APPLICATION OF THE BOUNDARY ELEMENT METHOD TO NUMERICAL MODELLING OF SOLIDIFICATION. PART II – THE MICRO-MACRO APPROACH

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In the paper a numerical model of solidification and cooling processes proceeding in the casting domain is discussed. The model is constructed on the basis of the boundary element method. The problem considered is treated as a boundary-initial one and it is formulated in a micro/macro convention; i.e. the component describing a capacity of internal heat sources in an adequate differential equation (the so-called source function) results from the analysis of crystallization process on a microscopic level.

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

1. Governing equations

The solidification process proceeding in the volume of pure metal or eutectic alloy can be treated as a boundary initial problem described by the partial differential equation (the Fourier equation) and adequate geometrical, physical, boundary and initial conditions. The non-steady temperature field in the considered domain D is represented by the following equation

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

where
c	–	specific heat
ρ	–	mass density
λ	–	thermal conductivity
q_V	–	source function (capacity of internal heat sources)
T, x, t	–	denote the temperature, spatial co-ordinates and time, respectively.

Because the solidification process proceeds in a comparatively short temperature interval constant mean values of the thermophysical parameters can be accepted and then the Eq (1.1) takes the form

$$x \in D \; : \quad \frac{\partial T(x,t)}{\partial t} = a\operatorname{div}[\operatorname{grad}T(x,t)] + \frac{q_V(x,t)}{c\rho} \tag{1.2}$$

where a is the diffusion coefficient.

The source function in Eqs (1.1) and (1.2) (cf Mochnacki and Suchy, 1995; Voller, 1991) can be written as follows

$$q_V(x,t) = L_V \frac{\partial f_S(x,t)}{\partial t} = -L_V \frac{\partial f_L(x,t)}{\partial t} \tag{1.3}$$

where

L_V — latent heat per unit of volume

f_L, f_S — liquid and solid state fractions in a neighbourhood of the point considered $x \in D$.

The courses of functions $f_L(x,t)$ and $f_S = 1 - f_L$ result from the assumed model of the crystallization process. In this paper the model presented, e.g., by Fraś (1992), Avdonin (1980), Majchrzak and Longa (1996) is applied. So, the number of nuclei appearing in the liquid sub-domain is proportional to the second power of undercooling below the solidification point T_c

$$N(x,t) = \Psi \Delta T^2(x,t) \tag{1.4}$$

where Ψ is the nucleation coefficient, while $\Delta T = T_c - T(x,t)$.

It should be assumed that the nucleation stops at the maximum of undercooling, i.e., if $\Delta T(x, t + \Delta t) < \Delta T(x,t)$ then $N(x, t + \Delta t) = N(x,t)$.

The theoretical considerations show, that the relation between derivative $dN/d\Delta T$ and undercooling ΔT can be described by normal distribution and the form of Eq (1.4) results from approximation of the initial fragment of Gaussian function distribution, see Fig.1.

The solid state growth (equiaxial grains) is determined by the formula

$$\frac{dR(x,t)}{dt} = \mu \Delta T^2(x,t) \tag{1.5}$$

where

R — grain radius

μ — growth coefficient.

In literature one can find the others formulas describing the growth (cf Fraś et al., 1996 – dendritic solidification).
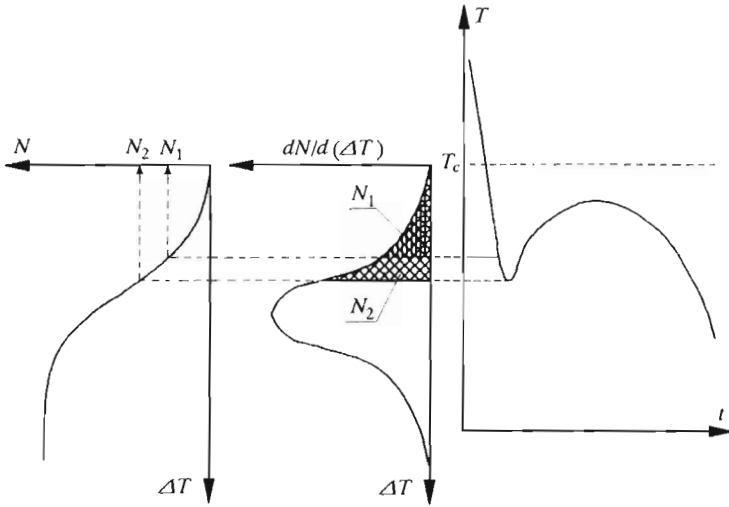
Fig. 1. Nucleation model

The relation between growth rate and solid state fraction is given by the Mehl-Johnson-Avrami-Kolmogorov equation (cf Kapturkiewicz, 1988).

$$f_S(x,t) = 1 - \exp\left\{-\frac{4}{3}\pi N(x,t)\left[\int_0^t dR(x,t)\right]^3\right\} = 1 - \exp(-\Omega) \qquad (1.6)$$

In reality the lower limit of integral (1.6) corresponds to the time t' for which the first portion of nuclei appears, because for $t < t' : dR = 0$.

So, the source function resulting from Eq $(1.3) \div (1.6)$ should be introduced into the energy equation (1.1) or (1.2).

On the outer surface of the system the boundary condition in a general form

$$x \in \Gamma : \quad \Phi[T(x,t), n \cdot \mathrm{grad}T(x,t)] = 0 \qquad (1.7)$$

is given. In this equation $n \cdot \mathrm{grad}T$ denotes the normal derivative. For $t = 0$

$$t = 0 : \quad T(x,t) = T_0(x) \qquad (1.8)$$

The presented above considerations can be extended on the case of alloys solidification. The energy equation constitutes the *natural* generalization of Eq (1.1), namely

$$x \in D : \quad c\rho\frac{\partial T(x,t)}{\partial t} = \mathrm{div}[\lambda\mathrm{grad}T(x,t)] + \sum_m q_V^{(m)}(x,t) \qquad (1.9)$$

where the index m identifies the successive phases. For example, in the case of cast iron solidification one can distinguish the austenite and eutectic phases (cf Skoczylas, 1991). Taking into account Eq (1.3) one obtains

$$x \in D : \quad c\rho \frac{\partial T(x,t)}{\partial t} = \text{div}[\lambda \text{grad} T(x,t)] + \sum_m L_V^{(m)} \frac{\partial f_S^{(m)}(x,t)}{\partial t} \quad (1.10)$$

If one assumes that the number of m phase nuclei at the point considered $x \in D$ is proportional, as previously, to the second power of undercooling then

$$N_m(x,t) = \Psi_m \Delta T_m^2(x,t) \quad (1.11)$$

where

Ψ_m –   nucleation coefficients for successive phases

ΔT_m –   undercooling of phase m, namely

$$\Delta T_m(x,t) = T_m - T(x,t) \quad (1.12)$$

It should be pointed out that the temperature T_1 is a function of local concentration of the alloy component, while the eutectic temperature T_2 is a constant value (cf Skoczylas, 1991).

The growth of each phase is determined by the formulas

$$\frac{dR_{(}x,t)}{dt} = \mu \Delta T^2(x,t) \quad (1.13)$$

The relation between growth rate and solid fraction for successive phases results from the system of Mehl-Johnson-Avrami-Kolmogorow equations (cf Kapturkiewicz, 1988; Skoczylas, 1991)

$$\frac{f_S^{(m)}(x,t)}{f_L(x,t) + f_S^{(m)}(x,t)} = 1 - \exp\left\{-\frac{4}{3}\pi N_m(x,t)\left[\int_0^t dR_m(x,t)\right]^3\right\} \quad (1.14)$$

while

$$f_L(x,t) + \sum_m f_S^{(m)}(x,t) = 1 \quad (1.15)$$

If one considers the case in which the successive phases are solidifying one after another, then

$$f_S^{(1)}(x,t) = 1 - \exp\left\{-\frac{4}{3}\pi N_1(x,t)\left[\int_0^t dR_1(x,t)\right]^3\right\} = 1 - \exp(-\Omega_1)$$

(1.16)

$$\frac{f_S^{(2)}(x,t)}{1 - f_S^{(1)}(x)} = 1 - \exp\left\{-\frac{4}{3}\pi N_2(x,t)\left[\int_0^t dR_2(x,t)\right]^3\right\} = 1 - \exp(-\Omega_2)$$

Since the solidification of the phases proceeds one after another, therefore $f_S^{(1)}$ in Eq $(1.16)_2$ is only the function of x.

In the general case, i.e. if one considers the simultaneous solidification, Eqs (1.16) should be written in the form

$$\frac{f_S^{(1)}(x,t)}{1 - f_S^{(2)}(x,t)} = 1 - \exp(-\Omega_1)$$

(1.17)

$$\frac{f_S^{(2)}(x,t)}{1 - f_S^{(1)}(x,t)} = 1 - \exp(-\Omega_2)$$

2. Numerical model of the source function evolution

In this section the model of pure metal solidification is discussed (cf Szopa, 1997).

Let us introduce the time grid defined as follows

$$0 = t^0 < t^1 < t^2 < ... < t^{f-1} < t^f < ... < t^F \qquad \Delta t = t^f - t^{f-1} \qquad (2.1)$$

while the domain of metal is divided into n parts (n control volumes V_i, $i = 1, 2, ..., n$).

The exponent Ω resulting from Eq (1.6) corresponds to the volume of solidified metal, in particular its local value associated with a control volume V_i can be expressed as a sum of successive portions of solidified material

$$\Omega_i^f = \delta V_i^1 + \delta V_i^2 + ... + \delta V_i^{f-1} + \delta V_i^f \qquad (2.2)$$

and then

$$f_L(x_i, t^f) = \exp(-\Omega_i^f) = \exp[-(\delta V_i^1 + \delta V_i^2 + ... + \delta V_i^f)] =$$

(2.3)

$$= \exp(-\delta V_i^1)\exp(-\delta V_i^2)...\exp(-\delta V_i^f) = (1 - \delta V_i^1)(1 - \delta V_i^2)...(1 - \delta V_i^f)$$

(there the approximation $\exp(-x) = 1 - x$ has been used and taking into account very small values of arguments the above simplification is fully acceptable).

The local value of the source function resulting from Eq (1.3) can be approximated as follows

$$q_V(x_i, t^f) = -L_V \frac{f_L(x_i, t^f) - f_L(x_i, t^{f-1})}{\Delta t} \tag{2.4}$$

Because

$$
\begin{aligned}
f_L(x_i, t^f) - f_L(x_i, t^{f-1}) &= \\
&= (1 - \delta V_i^1)(1 - \delta V_i^2)...(1 - \delta V_i^{f-1})\left[(1 - \delta V_i^f) - 1\right] = \\
&= -(1 - \delta V_i^1)(1 - \delta V_i^2)...(1 - \delta V_i^{f-1})\delta V_i^f = -f_L(x_i, t^{f-1})\delta V_i^f
\end{aligned}
\tag{2.5}
$$

therefore Eq (2.4) can be expressed as follows

$$q_V(x_i, t^f) = L_V f_L(x_i, t^{f-1}) \frac{\delta V_i^f}{\Delta t} \tag{2.6}$$

The most general model of the local source function evolution requires observation of the vicissitudes of successive grains generations.

Let us consider the control volume V_i for which at the interval Δt temperature decreases below the solidification point and the crystallization process starts. We find the number of the first *portion* of nuclei N_i^1 and the final radius of grains $R_i^1 = \Delta R_i^1$ (see Eq (1.5)). The first value of δV_i^1 is equal to

$$\delta V_i^1 = \frac{4}{3}\pi N_i^1 \Delta R_i^1 \tag{2.7}$$

In the second stage of crystallization process modelling we find the quantity $N_i = \Psi \Delta T_i^2$ and next we can estimate the size of the second generation, i.e. $N_i^2 = N_i - N_i^1$. We can also find a new increment of the grains radius ΔR_i^2. It should be pointed out that the current radiuses of first generation are equal to $\Delta R_i^1 + \Delta R_i^2$, while for the second generation: ΔR_i^2. The increment of solid state, i.e., δV_i^2 is determined by the formula

$$\delta V_i^2 = \frac{4}{3}\pi[N_i^1(\Delta R_i^1 + \Delta R_i^2)^3 + N_i^1(\Delta R_i^2)^3] - \delta V_i^1 \tag{2.8}$$

The next steps of crystallization process modelling result from generalization of the considerations presented above. It should be pointed out that after the passing by the maximum undercooling the number of nuclei in the control volume V_i is constant and this fact must be taken into account in an adequate numerical procedure. The model considered is shown in Fig.2.
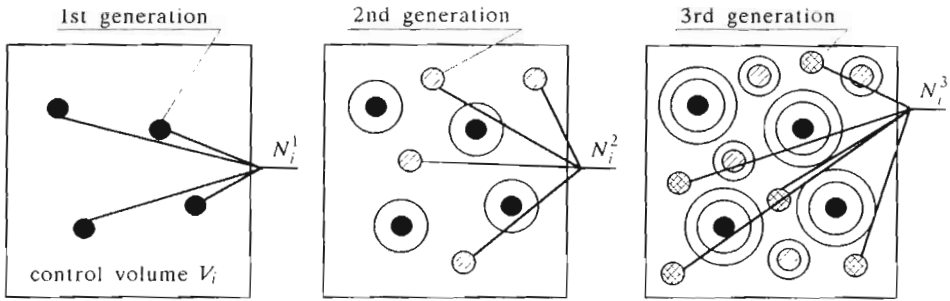
Fig. 2. Families of grains

3. BEM using discretization in time

In order to simplify the numerical model of the process discussed the 1D task is considered and the energy equation takes a form

$$x \in D : \quad \frac{\partial T(x,t)}{\partial t} = a\frac{\partial^2 T(x,t)}{\partial x^2} + \frac{q_V(x,t)}{c\rho} \qquad (3.1)$$

On the outer surface of the system the boundary condition (1.7), and for $t = 0$ the initial condition (1.8) are given.

In the simplest version of the BEM using discretization in time Eq (3.1) for the transition $t^{f-1} \to t^f$ is written in the form

$$x \in D : \quad \frac{T(x,t^f) - T(x,t^{f-1})}{\Delta t} = a\frac{\partial^2 T(x,t^f)}{\partial x^2} + \frac{q_V(x,t^f)}{c\rho} \qquad (3.2)$$

or

$$x \in D : \quad \frac{\partial^2 T(x,t^f)}{\partial x^2} - \frac{1}{a\Delta t}T(x,t^f) + \frac{1}{a\Delta t}T(x,t^{f-1}) + \frac{q_V(x,t^f)}{\lambda} \qquad (3.3)$$

The weighted residual method criterion (cf Brebbia et al., 1984) leads to the following formula

$$\int_0^L \left[\frac{\partial^2 T(x,t^f)}{\partial x^2} - \frac{1}{a\Delta t}T(x,t^f) + \frac{1}{a\Delta t}T(x,t^{f-1}) + \frac{q_V(x,t^f)}{\lambda}\right]T^*(\xi,x)\,dx = 0$$

$$(3.4)$$

where L is plate thickness, while $T^*(\xi,x)$ is a fundamental solution to the problem considered, and it is a function of the form

$$T^*(\xi,x) = \frac{\sqrt{a\Delta t}}{2}\exp\left(-\frac{|x - \xi|}{\sqrt{a\Delta t}}\right) \qquad (3.5)$$

while $\xi \in (0, L)$ is a point at which a concentrated heat source is applied.

The fundamental solution (3.5) fulfills the following equation

$$\frac{\partial^2 T^*(\xi, x)}{\partial x^2} - \frac{1}{a\Delta t}T^*(\xi, x) = -\delta(x - \xi) \tag{3.6}$$

where $\delta(x - \xi)$ is the Dirac function.

The heat flux resulting from the fundamental solution equals

$$q^*(\xi, x) = -\lambda \frac{\partial T^*(\xi, x)}{\partial x} = \frac{\lambda \operatorname{sgn}(x - \xi)}{2} \exp\left(-\frac{|x - \xi|}{\sqrt{a\Delta t}}\right) \tag{3.7}$$

Integrating twice by parts the first component of Eq (3.4) and taking into account the properties of fundamental solution (cf Brebbia et al., 1984) we have

$$T(\xi, t^f) + \left[\frac{1}{\lambda}T^*(\xi, x)q(x, t^f)\right]_0^L = \left[\frac{1}{\lambda}q^*(\xi, x)T(x, t^f)\right]_0^L + p(\xi) + z(\xi) \tag{3.8}$$

where

$$p(\xi) = \frac{1}{a\Delta t} \int_0^L T^*(\xi, x)T(x, t^{f-1}) \, dx$$

$$\tag{3.9}$$

$$z(\xi) = \frac{1}{\lambda} \int_0^L q_V(x, t^f)T^*(\xi, x) \, dx$$

For $\xi \to 0^+$ and for $\xi \to L^-$ one obtains the system of equations which can be written in the matrix form

$$\begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \begin{bmatrix} q(0, t^f) \\ q(L, t^f) \end{bmatrix} = \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} T(0, t^f) \\ T(L, t^f) \end{bmatrix} + \begin{bmatrix} p(0) \\ p(L) \end{bmatrix} + \begin{bmatrix} z(0) \\ z(L) \end{bmatrix} \tag{3.10}$$

where

$$g_{11} = -g_{22} = -\frac{\sqrt{\Delta t}}{2\sqrt{\lambda c}} \qquad\qquad g_{12} = -g_{21} = \frac{\sqrt{\Delta t}}{2\sqrt{\lambda c}} \exp\left(-\frac{L}{\sqrt{a\Delta t}}\right) \tag{3.11}$$

while

$$h_{11} = h_{22} = -\frac{1}{2} \qquad\qquad h_{12} = h_{21} = \frac{1}{2} \exp\left(-\frac{L}{\sqrt{a\Delta t}}\right) \tag{3.12}$$

Eq (3.10) allows one to determine the *missing* boundary values (temperatures and heat fluxes for $x = 0$ and $x = L$), while at the second step of computations the temporary temperatures in the set of internal points $\xi \in (0, L)$ can be found using Eq (3.8).
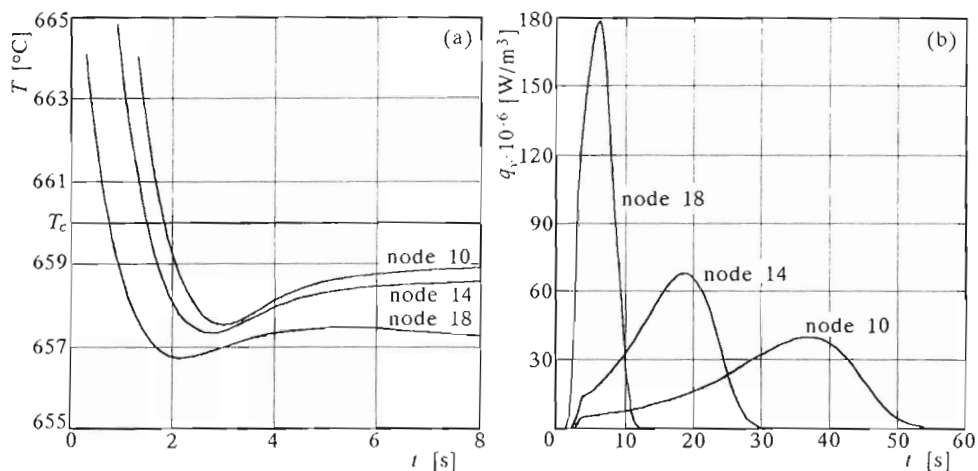
4.   Sample numerical simulation

Fig. 3. (a) – Cooling curves; (b) – Source function evolution

As the example for testing the algorithm proposed a problem of alumi-nium plate ($L = 0.02\,$m) solidification is solved. On the outer surface of the plate the boundary temperature $T_B = 655°$C, while for the axis of symmetry $q_B = 0$ are assumed. The growth coefficient is equal to $\mu = 3 \cdot 10^{-6}\,$m/(sK^2), at the same time the nucleation coefficient: $\psi = 10^{10}\,$m^{-3}K^2. Pouring tem-perature: $T_0 = 700°$C, solidification point: $T_c = 660°$C. In the domain of the plate 20 control volumes are distinguished. In Fig.3a the cooling curves at the points 10, 14 and 18 are presented, while in Fig.3b the evolutions of source function at the same points are shown.

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Zastosowanie metody elementów brzegowych do numerycznego modelowania procesu krzepnięcia. Część II – Model mikro-makro

Streszczenie

W pracy przedstawiono opis procesów cieplnych (krzepnięcie i krystalizacja) zachodzących w układzie odlew-forma. Model numeryczny zbudowano wykorzystując kombinowany wariant metody elementów brzegowych. Zadanie potraktowano jako problem brzegowo-początkowy sformułowany w konwencji mikro-makro, tzn. składnik opisujący wydajność źródeł wewnętrznych w równaniu energii wynika z analizy procesu krystalizacji na poziomie mikroskopowym.