchange, $\mathbf{x} = \mathbf{x}(t)$ is a column matrix including the temperature values in the nodes of the digitized body. The matrices \mathbf{C} , \mathbf{K} and \mathbf{R} are the functions of the unknown node temperatures \mathbf{x} .

To solve the equation (30), the known methods of the direct integration of equations of motion can be used, e.g. the Newmark's or Wilson's method, SS_{pj} (Zienkiewicz-Wood) method, finite differences method [Kleiber 1995]. Non-linearity of the equation (30), regardless of the applied method of the direct integration of equations of motion, forces the applying an iteration procedure.

EQUATIONS OF THE INCREMENTAL VERSION OF THE FINITE ELEMENTS METHOD

The process of heat flow within the time range $t_n \leq t \leq t_n + \Delta t$ is considered. It may be assumed that in an instant t_n a boundary-initial solution, i.e. the temperature field ${}^{t_n}\Theta$, is known as well as this actual configuration is at the same time the reference configuration.

At the beginning it is possible to make the following decomposition of each of the components of the equation (30):

$$\begin{aligned} {}^{t_n}\mathbf{x} &= {}^{t_n}\mathbf{x} + \Delta\mathbf{x} = {}^{t_n}\mathbf{x} + \Delta\mathbf{x} \\ {}^{t_n}\mathbf{C} &= {}^{t_n}\mathbf{C} + \Delta\mathbf{C} = {}^{t_n}\mathbf{C} + \Delta\mathbf{C} \\ {}^{t_n}\mathbf{K} &= {}^{t_n}\mathbf{K} + \Delta\mathbf{K} = {}^{t_n}\mathbf{K} + \Delta\mathbf{K} \\ {}^{t_n}\mathbf{R} &= {}^{t_n}\mathbf{R} + \Delta\mathbf{R} = {}^{t_n}\mathbf{R} + \Delta\mathbf{R} \\ t &\in \langle t_n, t_n + \Delta t \rangle \end{aligned} \quad (31)$$

where, for example, ${}^t_n\mathbf{C}$ denotes the matrix \mathbf{C} describing the state of a body in the instant t , referred to the configuration in the instant t_n , $\Delta\mathbf{C}$ is the increase of the matrix \mathbf{C} within the time range $\Delta t = t - t_n$. Then, the equation (30) may be written for the instants t_n and $t_{n+1} = t_n + \Delta t$:

$$\begin{aligned} {}^t_n\mathbf{C} {}^t_n\dot{\mathbf{x}} + {}^t_n\mathbf{K} {}^t_n\mathbf{x} + {}^t_n\mathbf{R} &= 0 \\ {}^t_{n+1}\mathbf{C} {}^t_{n+1}\dot{\mathbf{x}} + {}^t_{n+1}\mathbf{K} {}^t_{n+1}\mathbf{x} + {}^t_{n+1}\mathbf{R} &= 0 \end{aligned} \quad (32)$$

After the introduction of the decomposition formulas (31) and then – subtracting both sides of these equations from each other, it is possible to obtain an incremental equation in a form:

$$\left({}^t_n\mathbf{C} + \Delta\mathbf{C}\right)\Delta\dot{\mathbf{x}} + \left({}^t_n\mathbf{K} + \Delta\mathbf{K}\right)\Delta\mathbf{x} + \left(\Delta\mathbf{R} + \Delta\mathbf{C} {}^t_n\dot{\mathbf{x}} + \Delta\mathbf{K} {}^t_n\mathbf{x}\right) = 0 \quad (33)$$

If the solution for the instant t_n is known, it is possible to unambiguously determinate the matrices ${}^t_n\mathbf{C}$ and ${}^t_n\mathbf{K}$. Nonlinearity sticks, however, in the matrices $\Delta\mathbf{K}$, $\Delta\mathbf{C}$ and $\Delta\mathbf{R}$, which depend on unknown solutions for the instant t_{n+1} . It is convenient to write the equation (33) in another, equivalent, form:

$${}^t_n\mathbf{C}\Delta\dot{\mathbf{x}} + {}^t_n\mathbf{K}\Delta\mathbf{x} + \Delta\tilde{\mathbf{R}} = 0 \quad (34)$$

where

$$\Delta\tilde{\mathbf{R}} = \Delta\mathbf{R} + \Delta\mathbf{C}\left({}^t_n\dot{\mathbf{x}} + \Delta\dot{\mathbf{x}}\right) + \Delta\mathbf{K}\left({}^t_n\mathbf{x} + \Delta\mathbf{x}\right)$$

In case of small time increment Δt , the changes of the matrices $\Delta\mathbf{C}$ and $\Delta\mathbf{K}$ can be neglected, so the equation (34) can be linearized:

$${}^t_n\mathbf{C}\Delta\dot{\mathbf{x}} + {}^t_n\mathbf{K}\Delta\mathbf{x} + \Delta\mathbf{R} = 0 \quad (35)$$

The solution of the equation (34) or (35) allows to calculate the state of the system in the instant $t_{n+1} = t_n + \Delta t$, and this, subsequently, enables to skip to the another, analogical step of a calculation procedure.

The presented procedure refers to the description of heat flow in the actualized Lagrange's description.

RESUME

The paper considers the problem of non-linear heat flow in solids at large temperature gradients and variable material properties. At first, the equation of heat conduction has been generalized, then the equations of the finite elements method in two versions: non-incremental and incremental, have been formulated. These are the new and original elements of the work. There exists many of practical examples, when high and fast temperature changes occur, e.g. during a fire. There is no possibility in existing, known programs to solve such problems. Author is going to implement the presented calculation model into the FEM packet of ABAQUS.

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