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APPLICATION OF THE BOUNDARY ELEMENT METHOD TO NUMERICAL MODELLING OF SOLIDIFICATION. PART I – THE ONE DOMAIN APPROACH

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In the paper the numerical model of thermal processes proceeding in the system casting-mold is discussed – in particular, the solidification of alloys is analyzed. The model is constructed using the composition of the 1st and 2nd schemes of the BEM. The problem considered is treated as a boundary-initial one and it is formulated on the basis of the one domain method (fixed domain method) (cf Mochnacki and Suchy, 1995; Voller, 1991).

Key words: boundary element method, solidification of metals and alloys

1. Governing equations

The energy equation describing the thermal processes in the domain of solidifying alloy is the following

$$x \in D \; : \quad c(T)\frac{\partial T(x,t)}{\partial t} = \mathrm{div}[\lambda(T)\mathrm{grad}T(x,t)] + q_V(x,t) \tag{1.1}$$

where

D	–	casting domain
$c(T)$	–	specific heat per unit of volume
$\lambda(T)$	–	thermal conductivity
$q_V(x,t)$	–	so-called source function.

Additionally, it is assumed that the convective heat transfer in the domain of molten metal can be neglected.

The source function $q_V(x,t)$ determines the evolution of latent heat L_V [J/m^3] and

$$q_V(x,t) = -L_V \frac{\partial f_L(x,t)}{\partial t} = L_V \frac{\partial f_S(x,t)}{\partial t} \tag{1.2}$$

where $f_L(x,t)$ is a volumetric fraction of molten metal at the neighbourhood of the considered point x, at the same time $f_S(x,t) = 1 - f_L(x,t)$. In the case of solidification in an interval of temperature (e.g. solidification of typical alloys) the values of $f_S(x,t)$ from the range $(0,1)$ correspond to a mushy zone sub-domain.

The one domain model consists in the assumption that the volumetric fraction of solid state $f_S(x,t)$ in the mushy zone sub-domain is a certain function of temperature $f_S = f_S(T)$. Since

$$\frac{\partial f_S(x,t)}{\partial t} = \frac{df_S(T)}{dT}\frac{\partial T(x,t)}{\partial t} = F(T)\frac{\partial T(x,t)}{\partial t} \tag{1.3}$$

therefore Eq (1.1) can be written in the form (cf Mochnacki and Suchy, 1995; Voller 1991)

$$x \in D \; : \quad [c(T) - L_V F(T)]\frac{\partial T(x,t)}{\partial t} = \mathrm{div}[\lambda(T)\mathrm{grad}T(x,t)] \tag{1.4}$$

or

$$x \in D \; : \quad C(T)\frac{\partial T(x,t)}{\partial t} = \mathrm{div}[\lambda(T)\mathrm{grad}T(x,t)] \tag{1.5}$$

where

$$C(T) = c(T) - L_V F(T) \tag{1.6}$$

is the substitute thermal capacity of alloy considered.

One can notice that for liquid and solid state sub-domains the function $f_S(x,t)$ is equal to 0 or 1, respectively, and $F(T) = 0$. So, the thermal processes in a whole casting domain are described by Eq (1.5).

The function determining the substitute thermal capacity results from the assumptions about the course of function $f_S(T)$. In the literature (e.g. Mochnacki and Suchy, 1995; Borisov, 1961; Samoïlovitch, 1977; Mochnacki, 1984) one can find a lot of different hypotheses associated with the form of $f_S(T)$ (or directly $C(T)$).

It should be pointed out that the energy equation (1.5) is strongly nonlinear, in particular, the parameter $C(T)$ varies strongly with temperature.

So, the basic BEM algorithm must be supplemented by the additional procedure linearizing (at the stage of numerical computations) the problem discussed and in this paper the Temperature Field Correction Method (TFCM) (cf Mochnacki, 1996; Majchrzak and Mochnacki, 1996) is applied.

The non-steady temperature field in the mold sub-domain is represented by the following equation

$$x \in D_m \; : \quad c_m(T)\frac{\partial T_m(x,t)}{\partial t} = \lambda_m \mathrm{div}[\mathrm{grad}T_m(x,t)] \tag{1.7}$$

where c_m, λ_m are the specific heat and thermal conductivity of the mold material, respectively. On the contact surface between casting and mold the continuity condition in the form

$$x \in \Gamma_{cm} \; : \quad \begin{cases} -\lambda \boldsymbol{n} \cdot \mathrm{grad}T(x,t) = -\lambda_m \boldsymbol{n} \cdot \mathrm{grad}T_m(x,t) \\ T(x,t) = T_m(x,t) \end{cases} \tag{1.8}$$

is assumed, while on the outer surface of the system

$$x \in \Gamma_0 \; : \quad \Phi[T_m(x,t), \boldsymbol{n} \cdot \mathrm{grad}T_m(x,t)] = 0 \tag{1.9}$$

where $\boldsymbol{n} \cdot \mathrm{grad}T$ is the normal derivative at the point $x \in \Gamma_0$.

For $t = 0$: $T(x,0) = T_0$, $T_m(x,0) = T_{m0}$.

2. Temperature field correction method

The theoretical basis concerning the method discussed is presented in detail in Majchrzak and Mochnacki (1996). Let us introduce the time grid defined as follows

$$0 = t^0 < t^1 < \ldots < t^{f-1} < t^f < \ldots < t^F < \infty \tag{2.1}$$

The idea of TFCM consists in correction of the local temperature values for successive transitions $t^{f-1} - t^f$. The parameter $C(T)$ is approximated by a step function, i.e. for $U_e < T < U_{e+1}$: $C(T) = c_e = \mathrm{const}$. The computations are made for a homogeneous domain with the parameter c_0 (e.g. the molten metal). The internal point x_i is considered and the following denotations are introduced (cf Fig.1)

$$\begin{aligned} \Delta_e &= c_e[T(x_i, t^{f-1}) - U_{e+1}] \\ \Delta_{e+1} &= \Delta_e + c_{e+1}[U_{e+1} - U_{e+2}] \\ \Delta_{e+2} &= \Delta_{e+1} + c_{e+2}[U_{e+2} - U_{e+3}] \\ &\ldots \end{aligned} \tag{2.2}$$

From the physical point of view Δ_e, Δ_{e+1} etc. are the changes of unit enthalpy [J/m^3] corresponding to the changes of temperature ΔT_e, ΔT_{e+1} etc. shown in Fig.1.

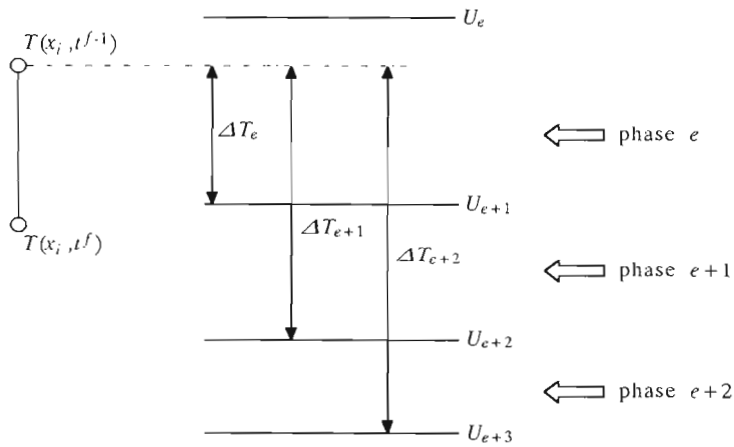

Fig. 1. Temperature field correction method

The procedure of temperature field correction method at the point x_i is the following (cf Majchrzak and Mochnacki, 1996).

If

$$c_0[T(x_i, t^{f-1}) - T(x_i, t^f)] < \Delta_e \tag{2.3}$$

then

$$\widehat{T}(x_i, t^f) = T(x_i, t^{f-1}) - \frac{c_0}{c_e}[T(x_i, t^{f-1}) - T(x_i, t^f)] \tag{2.4}$$

If

$$\Delta_e < c_0[T(x_i, t^{f-1}) - T(x_i, t^f)] < \Delta_{e+1} \tag{2.5}$$

then

$$\widehat{T}(x_i, t^{f+1}) = U_{e+1} + \frac{\Delta_e}{c_{e+1}} - \frac{c_0}{c_{e+1}}[T(x_i, t^{f-1}) - T(x_i, t^f)] \tag{2.6}$$

If

$$\Delta_{e+1} < c_0[T(x_i, t^{f-1}) - T(x_i, t^f)] < \Delta_{e+2} \tag{2.7}$$

then

$$\widehat{T}(x_i, t^{f+1}) = U_{e+2} + \frac{\Delta_{e+1}}{c_{e+2}} - \frac{c_0}{c_{e+2}}[T(x_i, t^{f-1}) - T(x_i, t^f)] \tag{2.8}$$

Similar formulas can be derived for further transitions, but in numerical realization such situations do not appear.

3. Boundary element method for parabolic equations

In this paper we confine ourselves to the presentation of numerical algorithms being a certain combination of the boundary element method for the system of linear parabolic equations (non-homogeneous domain) with additional procedures which allows one to take into account the solidification and cooling processes proceeding in casting volume.

The integral equation corresponding to the homogeneous domain D (or D_m) limited by the boundary Γ for which the normal heat flux $q(x,t)$ or temperature $T(x,t)$ is given, can be written in the form (cf Majchrzak, 1991; Brebbia et al., 1984)

$$B(\xi)T(\xi,t^F) + \frac{1}{c}\int_0^{t^F}\int_\Gamma T^*(\xi,x,t^F,t)q(x,t)\,d\Gamma dt = \tag{3.1}$$

$$= \frac{1}{c}\int_0^{t^F}\int_\Gamma q^*(\xi,x,t^F,t)T(x,t)\,d\Gamma dt + \int_D T^*(\xi,x,t^F,0)T(x,0)\,dD$$

where $T^*(\xi,x,t^F,t)$ *is the fundamental solution*

$$T^*(\xi,x,t^F,t) = \frac{1}{\sqrt{[4\pi a(t^F-t)]^d}}\exp\Big[-\frac{r^2}{4a(t^F-t)}\Big] \tag{3.2}$$

$q^*(\xi,x,t^F,t)$ is the heat flux resulting from the fundamental solution

$$q^*(\xi,x,t^F,t) = -\lambda\frac{\partial T^*(\xi,x,t^F,t)}{\partial n} \tag{3.3}$$

$B(\xi) = 1$ for an internal point $\xi \in D$, $B(\xi) \in (0,1)$ for a boundary point $\xi \in \Gamma$ and

$[0,t^F]$ – considered interval of time

d – problem dimension

r – distance from the considered point x to the point ξ where a concentrated heat source is applied.

The numerical approximation of Eq (3.1) consists in discretization of the considered interval of time $[0,t^F]$, and the boundary limiting the area D. If a non-zero initial condition is considered then the interior D must be discretized, too.

So, the boundary Γ is divided into N boundary elements Γ_j, $j = 1, 2, ..., N$ and the interior D into L internal cells D_l, $l = 1, 2, ..., L$.

Here two approaches can be taken into account. The first of them is called the 1st scheme of the BEM and its idea consists in the treatment of the transition from t^{f-1} to t^f as a certain separate problem with an adequate pseudo-initial condition; i.e. numerical approximation of Eq (3.1) has of the form

$$B(\xi^i)T(\xi^i,t^f) + \frac{1}{c}\sum_{j=1}^{N}\int_{\Gamma_j}\int_{t^{f-1}}^{t^f} T^*(\xi^i,x,t^f,t)q(x,t)\,d\Gamma_j dt =$$

$$= \frac{1}{c}\sum_{j=1}^{N}\int_{\Gamma_j}\int_{t^{f-1}}^{t^f} q^*(\xi^i,x,t^f,t)T(x,t)\,d\Gamma_j dt + \tag{3.4}$$

$$+ \sum_{l=1}^{L}\int_{D_l} T^*(\xi^i,x,t^f,t)T(x,t^{f-1})\,dD_l$$

In case of the 2nd scheme of the BEM the integration process starts from $t^0 = 0$ and then the knowledge of successive pseudo-initial conditions is not required but temporary values of the boundary temperatures and heat fluxes for $t = t^0$, $t = t^1$, ..., $t = t^{f-1}$ must be *registered*. The numerical approximation of Eq (3.1) for this scheme is as follows

$$B(\xi^i)T(\xi^i,t^f) + \frac{1}{c}\sum_{j=1}^{N}\sum_{s=1}^{f}\int_{\Gamma_j}\int_{t^{s-1}}^{t^s} T^*(\xi^i,x,t^f,t)q(x,t)\,d\Gamma_j dt =$$

$$= \frac{1}{c}\sum_{j=1}^{N}\sum_{s=1}^{f}\int_{\Gamma_j}\int_{t^{s-1}}^{t^s} q^*(\xi^i,x,t^f,t)T(x,t)\,d\Gamma_j dt + \tag{3.5}$$

$$+ \sum_{l=1}^{L}\int_{D_l} T^*(\xi_i,x,t^f,0)T(x,0)\,dD_l$$

It should be pointed out that for the initial condition $T(x,0) = 0$ the last component of Eq (3.5) is equal to zero, and the integration over D can be omitted. The same effect can be obtained in the case of initial condition of the form $T(x,0) = T_0 = \text{const}$ (cf Majchrzak, 1991).

As an example of the discussed schemes the numerical algorithm for 2D problem $x = \{x_1, x_2\}$ is presented (the constant elements are assumed). The

final form of resolving system in the case of the 1st scheme of the BEM is the following $(i = 1, 2, ..., N)$

$$\sum_{j=1}^{N} g_{ij} q(x^j, t^f) = \sum_{j=1}^{N} z_{ij} T(x^j, t^f) + \sum_{l=1}^{L} p_{il} T(x^l, t^{f-1}) \tag{3.6}$$

or

$$\mathbf{G}\mathbf{q}^f = \mathbf{Z}\mathbf{T}^f + \mathbf{P}\mathbf{T}^{f-1} \tag{3.7}$$

where $(i, j = 1, 2, ..., N)$

$$g_{ij} = \frac{1}{4\pi\lambda} \int_{\Gamma_j} \mathrm{Ei}\Big(\frac{r_{ij}^2}{4a\Delta t}\Big)\, d\Gamma_j \qquad \widehat{z}_{ij} = \frac{1}{2\pi} \int_{\Gamma_j} \frac{d_{ij}}{r_{ij}^2} \exp\Big(-\frac{r_{ij}^2}{4a\Delta t}\Big)\, d\Gamma_j$$

$$p_{il} = \frac{1}{4\pi a \Delta t} \int_{D_l} \exp\Big(-\frac{r_{il}^2}{4a\Delta t}\Big)\, dD_l \qquad z_{ij} = \begin{cases} \widehat{z}_{ij} & i \neq j \\ \widehat{z}_{ij} - B_i & i = j \end{cases}$$

and $\mathrm{Ei}(\zeta)$ is the expotential integral function, $\mathrm{Ei}(\zeta) = \int_{\zeta}^{\infty} \frac{1}{\zeta} \exp(-\zeta)\, d\zeta$. After computations of unknown boundary temperatures and heat fluxes Eq (3.4) can be applied (for $B(\xi^i) = 1$) in order to determine the temporary temperatures at an optional set of points from the interior D $(i = N+1, N+2, ..., N+L)$

$$T(\xi^i, t^f) = \sum_{j=1}^{N} z_{ij} T(x^j, t^f) - \sum_{j=1}^{N} g_{ij} q(x^j, t^f) + \sum_{l=1}^{L} p_{il} T(x^l, t^{f-1}) \tag{3.8}$$

The final form of resolving system in the case of the 2nd scheme of the BEM is the following $(i = 1, 2, ..., N)$

$$\begin{aligned} \sum_{j=1}^{N} g_{ij} q(x^j, t^f) &= \sum_{j=1}^{N} z_{ij} T(x^j, t^f) + \\ &+ \sum_{s=1}^{f-1} [z_{ij}^s T(x^j, t^{f-s}) - g_{ij}^s q(x^j, t^{f-s})] + \sum_{l=1}^{L} p_{il} T(x^l, t^0) \end{aligned} \tag{3.9}$$

or

$$\mathbf{G}\mathbf{Q}^f = \mathbf{Z}\mathbf{T}^f + \sum_{s=1}^{f-1} (\mathbf{Z}^s \mathbf{T}^{f-s} - \mathbf{G}^s \mathbf{Q}^{f-s}) + \mathbf{P}\mathbf{T}^0 \tag{3.10}$$

where

$$g_{ij}^{s} = \frac{1}{4\pi\lambda}\int_{\Gamma_j}\left[\mathrm{Ei}\left(\frac{r_{ij}^2}{4a(s+1)\Delta t}\right) - \mathrm{Ei}\left(\frac{r_{ij}^2}{4as\Delta t}\right)\right] d\Gamma_j$$

$$z_{ij}^{s} = \frac{1}{2\pi}\int_{\Gamma_j}\frac{d_{ij}}{r_{ij}^2}\left[\exp\left(-\frac{r_{ij}^2}{4a(s+1)\Delta t}\right) - \exp\left(-\frac{r_{ij}^2}{4as\Delta t}\right)\right] d\Gamma_j$$

The philosophy of solidification process modelling (presented in this paper) causes that for the casting domain only the 1st scheme of the BEM can be used. It results from the need for the temperature field correction at each step of time. The computations concerning the mold domain can be realized by means of both schemes. It turned out, that the best results from the point of view of solution accuracy one obtains by the combining of the 1st scheme for the casting domain with the 2nd scheme for the mold domain. The composition of two variants of BEM allow one to eliminate serious difficulties posed by the necessity for a proper choice of the time step Δt allowing good accuracy to be maintained of the numerical solution for two domains, thermophysical parameters of which differ essentially.

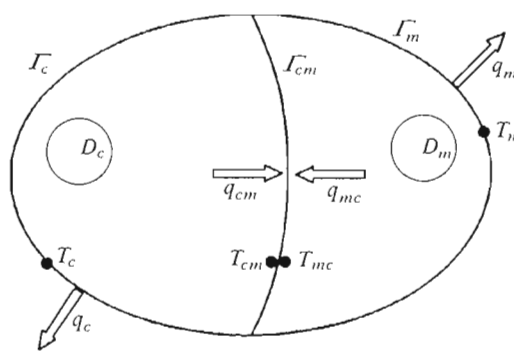

Fig. 2. Casting and mold sub-domains

For further considerations the following quantities are distinguished (Fig.2):

- $\mathbf{T}_c^f$, $\mathbf{q}_c^f$ denote the boundary temperatures and heat fluxes on the outer surface of the casting for $t = t^f$ and $\mathbf{T}_c^{f-1}$ internal temperatures for $t = t^{f-1}$
- $\mathbf{T}_m^f$, $\mathbf{q}_m^f$, $\mathbf{T}_m^{f-1}$ denote the same functions for the outer surface and interior of the mold

- $\mathbf{T}^f_{cm}$, $\mathbf{q}^f_{cm}$, $\mathbf{T}^f_{mc}\mathbf{q}^f_{mc}$ are the temperatures and heat fluxes on the contact surface (as it was mentioned $\mathbf{q}^f_{cm} = -\mathbf{q}^f_{mc}$, in the case of ideal contact $\mathbf{T}^f_{mc} = \mathbf{T}^f_{cm}$).

As results from the considerations presented in Section 3 the resolving system for casting is of the form $\mathbf{G}\mathbf{q}^f = \mathbf{Z}\mathbf{T}^f + \mathbf{P}\mathbf{T}^{f-1}$. In order to distinguish the part of the boundary for which the continuity condition is assumed, the system of equations determining the boundary values for $t \in [t^{f-1}, t^f]$ is written in the form

$$\begin{bmatrix} \mathbf{G}_c & \mathbf{G}_{cm} \end{bmatrix} \begin{bmatrix} \mathbf{q}^f_c \\ \mathbf{q}^f_{cm} \end{bmatrix} = \begin{bmatrix} \mathbf{Z}_c & \mathbf{Z}_{cm} \end{bmatrix} \begin{bmatrix} \mathbf{T}^f_c \\ \mathbf{T}^f_{cm} \end{bmatrix} + \mathbf{P}_c \mathbf{T}^{f-1}_c \tag{3.11}$$

while for the mold sub-domain

$$\begin{bmatrix} \mathbf{G}_m & \mathbf{G}_{mc} \end{bmatrix} \begin{bmatrix} \mathbf{q}^f_m \\ \mathbf{q}^f_{mc} \end{bmatrix} = \begin{bmatrix} \mathbf{Z}_m & \mathbf{Z}_{mc} \end{bmatrix} \begin{bmatrix} \mathbf{T}^f_m \\ \mathbf{T}^f_{mc} \end{bmatrix} + \tag{3.12}$$

$$+ \sum_{s=1}^{f-1} \left(\begin{bmatrix} \mathbf{Z}^s_m & \mathbf{Z}^s_{mc} \end{bmatrix} \begin{bmatrix} \mathbf{T}^{f-s}_m \\ \mathbf{T}^{f-s}_{mc} \end{bmatrix} - \begin{bmatrix} \mathbf{G}^s_m & \mathbf{G}^s_{mc} \end{bmatrix} \begin{bmatrix} \mathbf{q}^{f-s}_m \\ \mathbf{q}^{f-s}_{mc} \end{bmatrix} \right)$$

at the same time the initial condition for D_c should be in an adequate way rebuilt (a new reference level). Finally, one obtains the following resolving system for $D_c \cup D_m$

$$\begin{bmatrix} \mathbf{Z}_c & -\mathbf{Z}_{cm} & \mathbf{G}_{cm} & \mathbf{0} \\ \mathbf{0} & -\mathbf{Z}_{mc} & -\mathbf{G}_{mc} + \mathbf{Z}_{mc}\mathbf{R} & -\mathbf{Z}_m \end{bmatrix} \begin{bmatrix} \mathbf{T}^f_c \\ \mathbf{T}^f_{cm} \\ \mathbf{q}^f \\ \mathbf{T}^f_m \end{bmatrix} = \tag{3.13}$$

$$= \begin{bmatrix} -\mathbf{G}_c \mathbf{q}^f_c + \mathbf{P}_c \mathbf{T}^{f-1}_c \\ -\mathbf{G}_m \mathbf{q}^f_m + \sum_{s=1}^{f-1} \left(\begin{bmatrix} \mathbf{Z}^s_m & \mathbf{Z}^s_{mc} \end{bmatrix} \begin{bmatrix} \mathbf{T}^{f-s}_m \\ \mathbf{T}^{f-s}_{mc} \end{bmatrix} - \begin{bmatrix} \mathbf{G}^s_m & \mathbf{G}^s_{mc} \end{bmatrix} \begin{bmatrix} \mathbf{q}^{f-s}_m \\ \mathbf{q}^{f-s}_{mc} \end{bmatrix} \right) \end{bmatrix}$$

At the last stage of algorithm the internal temperatures are calculated for both sub-domains separately.

4. Example of numerical simulation

The hot spot shown in Fig.3 is considered. The casting is made of carbon steel. The thermophysical parameters of sub-domains are assumed according

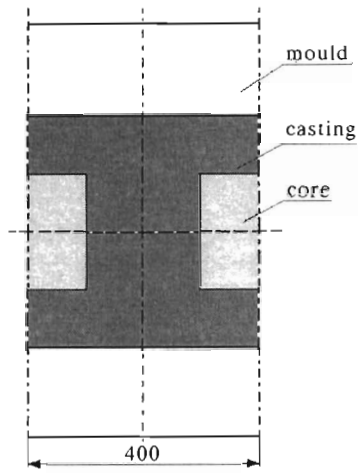

Fig. 3. Heterogeneous domain casting-mold-core

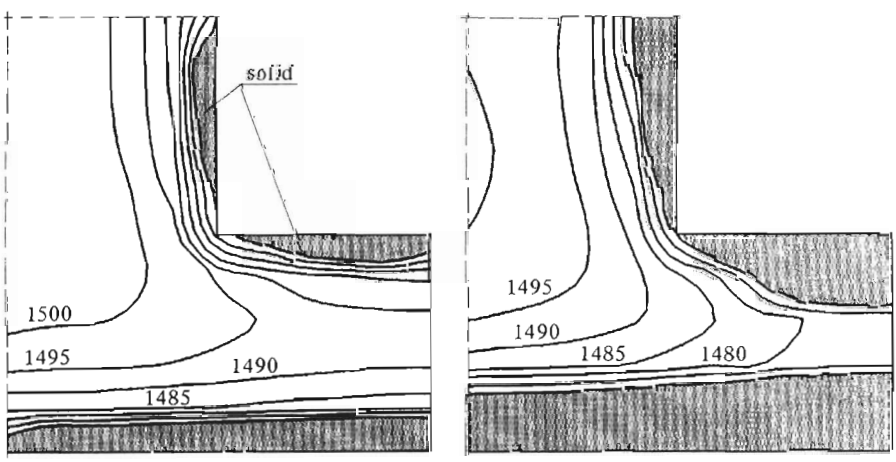

Fig. 4. Temperature field for times 10 and 20 minutes

to [10]. The symmetrical fragment of casting domain is divided into 75 square internal cells, the boundary is divided into 96 boundary elements.

In Fig.4 the temperature field and solid state sub-domain for times 10 and 20 minutes are shown.

Summing up, it should be pointed out that the method presented in this paper allows for effective application of typical BEM algorithms to solving the linear Fourier equation for numerical modelling of a large class of solidification problems.

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Zastosowanie metody elementów brzegowych do numerycznego modelowania procesu krzepnięcia. Część I – Metoda jednego obszaru

Streszczenie

W pracy przedstawiono opis procesów cieplnych zachodzących w układzie odlew-forma, w szczególności rozważono krzepnięcie stopów. Model numeryczny zbudowano wykorzystując tzw. I i II schemat metody elementów brzegowych Rozważany problem potraktowano jako zadanie brzegowo-początkowe opisane równaniami odpowiadającymi metodzie jednego obszaru (por. Mochnacki i Suchy, 1995; Voller, 1991).

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