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The BEM application for numerical solution of non-steady and nonlinear thermal diffusion problems

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Application of the boundary element method for approximate solution of non-steady and nonlinear thermal diffusion problems is not possible in a direct way. The fundamental solutions (being a basis of the BEM algorithm) are known only for linear problems — in particular the linear form of the Fourier equation is required. On the other hand, the numerous advantages of the boundary element method are a sufficient justification for the examinations concerning the adaptation of the method in this direction. In the paper, the numerical procedures "linearizing" the typical mathematical model of heat conduction process will be discussed. Combining the basic BEM algorithm for linear Fourier equation with procedures correcting the temporary solutions for successive values of time, we obtain a simple tool which allows us to solve a large class of the practical problems concerning the heat conduction processes. In this paper we will discuss in turn the algorithms called the *temperature field correction method* (TFCM), the *alternating phase truncation method* (APTM) and the *artificial heat source method* (AHSM). In the final part of the paper, some examples of numerical solutions will be presented.

1. Introduction

The nonlinear thermal diffusion problems can be divided into three groups [8], namely such that:

- the process is described by a linear differential equation, but the boundary conditions are nonlinear;
- the differential equation considered is nonlinear, but the boundary conditions are linear;
- both the differential equation as well the boundary conditions are nonlinear.

The models close to the real physical problems belong, as a rule, to the third group. Thermophysical parameters (specific heat, mass density, thermal conductivity) of typical materials are the functions of temperature, whereas the heat transfer coefficients appearing in the "natural" Robin boundary conditions determining the continuity of heat flux on the outer surface of the system are temperature-dependent, too.

It should be pointed out that from a numerical point of view, the nonlinear boundary conditions do not cause any essential difficulties connected with the construction of relatively exact and simple algorithms. In a case of non-steady heat conduction, the transition from time t to $t+\Delta t$ is analyzed. The coefficients in the suitable boundary conditions (natural convection and radiation are typical examples of such problems) can be determined for time t — in this way we consider the conditions for which the heat transfer coefficients (or thermal resistances) are known [18]. If necessary, in order to estimate the values of coefficients for time $t + \Delta t$, a certain iterative process can be applied [1].

More complex problems are connected with nonlinearities in the differential equation describing the heat conduction process in the domain considered. Temperature-dependent thermophysical

parameters can be, in a simple manner taken into account only in the case of application of the method of finite differences. On the other hand, however, the FDM is not the most effective and accurate method — particularly for the geometrically complex objects. The real shape of the boundary and the differential grid do not fit together. So, the approximation of boundary conditions is decidedly worse than in the case of FEM or BEM.

The basic algorithm of the finite element method can be adapted for numerical solution of nonlinear thermal diffusion problems, because the thermophysical parameters of the material can be in a certain way averaged in sub-domains of successive finite elements. Such type of the FEM algorithm was presented by the authors of this paper in [10, 12, 15]. The thermal diffussivity in domain of the finite element considered has been defined as an integral mean for the corresponding interval of temperature. The method was sufficiently accurate for moderate changes of thermophysical parameters, but e.g. in the case of modelling of the solidification process (a thermal diffussivity of the so-called *mushy* zone essentially differs from this parameter for solid and liquid sub-domains), certain additional correcting procedures should be introduced.

The boundary element method in its "natural" form can be used only for numerical simulation of heat conduction problems described by the linear differential equations [3, 21]. So, in order to apply the method for approximate solution of nonlinear problems, the suitable "linearizing" procedures must be worked out, and this will be the subject of the present paper. In particular, the methods called the *temperature field correction method* (TFCM), the *alternating phase truncation method* (APTM) and the *artificial heat source method* (AHSM) will be discussed (Secs. 3, 4 and 5). In Sec. 6 the 1st scheme of the BEM will be presented, while in Sec. 7 the examples of numerical simulations will be shown. The examples concern a strongly nonlinear problem, namely the phase transition process (treated as a so-called "fixed domain problem" [6, 23]) will be analyzed.

2. Governing equations

The equation describing non-steady state temperature field in a certain isobaric and isotropic domain Ω in which the heat is transported by conduction, is of the form

$$X \in \Omega : \quad c(T)\frac{\partial T(X,t)}{\partial t} = \operatorname{div}\left[\lambda(T)\operatorname{grad} T(X,t)\right] + q_V(X,t)\,, \tag{1}$$

where $c(T)$, $\lambda(T)$ are the thermophysical parameters (specific heat related to a unit of volume and thermal conductivity), q_V is the capacity of internal heat sources, T, X, t — denote temperature, spatial co-ordinate and time. In this paper we will consider the solenoidal temperature fields, and then $q_V = 0$.

Equation (1) is supplemented by boundary conditions in the general form

$$X \in \Gamma : \quad \Phi[T(X,t),\, n \cdot \operatorname{grad} T(X,t)] = 0\,, \tag{2}$$

and the initial condition

$$t = 0 : \quad T(X,0) = T_0(X)\,. \tag{3}$$

The symbol $n \cdot \operatorname{grad} T$ used in Eq. (2) denotes a normal derivative at the boundary point considered. Typical forms of the boundary condition (2) are the following:

- the first type of boundary condition

$$X \in \Gamma_1 : \quad T(X,t) = T_g(X,t)\,, \tag{4}$$

where T_g is a given boundary temperature;

- the second type of boundary condition

$$X \in \Gamma_{\mathrm{II}}: \quad -\lambda(T) n \cdot \operatorname{grad} T(X,t) = q_n(X,t), \tag{5}$$

where q_n is a given boundary heat flux;

- the third type of boundary condition

$$X \in \Gamma_{\mathrm{III}}: \quad -\lambda(T) n \cdot \operatorname{grad} T(X,t) = \alpha[T(X,t) - T^{\infty}], \tag{6}$$

where α is the heat transfer coefficient at the boundary point X, while T^{∞} is ambient temperature.

The basic mathematical model of the heat conduction process can be rebuilt by introducing to the considerations the physical enthalpy (related to a unit of volume), defined as follows:

$$H(T) = \int_{T_{\mathrm{r}}}^{T} c(\mu)\,\mathrm{d}\mu, \tag{7}$$

where T_{r} denotes a certain reference level.

The energy equation written in the enthalpy convention takes the form

$$X \in \Omega: \quad \frac{\partial H(X,t)}{\partial t} = \operatorname{div}[a(T) \operatorname{grad} H(X,t)], \tag{8}$$

where $a = \lambda/c$.

The structure of Eq. (8) is the same as the form of a typical Fourier equation. So, the numerical aspects of approximate solutions of the problems in which the enthalpy convention has been introduced are close to the problems appearing in the case of a classical approach.

It is easy to verify that the normal heat flux is equal to $q_n = -a\,n \cdot \operatorname{grad} H(X,t)$, and the typical boundary conditions written in enthalpy convention are of the form

$$X \in \Gamma_{\mathrm{I}}: \quad H(X,t) = H_{\mathrm{g}}(X,t), \tag{9}$$

$$X \in \Gamma_{\mathrm{II}}: \quad -a\,n \cdot \operatorname{grad} H(X,t) = q_n(X,t), \tag{10}$$

$$X \in \Gamma_{\mathrm{III}}: \quad -a\,n \cdot \operatorname{grad} H(X,t) = \alpha[T(H) - T^{\infty}]. \tag{11}$$

The boundary condition of the 3rd type is, to a certain degree, the "Achilles' heel" of the enthalpy convention. If the specific heat c is a constant value, then

$$H - H^{\infty} = \int_{T_{\mathrm{r}}}^{T} c\,\mathrm{d}\mu - \int_{T_{\mathrm{r}}}^{T^{\infty}} c\,\mathrm{d}\mu = c(T - T^{\infty}) \tag{12}$$

and we have $T - T^{\infty} = (H - H^{\infty})/c$, i.e.

$$-a\,n \cdot \operatorname{grad} H(X,t) = \alpha_H (H - H^{\infty}), \tag{13}$$

where $\alpha_H = \alpha/c$. In this case we obtain the formula analogous to Eq. (6). On the other hand, if the specific heat c is variable then the problem is more complicated. From Eq. (12) it results that

$$H - H^{\infty} = \int_{T_{\mathrm{r}}}^{T} c(\mu)\,\mathrm{d}\mu = c^*(T - T^{\infty}), \tag{14}$$

and at the same time c^* is the integral mean of the specific heat in the interval $\langle T^{\infty}, T\rangle$. In the corresponding condition

$$-a\,n \cdot \operatorname{grad} H(X,t) = \frac{\alpha}{c^*}(H - H^{\infty}) \tag{15}$$

additional nonlinearity appears, which in case of numerical analysis should be taken into account.

The last element of the discussed approach is the determination of the function describing the dependence between temperature and physical enthalpy of the material considered, because as a rule we want to obtain the results of computations in the form of time-dependent temperature fields. The details of this problem are presented in [17].

The other approach to the heat conduction problem consists in introducing to the considerations the function called the Kirchhoff transformation defined in the following way:

$$U(T) = \int_{T_r}^{T} \lambda(\mu)\,\mathrm{d}\mu\,. \tag{16}$$

From this definition it follows that $\lambda(T) = \mathrm{d}U(T)/\mathrm{d}T$ and it is easy to check that the right-hand side of the energy equation can be written in the form

$$X \in \Omega: \quad \operatorname{div}[\lambda(T)\operatorname{grad}T(X,t)] = \operatorname{div}[\operatorname{grad}U(X,t)]\,. \tag{17}$$

So, introduction of the function $U(T)$ linearizes the operator $\operatorname{div}(\lambda \operatorname{grad} T)$ and the equation describing the steady-state temperature field in domain Ω becomes linear. Because of this, Kirchhoff's transformation is very useful for computations connected with such problems. The function can be also used for mathematical description of nonsteady-state processes [12], as well as in the range of thermal theory of foundry [13].

The first step of the present considerations consists in the following reconstruction of the Fourier equation. The left-hand side of this equation will be written according to the enthalpy convention, while the right-hand side — in Kirchhoff's convention

$$\frac{\partial H(X,t)}{\partial t} = \operatorname{div}[\operatorname{grad}U(X,t)]\,. \tag{18}$$

Because $H = H(T)$ and $U = U(T)$ are functions of temperature and are monotonic, it is possible to find the relationship $H = \Psi(U)$.

It can be seen that

$$\frac{\partial H(X,t)}{\partial t} = \frac{\partial H(U)}{\partial U}\frac{\partial U(X,t)}{\partial t} = \Psi'(U)\frac{\partial U(X,t)}{\partial t}\,; \tag{19}$$

this means that a new form of energy equation is as follows

$$\Psi'(U)\frac{\partial U(X,t)}{\partial t} = \psi(U)\frac{\partial U(X,t)}{\partial t} = \operatorname{div}[\operatorname{grad}U(X,t)]\,. \tag{20}$$

The analytical determination of $\psi(U)$ and of its derivative is generally impossible. The specific heats and others thermophysical parameters of the materials are generally given in the form of tables, and the functions $H(T)$ and $U(T)$ must be found on the basis of numerical integration (e.g. the Simpson method). In this way we can find the discrete set of $H(T)$ and $U(T)$ values (Fig. 1). Next, for the specific values of T_i we obtain pairs of numbers (U_i, H_i) which determine (in discrete form) the course of $\psi(U)$. Its derivative can be found by means of numerical differentiation.

The construction of a mathematical model requires the suitable reconstruction of the boundary and initial conditions, and namely:

- The first type of conditions can be transformed immediately

$$X \in \Gamma_{\mathrm{I}}: \quad U(X,t) = U_{\mathrm{g}}(X,t)\,; \tag{21}$$

- In the case of the second type of boundary conditions, one can notice that the expression $-\lambda n \cdot \operatorname{grad}T(X,t)$ can be written as $-n \cdot \operatorname{grad}U(X,t)$, and finally

$$X \in \Gamma_{\mathrm{II}}: \quad -n \cdot \operatorname{grad}U(X,t) = q_n(X,t)\,; \tag{22}$$

- The third type condition is of the form

$$X \in \Gamma_{\mathrm{III}}: \quad -n \cdot \operatorname{grad} U(X,t) = \alpha(T - T^{\infty}). \tag{23}$$

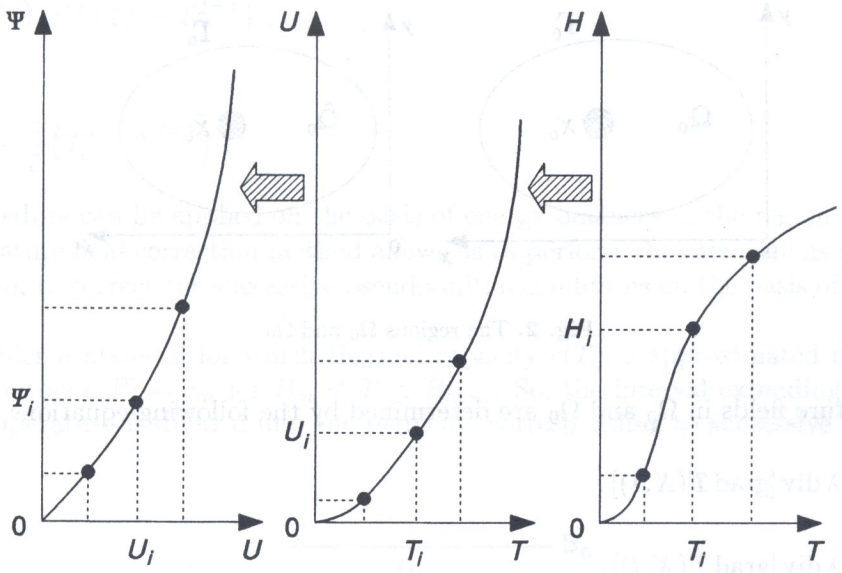

Fig. 1. Construction of $\psi(U)$

Let us repeat the considerations which have been exposed previously. We have

$$U - U^{\infty} = \int_{T_{\infty}}^{T} \lambda(\mu)\,\mathrm{d}\mu = \lambda^{*}(T - T^{\infty}). \tag{24}$$

For $\lambda = \text{const}$, $\lambda^{*} = \lambda$, whereas for $\lambda = \lambda(T)$, λ^{*} is the integral mean of the thermal conductivity for the interval $\langle T^{\infty}, T\rangle$. The boundary condition (23) can be rewritten in the form

$$-n \cdot \operatorname{grad} U(X,t) = \alpha_u(U - U^{\infty}), \tag{25}$$

where $\alpha_u = \alpha/\lambda^{*}$. As can be seen, the difficulties connected with a correct approximation of this condition are the same as in the case of application of the enthalpy convention.

Now we pass to the problems connected with construction of numerical algorithms "linearizing" the mathematical models of heat conduction problems.

3. The temperature field correction method (TFCM)

The temperature field correction method consists in the reconstruction of successive temporal solutions (for $t = t^1, t^2, \ldots$, etc.) corresponding to a certain linear problem, in order to take into account that in reality the nonlinear problem is analyzed.

The philosophy of approach to the problem of reconstructing the pseudo-initial condition for successive levels of time was presented by Szargut and Mochnacki [22], and next extended by Hong, Umeda and Kimura [4, 5], whereas the algorithm presented here was discussed by E.Majchrzak in [9].

The essence of the procedure of temperature field correction results from the following reasoning. Consider now two identical regions Ω_0 and $\hat{\Omega}_0$. The thermophysical parameters of Ω_0 are equal to

c, λ, whereas for $\hat{\Omega}_0$ we have $\hat{c}$, $\hat{\lambda}$. At the same time it is assumed that $\lambda = \hat{\lambda}$. The boundary conditions given on the contours Γ_0 and $\hat{\Gamma}_0$ are the same, i.e. (cf. Fig. 2)

$$X \in \Gamma_0 : \quad \Phi(T, \bar{n} \cdot \operatorname{grad} T) = 0, \qquad \hat{X} \in \hat{\Gamma}_0 : \quad \Phi[\hat{T}, \bar{n} \cdot \operatorname{grad} \hat{T}] = 0. \tag{26}$$

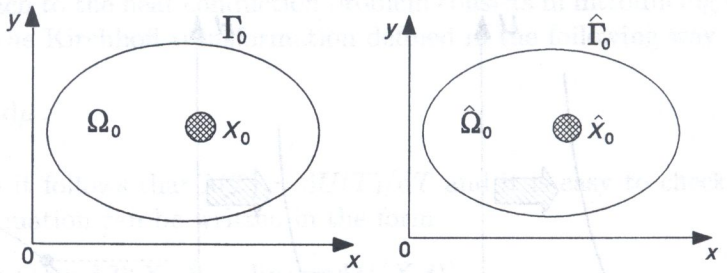

Fig. 2. The regions Ω_0 and $\hat{\Omega}_0$

The temperature fields in Ω_0 and $\hat{\Omega}_0$ are determined by the following equations

$$\begin{aligned} c\frac{\partial T(X,t)}{\partial t} &= \lambda \operatorname{div}[\operatorname{grad} T(X,t)], \\ \hat{c}\frac{\partial \hat{T}(X,t)}{\partial t} &= \hat{\lambda} \operatorname{div}[\operatorname{grad} \hat{T}(X,t)]. \end{aligned} \tag{27}$$

A new variable is introduced, $\tau = \frac{c}{\hat{c}}t$. Since $\frac{\partial \hat{T}}{\partial t} = \frac{\partial \hat{T}}{\partial \tau}\frac{\mathrm{d}\tau}{\mathrm{d}t} = \frac{c}{\hat{c}}\frac{\partial \hat{T}}{\partial \tau}$, therefore the equation for the second domain can be written in the form

$$\hat{c}\frac{\partial \hat{T}(X,\tau)}{\partial \tau} = \lambda \operatorname{div}[\operatorname{grad} \hat{T}(X,\tau)]. \tag{28}$$

It should be pointed out that equations describing the heat transfer processes in Ω_0 and $\hat{\Omega}_0$ are identical although the time in Ω_0 and $\hat{\Omega}_0$ "runs" in different way.

In Fig. 3 the curves of cooling at a selected point $X_0 \in \Omega_0$ and at the corresponding point $\hat{X}_0 \in \hat{\Omega}_0$ are shown.

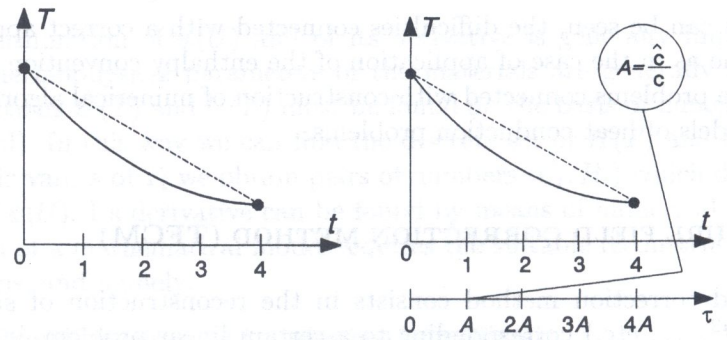

Fig. 3. The curves of cooling at points X_0 and $\hat{X}_0$

The slopes of the straight lines in Fig. 3 are the same:

$$\frac{\Delta T}{\Delta t} = \frac{\Delta \hat{T}}{\Delta \tau} = \frac{\hat{c}}{c}\frac{\Delta \hat{T}}{\Delta t}. \tag{29}$$

So,

$$c\Delta T = \hat{c}\Delta\hat{T}\,. \tag{30}$$

Equation (30) can be written in the form

$$c\left(T_0^f - T_0^{f+1}\right) = \hat{c}\left(\hat{T}_0^f - T_0^{f+1}\right)\,, \tag{31}$$

and

$$\hat{T}_0^{f+1} = T_0^f - \frac{c}{\hat{c}}\left(T_0^f - T_0^{f+1}\right)\,. \tag{32}$$

The same procedure can be applied on the basis of energy balances in the region of point X_0 [14].

The temperature field correction method allows us to perform the calculations in a homogenous region, and then, to correct the successive pseudo-initial conditions on the basis of equations of the (32) type.

Let us consider a material for which thermal capacity $c(T)$ is approximated by a certain step function, this means $c(T) = c_m$ for $B_m < T < B_{m+1}$. So, the interval extending from the initial to ambient temperature is divided into the segments corresponding to successive values of c_m (cf. Fig. 4).

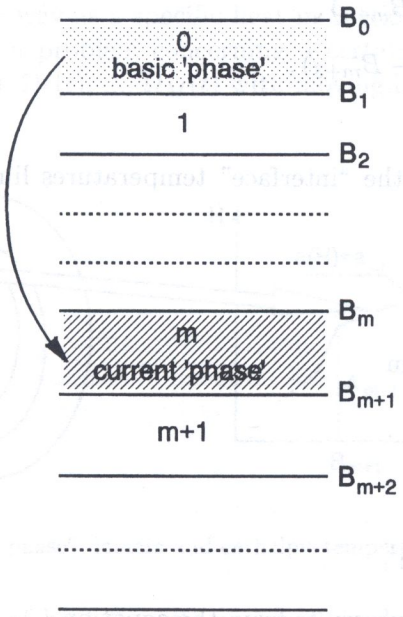

Fig. 4. Division

The time grid defined as follows

$$0 = t^0 < t^1 < \ldots < t^f < t^{f+1} < \ldots < t^F < \infty \tag{33}$$

is introduced, and the specific point X_0 of control volume V_0 is taken into account.

Let us assume that the cooling process is analyzed and the temperature at point X_0 has decreased from T_0^f to T_0^{f+1}; at the same time the computations have been executed for $c(T) = c_0$. The algorithm of temperature correction at the point considered is the following.

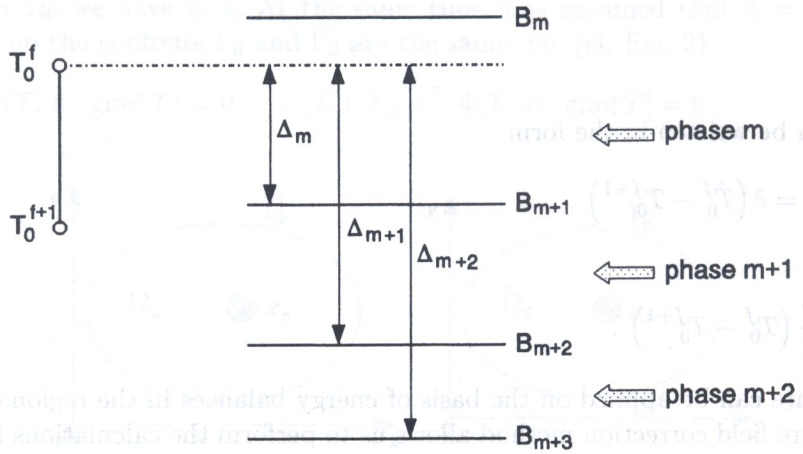

Fig. 5. The transition $f \to f+1$

Let (cf. Fig. 5)

$$\begin{aligned} \Delta_m &= c_m(T_0^f - B_{m+1})\,, \\ \Delta_{m+1} &= \Delta_m + c_{m+1}(B_{m+1} - B_{m+2})\,, \\ \Delta_{m+2} &= \Delta_{m+1} + c_{m+2}(B_{m+2} - B_{m+3})\,, \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots \end{aligned} \tag{34}$$

where B_m, B_{m+1}, B_{m+2}, ... are the "interface" temperatures limiting the successive "phases" of the material considered.

If

$$c_0(T_0^f - T_0^{f+1}) < \Delta_m\,, \tag{35}$$

then the formula (32) takes a form

$$\hat{T}_0^{f+1} = T_0^f - \frac{c_0}{c_m}\left(T_0^f - T_0^{f+1}\right). \tag{36}$$

For the case

$$\Delta_m < c_0\left(T_0^f - T_0^{f+1}\right) < \Delta_{m+1}\,, \tag{37}$$

the value of corrected temperature results from the equation

$$c_0\left(T_0^f - T_0^{f+1}\right) = c_m\Delta_m + c_{m+1}\left(B_{m+1} - \hat{T}_0^{f+1}\right) \tag{38}$$

and we obtain

$$\hat{T}_0^{f+1} = B_{m+1} + \frac{c_m}{c_{m+1}}\Delta_m - \frac{c_0}{c_{m+1}}\left(T_0^f - T_0^{f+1}\right). \tag{39}$$

If

$$\Delta_{m+1} < c_0\left(T_0^f - T_0^{f+1}\right) < \Delta_{m+2}\,, \tag{40}$$

then

$$c_0\left(T_0^f - T_0^{f+1}\right) = c_m\Delta_m + c_{m+1}(\Delta_{m+1} - \Delta_m) + c_{m+2}\left(B_{m+2} - \hat{T}_0^{f+1}\right) \tag{41}$$

and

$$\hat{T}_0^{f+1} = B_{m+2} + \frac{c_m}{c_{m+2}}\Delta_m + \frac{c_{m+1}}{c_{m+2}}(\Delta_{m+1} - \Delta_m) - \frac{c_0}{c_{m+2}}\left(T_0^f - T_0^{f+1}\right). \tag{42}$$

Similar formulas can be obtained for other possible transitions, but in practice these transitions do not appear (because of the small differences between T_0^f and T_0^{f+1}).

The algorithm presented above concerns the cooling processes and their reconstruction in the case of heating or a more general heat transfer problem is quite simple.

4. The alternating phase truncation method (APTM)

The basic algorithm of alternating phase truncation method was presented by Rogers, Berger and Ciment in [19, 20] and was used for numerical simulation of the Stefan problem (solidification at a constant temperature). The generalization of the APTM was presented in paper [7], while the approach which allows to adapt the method for a large class of nonlinear heat conduction problems was discussed in [11]. The APTM consists in conventional reduction of the considered domain Ω to a homogenous domain. So, the philosophy of APTM is close to the previously presented method of temperature field correction, but in numerical realization the APTM essentially differs in principles from the TFCM.

The method discussed requires the formulation of an adequate mathematical model using the enthalpy convention. If we assume that the thermal diffussivity $a(H)$ can be approximated by a certain step function (in the same way as a specific heat in Section 3), then the nonlinear problem considered can be replaced with a problem concerning a certain "multi-phase" domain being a composition of sub-domains $\Omega_0(t)$, $\Omega_1(t)$, ..., $\Omega_M(t)$ with moving boundaries $\Gamma_1(t)$, $\Gamma_2(t)$, ..., $\Gamma_M(t)$ (cf. Fig. 6).

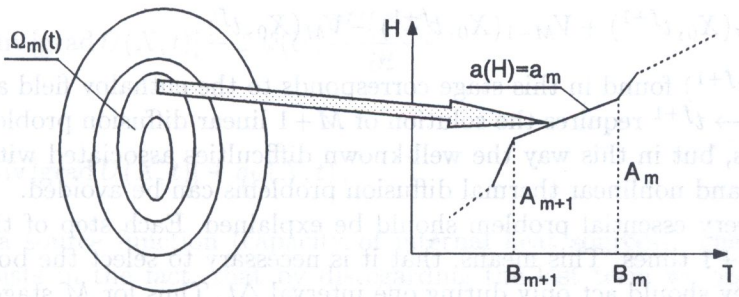

Fig. 6. "Multi-phase" domain and enthalpy–temperature diagram

The mathematical description of heat transfer processes in domain Ω (assuming that thermophysical parameters of sub-domains $\Omega_m(t)$ are constant) is

$$\left.\begin{aligned}
&X \in \Omega_m(t) \quad : \quad \frac{\partial H_m(X,t)}{\partial t} = a_m \operatorname{div}\left[\operatorname{grad} H_m(X,t)\right], \\
&X \in \Gamma_m(t) \quad : \quad \begin{cases} -a_m n \cdot \operatorname{grad} H_m(X,t) = -a_{m+1} n \cdot \operatorname{grad} H_{m+1}(X,t), \\ H_m(X,t) = H_{m+1}(X,t) = A_m, \end{cases} \\
&X \in \Gamma \quad : \quad \Phi[H(X,t),\, n \cdot \operatorname{grad} H(X,t)] = 0, \\
&t = 0 \quad : \quad H(X,t) = H_0(X).
\end{aligned}\right\} \tag{43}$$

Let us consider two separate levels of time t^f and t^{f+1}. The enthalpy distribution in region Ω at time t^f is known.

The first stage of computation concerns the hottest phase. The enthalpy distribution in the domain Ω at time t^f is transformed in this way

$$X_0 \in \Omega : \quad V_0(X_0, t^f) = \max[A_1, H(X_0, t^f)]. \tag{44}$$

This new pseudo-initial condition corresponds to a structural reduction of the whole area Ω to the "hottest phase" domain. Next, on the basis of numerical methods, the transition $t^f \rightarrow t^{f+1}$ is calculated. The solution for time t^{f+1} : $V_0^*(X_0, t^{f+1})$ is corrected according to the formula

$$V_0(X_0, t^{f+1}) = V_0^*(X_0, t^{f+1}) + H(X_0, t^f) - V_0(X_0, t^f) \tag{45}$$

and the first stage of computations comes to an end.

If we consider an arbitrary stage m ($m = 1, 2, ..., M-1$) then the enthalpy distribution $V_{m-1}(X_0, t^{f+1})$ is known. Reduction of domain Ω to Ω_m corresponds to acceptance of the following pseudo- initial condition

$$V_m(X_0, t^f) = \min\left\{A_m, \max[A_{m+1}, V_{m-1}(X_0, t^{f+1})]\right\}. \tag{46}$$

If $V_m^*(X_0, t^{f+1})$ denotes the enthalpy field calculated in this stage, then the final effect of its realization follows from the formula

$$V_m(X_0, t^{f+1}) = V_m^*(X_0, t^{f+1}) + V_{m-1}(X_0, t^{f+1}) - V_m(X_0, t^f). \tag{47}$$

At the last stage ($m = M$), the following pseudo-initial condition is assumed

$$V_{M-1}(X_0, t^f) = \min[A_M, V_{M-1}(X_0, t^{f+1})]. \tag{48}$$

After the computation of $V_M^*(X_0, t^{f+1})$ one obtains

$$H(X_0, t^{f+1}) = V_M^*(X_0, t^{f+1}) + V_{M-1}(X_0, t^{f+1}) - V_M(X_0, t^f). \tag{49}$$

The solution $H(X_0, t^{f+1})$ found in this stage corresponds to the enthalpy field at time $t = t^{f+1}$.

The transition $t^f \rightarrow t^{f+1}$ requires the solution of $M+1$ linear diffusion problems in structurally homogenous domains, but in this way the well-known difficulties associated with numerical simulation of non-steady and nonlinear thermal diffusion problems can be avoided.

At this point, a very essential problem should be explained. Each step of time in the APTM algorithm is done $M+1$ times. This means, that it is necessary to select the boundary conditions carefully, because they should act only during one interval Δt. Thus for M stages the boundary Γ should be insulated (the adiabatic condition). The "real" boundary condition "acts" only for this phase which corresponds to the current boundary temperature.

5. THE ARTIFICIAL HEAT SOURCE METHOD (AHSM)

In this section a certain algorithm will be discussed, which can be called the artificial heat source method (AHSM). A proposed approach can be useful in the case of nonlinear and non-steady heat conduction problems, as well as in numerical modelling of the solidification process. The method has been presented by B. Mochnacki and E. Majchrzak in [16]. The AHSM can be a very effective supplementary algorithm, first of all in the case of the BEM application to solution of the nonlinear problems.

Let us consider the boundary-initial problem described by energy equation (20), boundary conditions (21), (22), (23) and the initial condition $t = 0 : U(X, 0) = U_0(X)$. The method of construction of $\psi(U)$ was presented in Sec. 2, while Fig. 7 presents the course of derivative $\psi(U)$ for the carbon steel: C = 0.08, Mn = 0.31, Si = 0.08, Cr = 0.045, Ni = 0.07, Mo = 0.02, S = 0.05, Cr = 0.045 (the range of function $\Psi'(U)$ corresponds to the interval of temperatures $[0, 700\,^{\circ}\mathrm{C}]$).

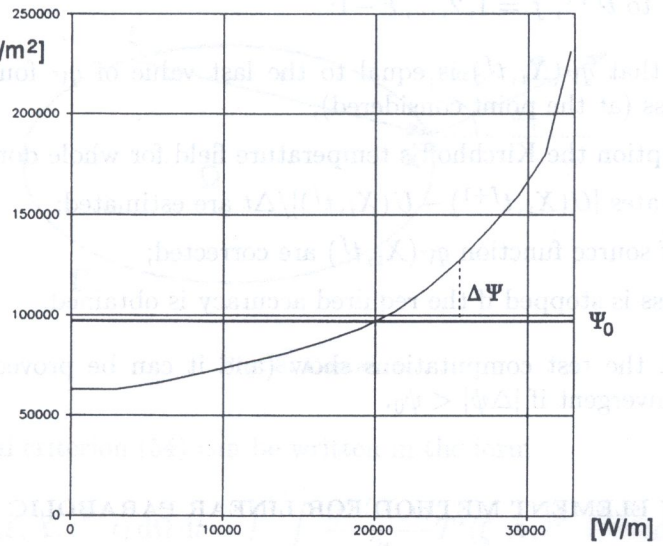

Fig. 7. The course of function $\Psi'(U)$

Consider now a function $\psi(U)$ which is conventionally expressed as a sum of two components, this means a constant part ψ_0 and a certain increment $\Delta\psi$,

$$\psi(U) = \psi_0 + \Delta\psi(U)\,. \tag{50}$$

The energy equation (20) can be written in the form

$$\psi_0 \frac{\partial U(X,t)}{\partial t} = \operatorname{div}\left[\operatorname{grad} U(X,t)\right] - \Delta\psi(U)\frac{\partial U(X,t)}{\partial t} \tag{51}$$

or

$$\psi_0 \frac{\partial U(X,t)}{\partial t} = \operatorname{div}\left[\operatorname{grad} U(X,t)\right] + q_V(X,t)\,, \tag{52}$$

where $q_V(X,t)$ is a source function (capacity of internal heat sources). The essential feature of equation (52) consists in the fact, that by disregarding the last term we obtain the linear form of energy equation. Taking into account the possible application of the boundary element method in the range of non-steady problems modelling, this is a very convenient form of basic differential equation (nonlinearity appears only in the component determining the internal heat sources, and the function describing the fundamental solution for the problem considered is well-known). The calculation of a source function requires, of course, the introduction of a certain iterative procedure. It should be pointed out that if $|\Delta\psi| < \psi_0$, then the corresponding iterative algorithm is convergent.

The iterative process of determining the source function is the following.

1. Transition from $t^0 = 0$ to $t^1 = t^0 + \Delta t$:

   - It is assumed that $q_V(X_i, t^0) = 0$, while X_i denote the central points of internal control volumes V_i selected in domain Ω;
   - Under this assumption the distribution of function U in the whole domain is calculated;
   - Local cooling rates $[U(X_i, t^1) - U(X_i, t^0)]/\Delta t$ are estimated;
   - Local values of source function $q_V(X_i, t^0)$ are corrected;
   - Iterative process is stopped if the required accuracy is obtained.

2. Transition from t^f to t^{f+1}, $f = 1, 2, ..., F-1$:

- It is assumed that $q_V(X_i, t^f)$ is equal to the last value of q_V found during the previous iterative process (at the point considered);
- For this assumption the Kirchhoff's temperature field for whole domain is calculated;
- Local cooling rates $[U(X_i, t^{f+1}) - U(X_i, t^f)]/\Delta t$ are estimated;
- Local values of source function $q_V(X_i, t^f)$ are corrected;
- Iterative process is stopped if the required accuracy is obtained.

As it was mentioned, the test computations show (and it can be proved analytically) that the iterative process is convergent if $|\Delta\psi| < \psi_0$.

6. THE BOUNDARY ELEMENT METHOD FOR LINEAR PARABOLIC EQUATIONS

In this chapter we shall discuss the problem of the BEM application for the case of a domain Ω which is characterized by constant thermophysical parameters (a linear problem). The object is placed in a rectangular coordinate system. The boundary-initial problem considered is described by the equation (cf. equation (1))

$$X \in \Omega : \quad \frac{\partial T(X,t)}{\partial t} = a\nabla^2 T(X,t) + \frac{q_V(X,t)}{c}, \tag{53}$$

boundary conditions (2) and initial condition (3).

Initially, we formulate the weighted residual criterion for the problem analyzed

$$\int_{t^0}^{t^F} \int_{\Omega} \left[a\nabla^2 T(X,t) - \frac{\partial T(X,t)}{\partial t} - \frac{q_V(X,t)}{c} \right] T^*(\xi, X, t^F, t)\, \mathrm{d}\Omega\, \mathrm{d}t, \tag{54}$$

where T^* is a fundamental solution of the form

$$T^*(\xi, X, t^F, t) = \frac{1}{[4\pi a(t^F - t)]^{w/2}} \exp\left[-\frac{r^2}{4a(t^F - t)} \right], \tag{55}$$

where ξ denotes the point in which the concentrated heat source is applied, while r is the distance from the considered point X to the point ξ, w is the problem dimension. The normal heat flux of fundamental solution should be found from the formula

$$q^*(\xi, X, t^F, t) = -\lambda \frac{\partial T^*(\xi, X, t^F, t)}{\partial n}, \tag{56}$$

If we consider the 2D problem ($X = (x_1, x_2)$, $\xi = (\xi_1, \xi_2)$), then we obtain the following expression

$$q^* = -\lambda \left(\frac{\partial T^*}{\partial x_1} \cos\alpha_1 + \frac{\partial T^*}{\partial x_2} \cos\alpha_2 \right) = \frac{\lambda d}{8\pi a^2 (t^F - t)^2} \exp\left[-\frac{r^2}{4a(t^F - t)} \right], \tag{57}$$

where

$$d = (x_1 - \xi_1)\cos\alpha_1 + (x_2 - \xi_2)\cos\alpha_2, \tag{58}$$

while $\cos\alpha_1$, $\cos\alpha_2$ are the directional cosines of the normal boundary vector (Fig. 8).

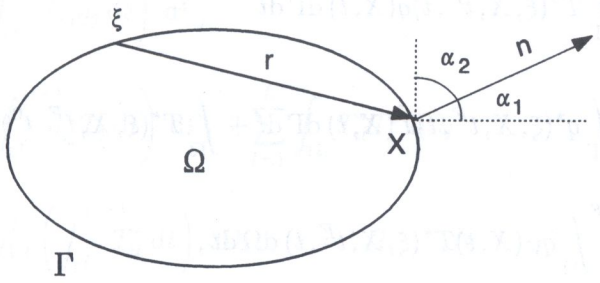

Fig. 8. Domain Ω

The weighted residual criterion (54) can be written in the form

$$\int_{t^0}^{t^F}\int_{\Omega} a\nabla^2 T(X,t)T^*(\xi,X,t^F,t)\,\mathrm{d}\Omega\,\mathrm{d}t - \int_{t^0}^{t^F}\int_{\Omega}\frac{\partial T(X,t)}{\partial t}T^*(\xi,X,t^F,t)\,\mathrm{d}\Omega\,\mathrm{d}t$$
$$-\frac{1}{c}\int_{t^0}^{t^F}\int_{\Omega} q_V(X,t)T^*(\xi,X,t^F,t)\,\mathrm{d}\Omega\,\mathrm{d}t = 0\,. \tag{59}$$

In order to construct the integral equation corresponding to the problem considered, we apply the 2nd Green's formula for the first component of equation (59) [3]

$$\int_{t^0}^{t^F}\int_{\Omega} a\left(\nabla^2 T\right)T^*\,\mathrm{d}\Omega\,\mathrm{d}t = \int_{t^0}^{t^F}\int_{\Omega} a\left(\nabla^2 T^*\right)T\,\mathrm{d}\Omega\,\mathrm{d}t - \frac{1}{c}\int_{t^0}^{t^F}\int_{\Gamma}(T^*q - Tq^*)\,\mathrm{d}\Gamma\,\mathrm{d}t\,. \tag{60}$$

The second component of the equation (59) is integrated by parts

$$\int_{t^0}^{t^F}\int_{\Omega}\frac{\partial T}{\partial t}T^*\,\mathrm{d}\Omega\,\mathrm{d}t = \left[\int_{\Omega} TT^*\,\mathrm{d}\Omega\right]_{t=t^0}^{t=t^F} - \int_{t^0}^{t^F}\int_{\Omega}\frac{\partial T^*}{\partial t}T\,\mathrm{d}\Omega\,\mathrm{d}t \tag{61}$$

and the equation (59) takes the form

$$\int_{t^0}^{t^F}\int_{\Omega}\left(a\nabla^2 T^* + \frac{\partial T^*}{\partial t}\right)T\,\mathrm{d}\Omega\,\mathrm{d}t - \left[\int_{\Omega} TT^*\,\mathrm{d}\Omega\right]_{t=t^0}^{t=t^F}$$
$$-\frac{1}{c}\int_{t^0}^{t^F}\int_{\Gamma}(T^*q - Tq^*)\,\mathrm{d}\Gamma\,\mathrm{d}t - \frac{1}{c}\int_{t^0}^{t^F}\int_{\Omega} q_V T^*\,\mathrm{d}\Omega\,\mathrm{d}t = 0\,. \tag{62}$$

Using the properties of the fundamental solution [3, 9] we finally obtain the following integral equation

$$T(\xi,t^F) + \frac{1}{c}\int_{t^0}^{t^F}\int_{\Gamma} T^*(\xi,X,t^F,t)q(X,t)\,\mathrm{d}\Gamma\,\mathrm{d}t$$
$$= \frac{1}{c}\int_{t^0}^{t^F}\int_{\Gamma} q^*(\xi,X,t^F,t)T(X,t)\,\mathrm{d}\Gamma\,\mathrm{d}t + \int_{\Omega} T^*(\xi,X,t^F,t^0)T(X,t^0)\,\mathrm{d}\Omega$$
$$+\frac{1}{c}\int_{t^0}^{t^F}\int_{\Omega} q_V(X,t)T^*(\xi,X,t^F,t)\,\mathrm{d}\Omega\,\mathrm{d}t\,. \tag{63}$$

For $\xi \to \Gamma$ the last equation is transformed to the boundary integral equation, which is of the form [3, 9]

$$C(\xi)T(\xi,t^F)+\frac{1}{c}\int_{t^0}^{t^F}\int_{\Gamma}T^*(\xi,X,t^F,t)q(X,t)\,\mathrm{d}\Gamma\,\mathrm{d}t$$

$$=\frac{1}{c}\int_{t^0}^{t^F}\int_{\Gamma}q^*(\xi,X,t^F,t)T(X,t)\,\mathrm{d}\Gamma\,\mathrm{d}t+\int_{\Omega}T^*(\xi,X,t^F,t^0)T(X,t^0)\,\mathrm{d}\Omega$$

$$+\frac{1}{c}\int_{t^0}^{t^F}\int_{\Omega}q_V(X,t)T^*(\xi,X,t^F,t)\,\mathrm{d}\Omega\,\mathrm{d}t, \tag{64}$$

where $C(\xi)\in(0,1)$. The value of coefficient $C(\xi)$ results from the position of the boundary point ξ considered; for example, for the smooth fragment of the boundary $C(\xi)=0.5$. It should be pointed out that for $\xi\in\Omega$: $C(\xi)=1$.

The numerical approximation of integral equation (64) consists in discretization of the considered interval of time $[t^0,t^F]$, and the boundary of the region Ω. In the case of nonsteady-state problems the interior of domain Ω must be also discretized.

So, the time grid is introduced (cf. equation (33)), while the boundary Γ is divided into N boundary elements Γ_j, $j=1,2,...,N$. Here we can assume a different approximation for the boundary values of individual elements. For example, we can consider a constant value of temperature and heat flux along the boundary element, or a linear distribution of T and q — Fig. 9. We can also introduce the boundary elements of higher order (e.g. parabolic elements).

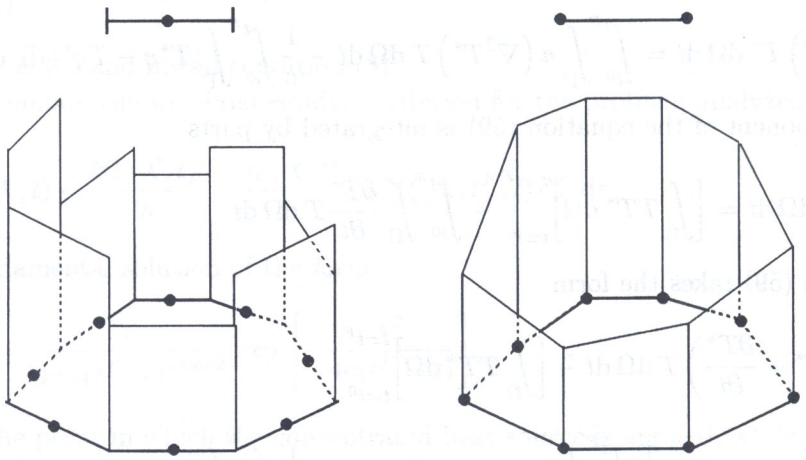

Fig. 9. Constant and linear boundary elements (2D problem)

The interior of Ω is divided into L internal cells Ω_l, $l=1,2,...,L$. Just as in the case of boundary elements, we can consider constant, linear and higher-order internal cells.

Here two approaches can be taken into account, i.e. the 1st or the 2nd scheme of the BEM. The idea of the 1st scheme consists in treatment of the transition from t^f to t^{f+1} as a certain separate problem with suitable pseudo-initial condition. In the case of the 2nd scheme of the BEM, the integration process starts from $t=t^0$ and then the knowledge of successive pseudo-initial conditions is needless, but consecutive values of boundary temperatures and heat fluxes for $t=t^0$, $t=t^1$, ..., $t=t^f$ must be "registered".

In this paper the 1st scheme of the BEM has been applied, because this algorithm allows us to combine the BEM with the procedures "linearizing" the nonlinear and non-steady heat conduction problems. In this case the numerical approximation of equation (64) is of the form

$$C_i T_i^{f+1} + \frac{1}{c}\sum_{j=1}^{N}\int_{\Gamma_j}\left(\int_{t^f}^{t^{f+1}} T_{ij}^* q_j \,\mathrm{d}t\right)\mathrm{d}\Gamma_j$$

$$= \frac{1}{c}\sum_{j=1}^{N}\int_{\Gamma_j}\left(\int_{t^f}^{t^{f+1}} q_{ij}^* T_j \,\mathrm{d}t\right)\mathrm{d}\Gamma_j + \sum_{l=1}^{L}\int_{\Omega_l} T_{il}^* T_l^f \,\mathrm{d}\Omega_l$$

$$+\frac{1}{c}\sum_{l=1}^{L}\int_{\Omega_l} q_{Vl}^f\left(\int_{t^f}^{t^{f+1}} T_{il}^* \,\mathrm{d}t\right)\mathrm{d}\Omega_l\,, \quad i = 1,2,\ldots,N, \tag{65}$$

where $T_{ij}^* = T^*(\xi^i, X^j, t^{f+1}, t)$, $q_{ij}^* = q^*(\xi^i, X^j, t^{f+1}, t)$, $T_j = T(X^j, t)$, $q_j = q(X^j, t)$, $T_l^f = T(X^l, t^f)$, $q_{Vl}^f = q_V(X^l, t^f)$.

If we assume the constant boundary elements and internal cells, then equation (65) can be written in the form

$$\sum_{j=1}^{N} G_{ij} q_j^{f+1} = \sum_{j=1}^{N} H_{ij} T_j^{f+1} + \sum_{l=1}^{L} P_{il} T_l^f + \sum_{l=1}^{L} Z_{il} q_{Vl}^f\,, \quad i = 1,2,\ldots,N\,, \tag{66}$$

where

$$G_{ij} = \frac{1}{c}\int_{\Gamma_j}\left(\int_{t^f}^{t^{f+1}} T_{ij}^* \,\mathrm{d}t\right)\mathrm{d}\Gamma_j\,, \tag{67}$$

$$H_{ij} = \begin{cases} \dfrac{1}{c}\displaystyle\int_{\Gamma_j}\left(\int_{t^f}^{t^{f+1}} q_{ij}^* \,\mathrm{d}t\right)\mathrm{d}\Gamma_j\,, & i \neq j \\ \dfrac{1}{c}\displaystyle\int_{\Gamma_j}\left(\int_{t^f}^{t^{f+1}} q_{ij}^* \,\mathrm{d}t\right)\mathrm{d}\Gamma_j - C_i\,, & i = j \end{cases}, \tag{68}$$

$$P_{il} = \int_{\Omega_l} T_{il}^* \,\mathrm{d}\Omega_l\,, \tag{69}$$

$$Z_{il} = \frac{1}{c}\int_{\Omega_l}\left(\int_{t^f}^{t^{f+1}} T_{il}^* \,\mathrm{d}t\right)\mathrm{d}\Omega_l\,. \tag{70}$$

It should be pointed out that the integration with respect to time can be done analytically [9], while the integration over the boundary and internal elements must be performed numerically (e.g. by the Gauss quadratures).

The resolving system (66) corresponding to transition from t^f to t^{f+1} can be written in the matrix form

$$\mathbf{G}\cdot\mathbf{q}^{f+1} = \mathbf{H}\cdot\mathbf{T}^{f+1} + \mathbf{P}\cdot\mathbf{T}^f + \mathbf{Z}\cdot\mathbf{q}_V^f\,. \tag{71}$$

After determination of the unknown boundary temperatures and heat fluxes, the equation (65) can be applied in order to find the temperatures at an optional set of points from the interior of Ω ($i = N+1$, $i = N+2$, ...):

$$T_i^{f+1} = \sum_{j=1}^{N} H_{ij} T_j^{f+1} - \sum_{j=1}^{N} G_{ij} q_j^{f+1} + \sum_{l=1}^{L} P_{il} T_l^f + \sum_{l=1}^{L} Z_{il} q_{Vl}^f\,. \tag{72}$$

To sum up, if we solve the nonlinear problem using the temperature field correction method or the alternating phase truncation method, then we consider the linear parabolic equation for which $q_V = 0$, and in this case the resolving system (71) contains only the matrices $\mathbf{G}$, $\mathbf{H}$ and $\mathbf{P}$. Application of the artificial heat source method leads to the non-zero component $\mathbf{q}_V^f$ and the final form of the resolving system is more complex.

7. THE EXAMPLES OF NUMERICAL COMPUTATION

The examples presented below have been chosen so as to assure the possibility of comparison of the results. As a basis, the FDM solution was taken into account, because the simple shape of the object, regular square grid, high order of approximation of the boundary conditions and application of the algorithm (verified by the authors) for nonlinear heat conduction problems [18], allows us to treat this solution as a sufficiently exact one.

In particular, the cooling processes in the domain of steel ingot during its heat treatment were analyzed. The 2D problem has been considered. Boundary conditions of the 3rd type have been assumed:

$$X \in \Gamma: \quad -\lambda(T) n \cdot \operatorname{grad} T = \alpha(T - T^{\infty}) . \tag{73}$$

The heat transfer coefficient: $\alpha = 250\ \mathrm{W/m^2\,K}$, while the cooling water temperature was equal to $T^{\infty} = 20\,^{\circ}\mathrm{C}$. The initial temperature of the domain Ω: $T(X,0) = 800\,^{\circ}\mathrm{C}$.

The physical conditions were the following:

$$C(T) = \begin{cases} 4.680 \cdot 10^6\ \mathrm{J/m^3K}, & T > 750\ [^{\circ}\mathrm{C}], \\ 9.550 \cdot 10^6, & 700 \leq T \leq 750, \\ 4.125 \cdot 10^6, & T < 700. \end{cases}$$

It should be pointed out that the problem discussed is strongly nonlinear and it constitutes a "drastic" test of correctness and effectiveness of the algorithms presented in this paper. The thermal conductivity of the ingot domain was assumed to be constant, $\lambda_1 = \lambda_2 = \lambda_3 = 35\ \mathrm{W/mK}$. On the basis of the above data functions $H = H(T)$, $H = H(U)$ and the other parameters appearing in Secs. 4 and 5 have been determined.

Consider a quarter of the lateral section of a steel ingot 0.2×0.6 m — cf. Fig. 10.

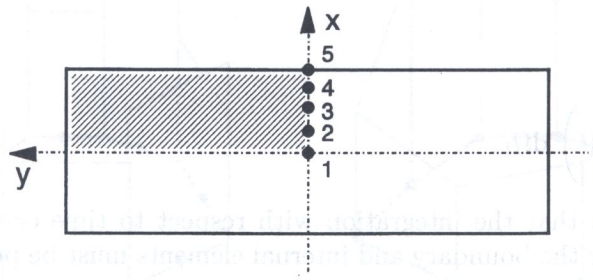

Fig. 10. Lateral cross-section

The temperature fields corresponding to times 2, 5, 10 and 15 mins. are shown in Fig. 11.

The curves of cooling shown in Figures 12 (TFCM), 13 (APTM) and 14 (AHSM) were found for points located along the axis of geometrical symmetry (as in Fig. 10). Solid lines correspond to "exact" solution, while the small squares and triangles denote the solutions obtained by means of the methods presented in the paper.

One can see that the obtained results are practically the same and they do not differ from the "exact" solution. The very good agreement of all numerical solutions was also surprising for the authors, because the philosophy of each algorithm was quite different. So, we should discuss the question which of the methods is recommendable.

From the numerical point of view, the first method (TFCM) is the simplest. The procedure correcting the values of temperature acts very quickly and leads to an additional loop placed directly after the main loop realizing the transition $t \to t + \Delta t$ for a linear task. On the other hand,

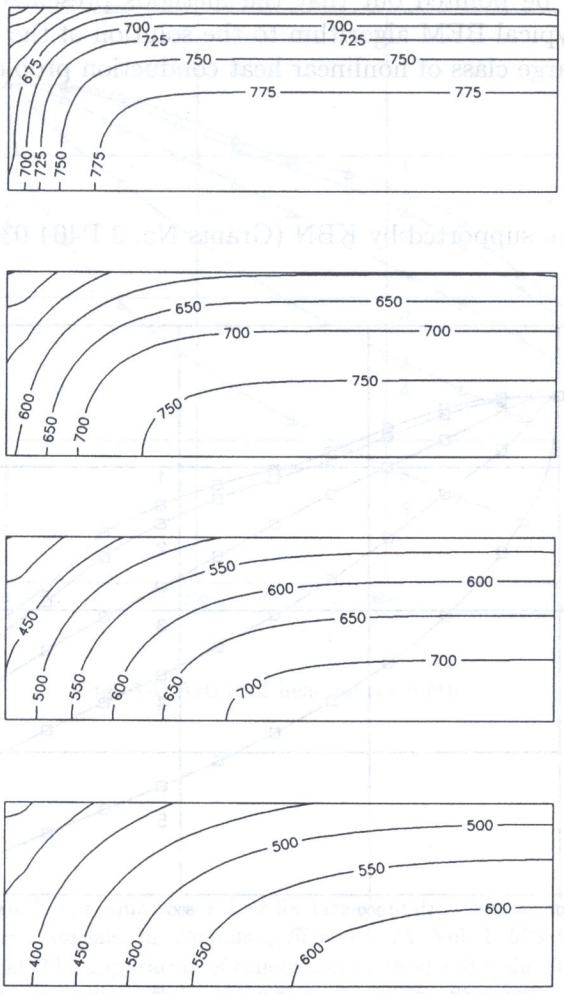

Fig. 11. Temperature fields for times 2, 5, 10 and 15 mins.

however, the method is entirely correct only in the case of constant value of thermal conductivity, and it can be used unconditionally only under this assumption.

The APTM requires an initial approximation of the real course of thermal diffussivity by a certain step function, because for successive "phases" the necessary energy equations must be linear. It seems that such approximation does not cause any essential troubles. The main loop of the computations connected with transition $t \to t + \Delta t$ is used repeatedly (for successive "phases"), and at the same time it must be supplemented by the procedure "rebuilding" the pseudo-initial conditions (formulae (44), (46) and (48)), the procedure "controlling" the addition of boundary conditions on the outer surface of the system (adiabatic or real ones), and the procedure realizing the correction of the obtained enthalpy fields (formulae (45), (47) and (49)). So, the computer program is rather complicated and the run time is considerably longer than in the case of TFCM. The last method (AHSM) does not require any initial preparations of the input data, because the derivative $\psi(U)$ can be an arbitrary function. It is the essential advantage of the method. Unfortunately, in the case of large values of $\Delta\psi(U)$, the iterative process is slowly convergent — it was shown during the computations concerning the discussed example (Fig. 14). On the other hand, the problem considered was extremely inconvenient from the point of view of the method discussed.

Summing up, it should be pointed out that the methods presented in this paper enable the effective application of a typical BEM algorithm to the solution of the linear Fourier equation for numerical modelling of a large class of nonlinear heat conduction problems.

ACKNOWLEDGEMENT

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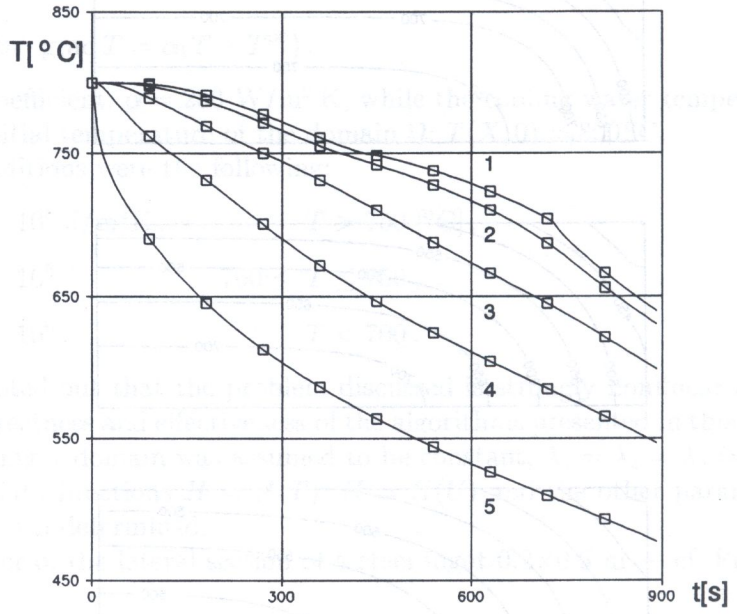

Fig. 12. Temperature field correction method

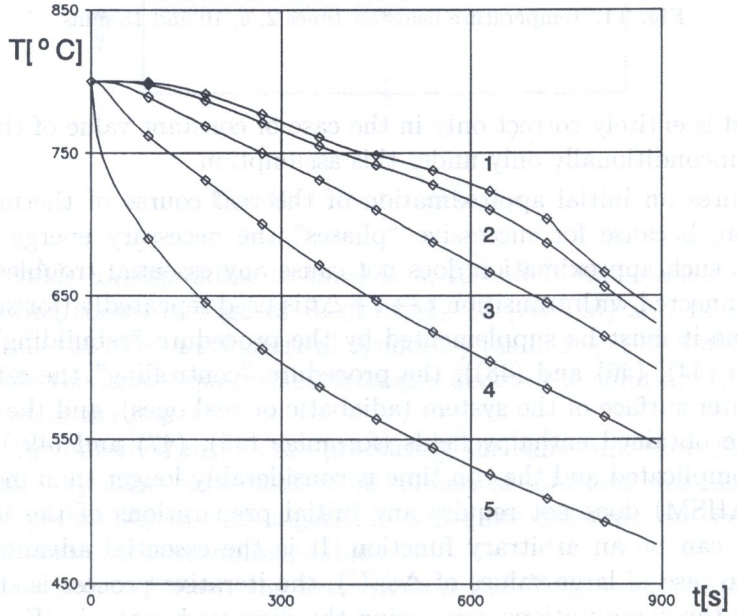

Fig. 13. Alternating phase truncation method

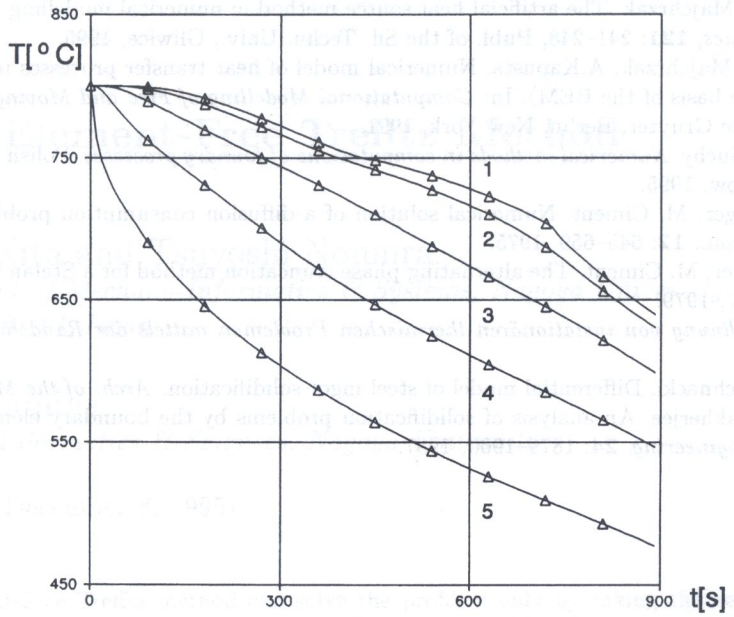

Fig. 14. Artificial heat source method

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