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Numerical Modeling of Solidification Process

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1. Introduction

This chapter is devoted to the problems connected with numerical modeling of moving boundary ones. In particular the solidification and cooling processes proceeding in the system casting-mould are considered. The subject matter of solidification process modeling is very extensive and only the selected problems from this scope will be here discussed. From the mathematical point of view the thermal processes proceeding in the domain considered (both in macro and micro/macro scale) are described by a system of partial differential equations (energy equations) supplemented by the geometrical, physical, boundary and initial conditions. The typical solidification model bases on the Fourier-Kirchhoff type equations, but one can formulate the more complex (coupled with the basic model) ones concerning the heat convection in a molten metal sub-domain, the changes of local chemical constitution of solidifying alloy (segregation process) etc. Here we limit oneself only to the tasks connected with the predominant heat conduction process, and (as the examples of various problems) the macro models of alloys solidification and the micro/macro models of pure metals crystallization will be presented, at the same time the direct and inverse problems will be discussed.

In order to construct a numerical model and an adequate computer program simulating the course of problem considered, one must accept a certain mathematical description of the process (the governing equations). The next step is the transformation of this mathematical model into a form called the re-solving system constructed on the basis of a selected numerical method.

After transformation of the algorithm developed into a computer program and supplementing it with suitable pre- and post-processing procedures (input data loading, graphic presentation of results, print-outs etc.), and carrying out of computations, one obtains the results including information concerning the transient temperature field, kinetics of solidification process, the temporary shapes of sub-domains etc. They may have a form of numerical print-outs, e.g., giving the temperature field at distinguished set of points or the volumetric fraction of solid state at the neighbourhood of these points.

Numerical modeling of the heat and mass transfer in solidifying metal is a typical interdisciplinary problem and requires particular knowledge in the field of foundry practice, mathematics (a course in mathematical analysis offered in technical schools is quite sufficient here), thermodynamics (in particular heat transfer), numerical methods and, in the final stage, also programming and operation of computer equipment.

2. Heat transfer in the system casting – mould

2.1 Description of the process

At first, we will consider the heat transfer processes in a system casting-mould-environment The solidification and cooling of casting material (alloy or pure metal) can be described by the following energy equation

$$c(T)\frac{\partial T(x,t)}{\partial t} = \nabla\left[\lambda(T)\nabla T(x,t)\right] + L\frac{\partial f_S(x,t)}{\partial t} \tag{1}$$

where $c(T)$ is a volumetric specific heat of casting material, $\lambda(T)$ is a thermal conductivity, L is a volumetric latent heat, $T = T(x, t)$, $f_S = f_S(x, t)$ denote the temperature and the local volumetric fraction of solid state, x denotes the spatial co-ordinates, t is a time. One can see, that only heat conduction in a casting volume is considered. The energy equation can constitute a base both in a case of macro-scale modeling and micro/macro one (Stefanescu, 1999; Mochnacki & Majchrzak, 2007a; Mochnacki & Suchy, 1995). The differences appear on a stage of solidification rate $\partial f_S/\partial t$ computations.

The equation determining the course of thermal processes in a mould sub-domain is of the form

$$c_m(T)\frac{\partial T_m(x,t)}{\partial t} = \nabla\left[\lambda_m(T)\,\nabla T_m(x,t)\right] \tag{2}$$

where the index m identifies the mould sub-domain, the non-homogeneous mould can be also considered.

On the external surface of mould the continuity condition (3rd type of boundary condition)

$$-\lambda_m\frac{\partial T_m(x,t)}{\partial n} = \alpha\left[T_m(x,t) - T_a\right] \tag{3}$$

is, as a rule, accepted. Here α is a heat transfer coefficient, T_a is an ambient temperature, $\partial/\partial n$ denotes a normal derivative.

On the contact surface between casting and mould the continuity condition is given

$$-\lambda\frac{\partial T(x,t)}{\partial n} = \frac{T(x,t) - T_m(x,t)}{R(x,t)} = -\lambda_m\frac{\partial T_m(x,t)}{\partial n} \tag{4}$$

where R is a thermal resistance. For $R = 0$ (a such assumption can be done in the case of sand mix mould) the last equation takes a form

$$\begin{cases} -\lambda\dfrac{\partial T(x,t)}{\partial n} = -\lambda_m\dfrac{\partial T_m(x,t)}{\partial n} \\ T(x,t) = T_m(x,t) \end{cases} \tag{5}$$

The initial temperature distribution for $t = 0$ is also known

$$t = 0: \quad T(x,0) = T_0(x)\,, \quad T_m(x,0) = T_{m0}(x) \tag{6}$$

The mathematical model presented above can be more complicated. One can consider the convectional component of heat transfer which appear in the molten metal sub-

domain. In the case of alloys solidification the segregation effects can be also taken into account, etc.

2.2 Macro models of solidification

In this sub-chapter the model called the one domain approach will be discussed (Mochnacki & Suchy, 1995). Let us denote the temperatures corresponding to the beginning and the end of solidification process as T_L and T_S . If one considers the solidification of pure metals or eutectic alloys then the border temperatures can be introduced in an artificial way substituting the solidification point T^* by a certain temperature interval $[T^* - \Delta T,\ T^* + \Delta T]$. Numerical experiments show that the assumed values of ΔT (in reasonable limits) are not very essential, and the results of numerical simulations of solidification process are similar.

One assumes the knowledge of temperature-dependent function f_S for interval $[T_S,\ T_L]$ and then

$$\frac{\partial f_S(x,t)}{\partial t} = \frac{\mathrm{d} f_S}{\mathrm{d}T}\frac{\partial T(x,t)}{\partial t} \tag{7}$$

Introducing this formula to equation (1) one obtains

$$C(T)\frac{\partial T(x,t)}{\partial t} = \nabla\left[\lambda(T)\nabla T(x,t)\right] \tag{8}$$

where $C(T) = c(T) - L\ \mathrm{d}f_S/\mathrm{d}T$ is called 'a substitute thermal capacity'. This parameter can be defined in the different ways.

Introducing the following definition of substitute thermal capacity

$$C(T) = \begin{cases} c_L & T > T_L \\ c_P - L\dfrac{\mathrm{d} f_S}{\mathrm{d}T} & T_S \le T \le T_L \\ c_S & T < T_S \end{cases} \tag{9}$$

where c_L, c_P, c_S are the volumetric specific heats of molten metal, mushy zone and solid state sub-domains, one can use the equation (9) as the model of thermal processes proceeding in the whole, conventionally homogeneous, casting domain. It is the reason that the approach presented is called 'a one domain method'.

The function f_S must fulfill the conditions $f_S(T_L) = 0$ and $f_S(T_S) = 1$, additionally for $T < T_S$: $f_S = 0$, for $T > T_L$: $f_S = 0$.

The integral

$$\int_{T_S}^{T_L} C(T)\,\mathrm{d}T = c_P(T_L - T_S) + L \tag{10}$$

corresponds to the change of volumetric physical enthalpy for $[T_S, T_L]$ gives the additional information assuring the proper choice of f_S .

As an example the following function can be considered

$$f_S(T) = \left(\frac{T_L - T}{T_L - T_S} \right)^n \tag{11}$$

and then

$$\frac{\mathrm{d} f_S(T)}{\mathrm{d}T} = -\frac{n}{T_L - T_S} \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \tag{12}$$

Finally

$$C(T) = c_P + \frac{L}{T_L - T_S} \; n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \tag{13}$$

The quotient $L/(T_L - T_S) = c_{sp}$ is called 'a spectral latent heat'. Introducing this parameter one has

$$C(T) = c_P + c_{sp} \; n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \tag{14}$$

It is easy to check that

$$\int_{T_S}^{T_L} \left[c_P + c_{sp} \; n \left(\frac{T_L - T}{T_L - T_S} \right)^{n-1} \right] \mathrm{d}T = c_P (T_L - T_S) + L \tag{15}$$

Above formulas are very often used for exponent $n = 1$ and then

$$C(T) = c_P + \frac{L}{T_L - T_S} = c_P + c_{sp} \; , \quad T \in [T_S, T_L] \tag{16}$$

So, the linear course of f_S leads to the constant value of mushy zone thermal capacity. Assuming additionally the constant values of c_S and c_L one obtains the staircase function as an approximation of $C(T)$. In Figure 1 this type of function is shown. If the changes of border temperatures are taken into account (macrosegregation effect) then the families of functions $C(T)$ should be considered (Szopa, 1999).

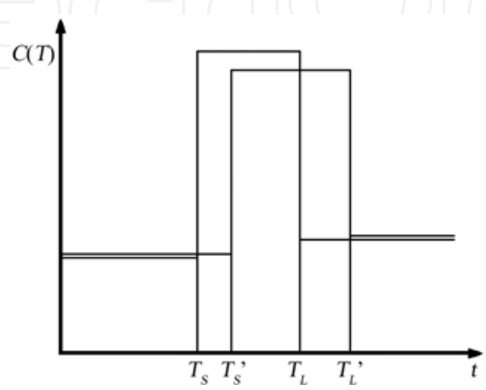

Fig. 1. Substitute thermal capacity

2.3 Introduction of enthalpy function and Kirchhoff transformation

Let us introduce the physical enthalpy of alloy defined in the following way

$$H(T) = \int_{T_r}^{T} C(\mu)\, \mathrm{d}\mu \tag{17}$$

where the lower limit of integration corresponds to the optional reference level.
The energy equation (8) written using the function (17) takes a form

$$\frac{\partial H(x,t)}{\partial t} = \nabla\left[a(T)\nabla H(x,t)\right], \qquad a(T) = \frac{\lambda(T)}{C(T)} \tag{18}$$

In Figure 2 the course of enthalpy function for carbon steel (0.44%C) under the assumption that the substitute thermal capacity $C(T)$ is approximated by piece-wise constant function (equation (16)) is shown.

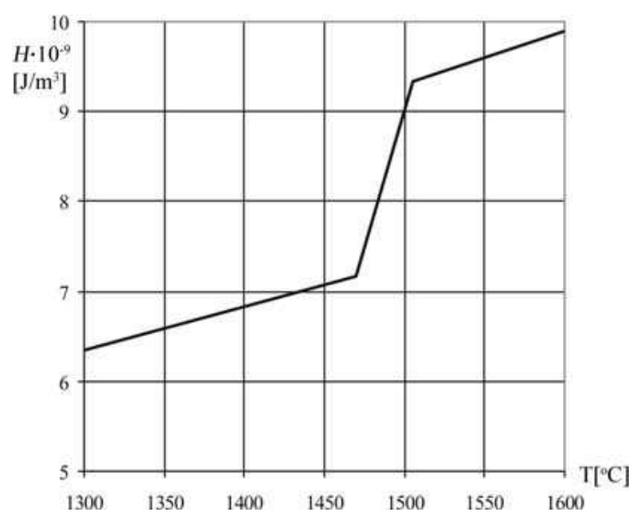

Fig. 2. Enthalpy function.

The transformation of typical boundary and initial conditions supplementing the equation (18) can be found, among others, in (Mochnacki & Suchy, 1995).
The mathematical model of solidification basing on the enthalpy function is often used at the stage of numerical modeling. In particular, the approach discussed seems to be very effective in a case of more complex courses of phase changes (e.g. solidification of cast iron, the process proceeds partially at the constant temperature and partially at the interval of temperature and then the introduction of enthalpy function and the application of numerical procedure called the Alternating Phase Truncation Method (Mochnacki & Suchy, 1995; Majchrzak & Mochnacki, 1995; Majchrzak & Mendakiewicz, 1993) leads to the simple and effective numerical algorithm).
The other form of energy equation determining the thermal processes in domain of solidifying alloy can be obtained using the Kirchhoff transformation, this means

$$U(T) = \int_{T_r}^{T} \lambda(\mu)\, \mathrm{d}\mu \tag{19}$$

It is easy to check that the introduction of function (19) Leeds to the following form of equation (8)

$$\phi\,[T(U)]\frac{\partial U(x,t)}{\partial t} = \nabla^2 U(x,t)\ , \qquad \phi\,(U) = \frac{C\,[T(U)]}{\lambda\,[T(U)]} \tag{20}$$

One can see, that the right hand side of energy equation (20) becomes a linear one and it can be essential at the stage of numerical modeling. The details concerning this approach and also the transformed form of typical boundary and initial conditions can be found in (Mochnacki & Suchy, 1995; Szopa, 1999).

3. Micro/macro models of solidification

A generalized form of solidification model belonging to the second generation ones (Stefanescu, 1999) will be here discussed. The equation describing the thermal processes proceeding in domain of solidifying metal contains the term (source function) controlling the course of latent heat evolution. A capacity of internal heat sources is proportional to crystallization rate, more precisely, to time derivative of function $f_S(x, t)$ corresponding to the local and temporary volumetric fraction of solid state at the point considered (Majchrzak et al., 2006; Mochnacki & Szopa, 2007; Fraś et al., 1993; Lupa et al. 2004) see: equation (1). If the micro/macro approach is taken into account, then the changes of f_S result from the crystallization laws in a micro scale (nucleation and nuclei growth). In this way the macro model basing on the Kirchhoff-Fourier-type equation is coupled with the model describing the processes proceeding on the level of single grains.

In literature one can find two basic models determining the mutual connections between f_S and temporary volume of grains. In particular, the following function is introduced

$$\omega(x,t) = N(x,t)\,V(x,t) \tag{21}$$

where N is a nuclei density [nuclei/m^3], V is a single grain volume. If one assumes $f_S(x, t) = \omega(x, t)$ then the linear model is considered (Majchrzak et al., 2006), while if $f_S(x, t) = 1 - \exp[-\omega(x, t)]$ then the exponential one is taken into account (Fraś et al., 1993; Lupa et al. 2004). In this place one can see that for the small values of ω, both models lead to the same results because $\exp(-\omega) \Rightarrow 1-\omega$ and $1 - \exp(-\omega) \Rightarrow \omega$. During the final stages of solidification the models discussed give the different results. The assumption of exponential changes of ω allows, in a certain way, to take into account the mutual geometrical interactions between the grains.

In this sub-chapter the generalization of the models previously presented will be shown. The differential equation from which linear and exponential models result, will be modified and in this way the new possibilities of f_S definition will appear.

As was mentioned, the micro/macro models of solidification discussed below require the introduction of function being the product of nuclei density and single grain volume. In a practical realization the exponent ω (equation (21)) is determined by the following formula (Mochnacki & Szopa, 2007; Fraś et al., 1993)

$$\omega(x,t) = \frac{4}{3}\pi\, v\, N(x,t)\left[\int_0^t u(\tau)\,\mathrm{d}\tau\right]^3 \tag{22}$$

where $u = \partial R/\partial t$ is a crystallization rate (R is a grain radius), N is nuclei density, v is a coefficient which equals 1 in case of spherical grains or $v < 1$ (e.g. dendritic growth, as in Figure 3 (Majchrzak & Piasecka, 1997)).

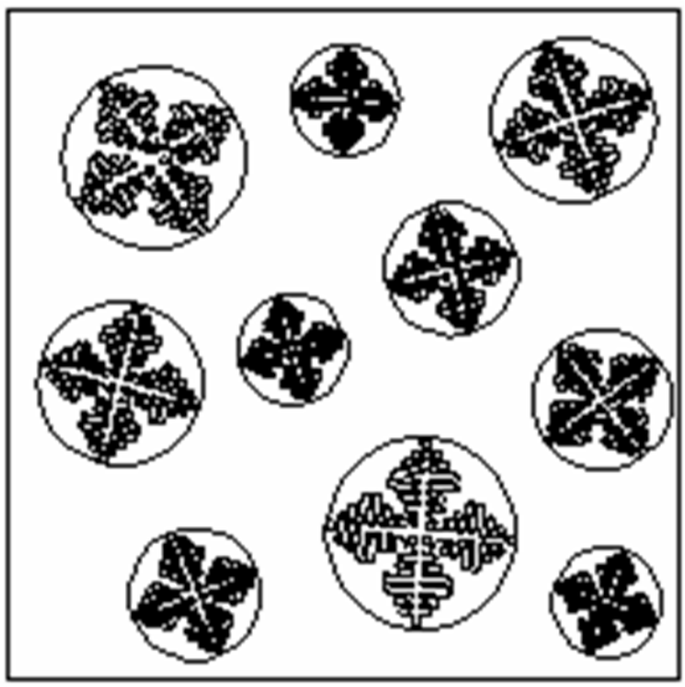

Fig. 3. Dendritic growth.

In the case of so-called linear model we have

$$f_S(x, t) = \omega(x, t) \tag{23}$$

and if $f_S = 1$ then the crystallization process stops.
The derivative of f_S with respect to time equals

$$\frac{\partial f_S(x, t)}{\partial t} = \frac{\partial \omega(x, t)}{\partial t} \tag{24}$$

The model above discussed determines the geometrical volume (volume fraction) and it is the correct assumption on the first stages of crystallization.
In order to take into account the limitations of growth in the final stages of the process one introduces the following modification of equation (24)

$$\frac{\partial f_S(x, t)}{\partial t} = \frac{\partial \omega(x, t)}{\partial t}\left[1 - f_S(x, t)\right] \tag{25}$$

Then

$$\frac{\mathrm{d} f_S(\omega)}{1 - f_S(\omega)} = \mathrm{d}\omega \tag{26}$$

next

$$f_S(\omega) = 1 + C\exp(-\omega) \tag{27}$$

Because for ω = 0: $f_S = 0$ therefore $C = -1$ and finally

$$f_S(\omega) = 1 - \exp(-\omega) \tag{28}$$

The last equation corresponds to the well known exponential model (the Kolmogoroff formula).
Here, the following modification of equation (24) can be proposed (Mochnacki & Szopa, 2007; Mochnacki & Szopa, 2010)

$$\frac{\partial f_S(x,t)}{\partial t} = \frac{\partial \omega(x,t)}{\partial t}\left[1 - f_S(x,t)\right]^n \tag{29}$$

where $n \geq 0$. From the physical point of view the same conditions as in previous case are fulfilled and the component $1 - f_S$ changes from 0 to 1.
So, we have

$$\frac{\mathrm{d} f_S(\omega)}{\left[1 - f_S(\omega)\right]^n} = \mathrm{d}\omega \tag{30}$$

It is easy to check that the solution fulfilling the condition ω = 0: $f_S = 0$ is of the form

$$f_S(\omega) = 1 - \left[(n-1)\omega + 1\right]^{\frac{1}{1-n}} \tag{31}$$

One can see that the last power-type formula constitutes the generalization of linear and exponential models. For $n = 0$ one obtains the linear one, while for $n = 1$ one has

$$\lim_{n\to 1} 1 - \left[(n-1)\omega + 1\right]^{\frac{1}{1-n}} = 1 - \exp(-\omega) \tag{32}$$

The others values of n can be also introduced. For example

$$\begin{aligned} n = 2: &\quad f_S = 1 - \frac{1}{\omega + 1} \\ n = 3: &\quad f_S = 1 - \frac{1}{\sqrt{2\omega + 1}} \\ n = \frac{1}{2}: &\quad f_S = 1 - \left(1 - \frac{\omega}{2}\right)^2 \end{aligned} \tag{33}$$

It should be pointed out that if $n \geq 1$ then for $\omega \to \infty$: $f_S \to 1$. This property is not fulfilled for $n < 1$ and it must be taken into account on the stage of numerical simulation. For example if $n = 1/2$ then solidification process takes place only for $\omega \leq 2$, the values $\omega > 2$ are not physically correct.
Now, the way of function ω modeling will be discussed.
A driving force of nucleation and nuclei growth is an undercooling below solidification point T^*. We assume that a local and temporary number of nuclei is proportional to the

second power of undercooling below the solidification point T^* (Mochnacki & Szopa, 2007; Fraś et al., 1993; Lupa et al. 2004)

$$N(x,t) = \eta\ \Delta T(x,t)^2 = \eta\left[T^* - T(x,t)\right]^2 \tag{34}$$

where η is the nucleation coefficient. The nucleation stops when $\Delta T(x, t + \Delta t) < \Delta T(x, t)$, additionally for $T(x, t) > T^*$: $N(x, t) = 0$ (Figure 4).

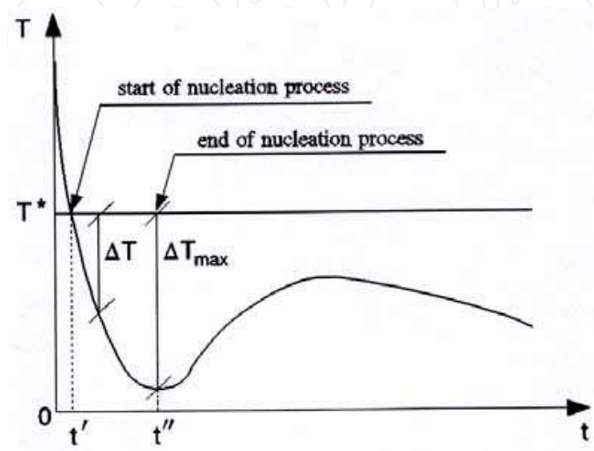

Fig. 4. Undercooling below point T^*

The solid phase growth (equiaxial grains) is determined by

$$\frac{\mathrm{d}R(x,t)}{\mathrm{d}t} = \mu\ \Delta T(x,t)^m \tag{35}$$

where μ is the growth coefficient, $m \in [1, 2]$. In literature one can also find the following equation

$$u(x,t) = \frac{\mathrm{d}R(x,t)}{\mathrm{d}t} = \mu_1\ \Delta T(x,t)^2 + \mu_2\ \Delta T(x,t)^3 \tag{36}$$

where μ_1, μ_2 are the growth coefficients.
Now, the certain aspects of function ω modelling will be discussed.
Because the problem considered is non-steady one, so one introduces the time grid defined as follows

$$0 = t^0 < t^1 < t^1 < \ldots < t^{s-1} < t^s < \ldots < t^S\ ,\quad \Delta t = t^s - t^{s-1} \tag{37}$$

while the metal domain is divided into m control volumes .
Let us consider the control volume ΔV_i from casting domain. During a certain interval of time the temperature at central point of ΔV_i decreases below the solidification point and the crystallization process starts.
We find a number of the first 'portion' of nuclei $N_i^{(1)}$ (using equation(34)) and the final radius of grains (formula (35)).
The first value of ω is equal to

$$\omega_i^{(1)} = \frac{4}{3}\pi v N_i^{(1)} \Delta R_i^{(1)} \tag{38}$$

This value is introduced into the macro model for transition corresponding to the next time interval.

In the second stage of crystallization process modeling we find the quantity N_i using the equation (34) and next we can estimate the size of the second generation, this means $N_i^{(2)} = N_i - N_i^{(1)}$. We can also find the new increment of the grains radius $\Delta R_i^{(2)}$. It should be pointed out that the current radii of the first generation are equal to $\Delta R_i^{(1)} + \Delta R_i^{(2)}$, while for the second generation: $\Delta R_i^{(2)}$.

The new value of function ω is determined by the formula

$$\omega_i^{(2)} = \frac{4}{3}\pi v \left[N_i^{(1)} \left(\Delta R_i^{(1)} + \Delta R_i^{(2)} \right)^3 + N_i^{(2)} \Delta R_i^{(2)3} \right] \tag{39}$$

The next steps of crystallization process modeling result from the generalization of considerations above presented. It should be pointed out that after the transition by the maximum undercooling, the number of nuclei at control volume ΔV_i is constant and this fact must be taken into account in adequate numerical procedure. The knowledge of two successive values of $\omega_i^{(k)}$ allows to estimate the source term in equation (1) using the differential quotient, in particular

$$L\frac{\partial f_S(x,t)}{\partial t} = L\frac{\mathrm{d} f_S}{\mathrm{d}\omega}\frac{\partial \omega(x,t)}{\partial t} \approx L[(n-1)\omega + 1]^{\frac{n}{1-n}} \frac{\Delta \omega}{\Delta t} \tag{40}$$

4. Examples of numerical methods application

In this sub-chapter only the selected problems connected with numerical modelling of solidification process will be discussed. In particular a certain version of control volume method and next the algorithms basing on the boundary element method will be here presented.

So, the first part of considerations is devoted to the application of control volume method (CVM) for numerical simulation of solidification process both in the macro and micro/macro scale. The control volume method (Mochnacki & Suchy, 1995; Domański et al., 2009a; Domański et al., 2009b; Mochnacki & Ciesielski, 2007) constitutes an effective tool for numerical computations of the heat transfer processes. The domain analyzed is divided into N volumes. The CVM algorithm allows to find the transient temperature field at the set of nodes corresponding to the central points of the control volumes. The nodal temperatures can be found on the basis of energy balances for the successive volumes. In order to assure the correctness and exactness of the algorithm proposed the control volumes are generated in the shape of the Voronoi polygons (see: Fig. 5).

Let us consider the control volume ΔV_0 with the central node x_0. It is assumed here that the thermal capacities and capacities of the internal heat sources are concentrated in the nodes representing elements, while thermal resistances are concentrated in the sectors joining the nodes

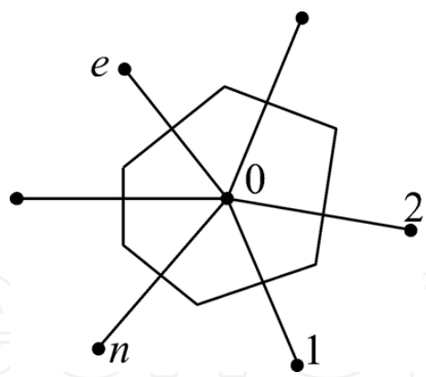

Fig. 5. Control volume ΔV_0

The energy balance for the control volume ΔV_0 can be written in the form

$$\Delta H_0 = \sum_e Q_e + |\Delta V_0| q_V \, \Delta t \tag{41}$$

where ΔH_0 is a change of control volume enthalpy during the time interval Δt, Q_e is a heat conducted at the time Δt from the adjoining nodes to the node x_0, q_V is a mean capacity of internal heat sources resulting from the evolution of latent heat in the control volume ΔV_0.
If one assumes that the heat fluxes flowing to the element ΔV_0 are proportional to the temperature differences at the moment $t = t^f$, then we shall obtain a solving system of the type 'explicit scheme'. So

$$Q_e = \frac{T_e^f - T_0^f}{R_{0e}^f} \Delta A_e \, \Delta t \tag{42}$$

where R_{0e}^f is the thermal resistance between points x_0 and x_e (Majchrzak & Mendakiewicz, 1993), ΔA_e surface limiting the domain ΔV_0 in the direction e. If we denote by h_e the distance between the nodes x_0, x_e then

$$R_{0e}^f = \frac{h_e}{2\lambda_0^f} + \frac{h_e}{2\lambda_e^f} \tag{43}$$

where λ_0^f and λ_e^f are the thermal conductivities in the control volumes ΔV_0 and ΔV_e at the moment $t = t^f$. The other definition of thermal resistance should be introduced for the boundary volumes (Mochnacki & Suchy, 1995). In a case of no-flux boundary condition (see: example presented) one assumes $R_{0e}^f = \infty$ (in numerical realization e.g. $R_{0e}^f = 10^{10}$) if the surface limiting the domain ΔV_0 in direction e is a part of 'adiabatic' boundary.
The change of enthalpy of the control volume ΔV_0 during the time Δt equals (Domański et al., 2009a; Domański et al., 2009b; Mochnacki & Ciesielski, 2007)

$$\Delta H_0 = C_0^f \left(T_0^{f+1} - T_0^f \right) |\Delta V_0| \tag{44}$$

where $C_0 f$ is the volumetric specific heat (substitute thermal capacity), f, f+1 denotes two successive time levels.
Let us write the balance equation using the explicit scheme

$$C_0^f\left(T_0^{f+1}-T_0^f\right)\left|\Delta V_0\right|=\sum_e \frac{T_e^f-T_0^f}{R_{0e}^f}\Delta A_e\,\Delta t+\left|\Delta V_0\right|q_V\,\Delta t \tag{45}$$

or

$$T_0^{f+1}=\sum_{e=0}^{n} W_e T_e^f+\frac{q_V\,\Delta t}{C_0^f} \tag{46}$$

where

$$W_e=\frac{\Delta t\,\Delta A_e}{C_0^f R_{0e}^f\left|\Delta V_0\right|},\quad e=1,\ldots,n \tag{47}$$

$$W_0=1-\sum_{e=1}^{n} W_e \tag{48}$$

In order to assure the stability of the above explicit scheme the coefficient W_0 must be positive.

It was mentioned above that the control volumes have been constructed in the form of Voronoi polygons (Thiessen cells). A single polygon is defined by the lines that bisect the lines between the central point and its surrounding points. The bisecting lines and the connection lines are perpendicular to each other and this property is very essential when the control volume method is used.

Many algorithms to construct the Voronoi polygons can be found in literature. One popular method is based on the Delaunay triangulation (Domański et al., 2009b; Mochnacki & Ciesielski, 2007) and this method has been used at the stage of 'in house' computer program construction. The aim of computations was the analysis of thermal processes in domain of solidifying cast composite made from Al-Si alloy (metal matrix) and silicon (fibres). In particular the problem of 'spontaneous' solidification of matrix due to presence of fibres has been analyzed.

In Figure 6 an example of the structure of cast composite with 40% fibres is shown. The geometrical parameters of a matrix-fibres system are chosen on the basis of the optical micrographs presented in (Domański et al., 2009b). It can be seen that the fibres diameters are different, and also their mutual positions are rather incidental. The only unquestionable information concerning the geometry of the system results from the volumetric fraction of the fibres in the domain analyzed. So, the numerical procedure realizing the mesh generation, fibres localization, values of fibres radii bases on the application of random numbers generation. The sub-domain presented in Figure 6 corresponds to the central part of composite (side of square equals 100 μm) and on the external surface the no-flux conditions have been assumed. It turned out that the spontaneous solidification takes place for 55% fraction of fibres. The kinetics of solidification in this case is shown in Figure 7. The input data concerning the parameters of cast composite components can be found in (Domański et al., 2009b).

A similar algorithm basing on the control volume method can be used also in a case of macro/micro modelling of solidification. One can see that the shapes of Thiessen cells are similar to the primary structure of casting and it was a reason of investigations connected with the application of presented version of CVM in a scope of macro/micro problems.

As an example the results of computations concerning the solidification of aluminium casting (2D problem) are presented. The macro control volume shown in Figure 8 (Mochnacki & Ciesielski, 2007) has been divided into micro control volumes. The heat fluxes (the Neumann boundary conditions) given on the periphery of macro control volume result from the solution of macroscopic problem (here the finite difference method has been applied). The micro model has been solved using the CVM under the assumption that the nuclei density is a constant value (this assumption is often used), the nuclei growth results from equation (35) for $m = 2$, while the changes of solid state fraction are determined by the Kolmogoroff formula. The result (cooling curve) shown in Figure 9 concerns the central point of macro control volume being in the direct thermal contact with sand mould sub-domain. The micro/macro approach allows one to observe the undercooling below the solidification point and next, the growth of local temperature. This effect cannot be observed when the numerical solution bases on the macro approach.

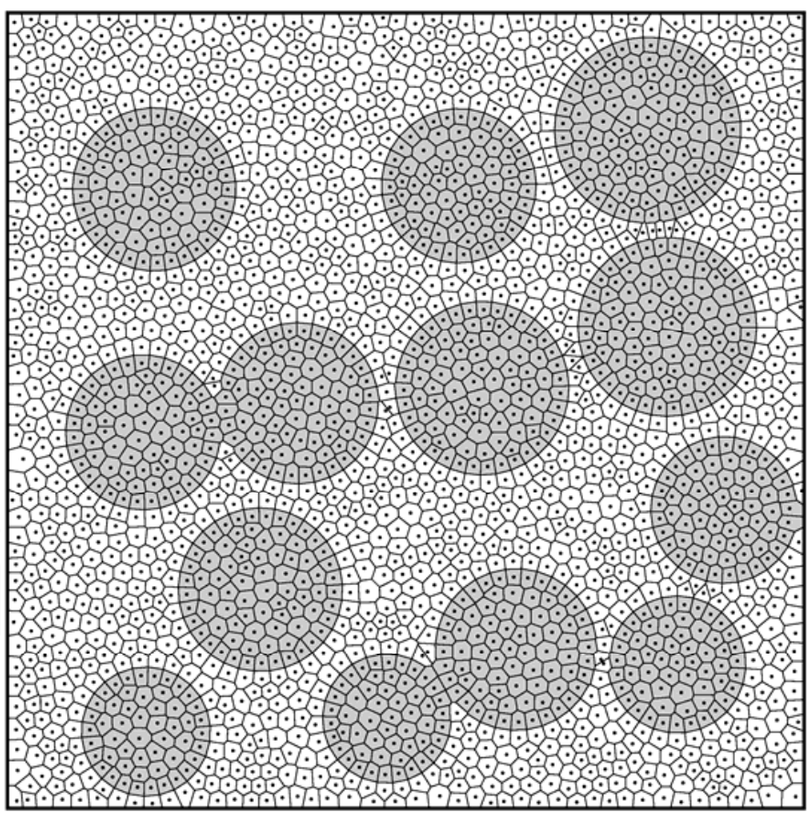

Fig. 6. Example of structure and its discretization.

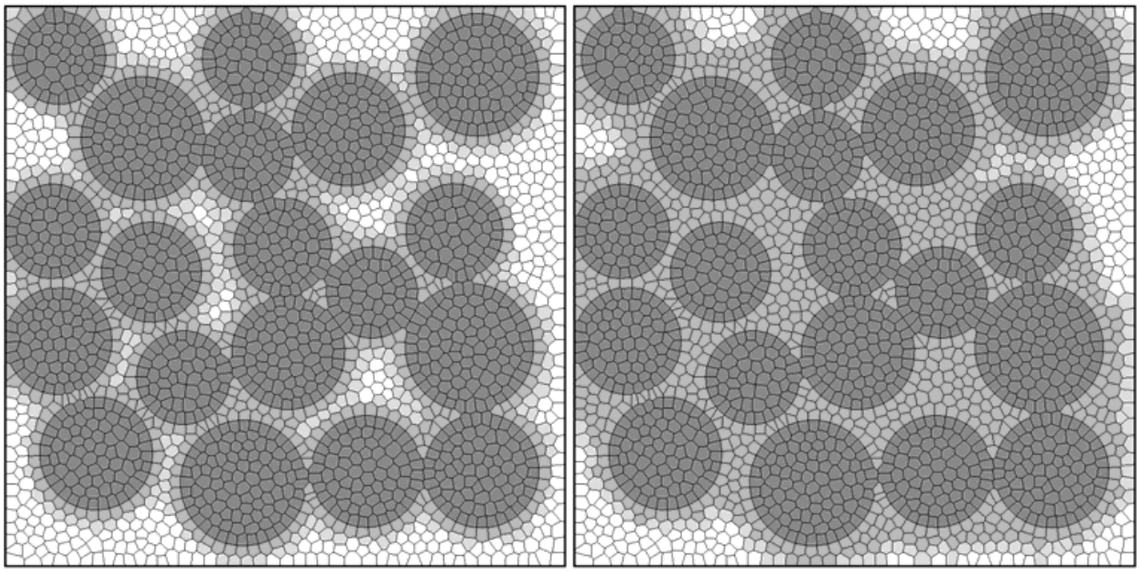

Fig. 7. Kinetics of composite solidification.

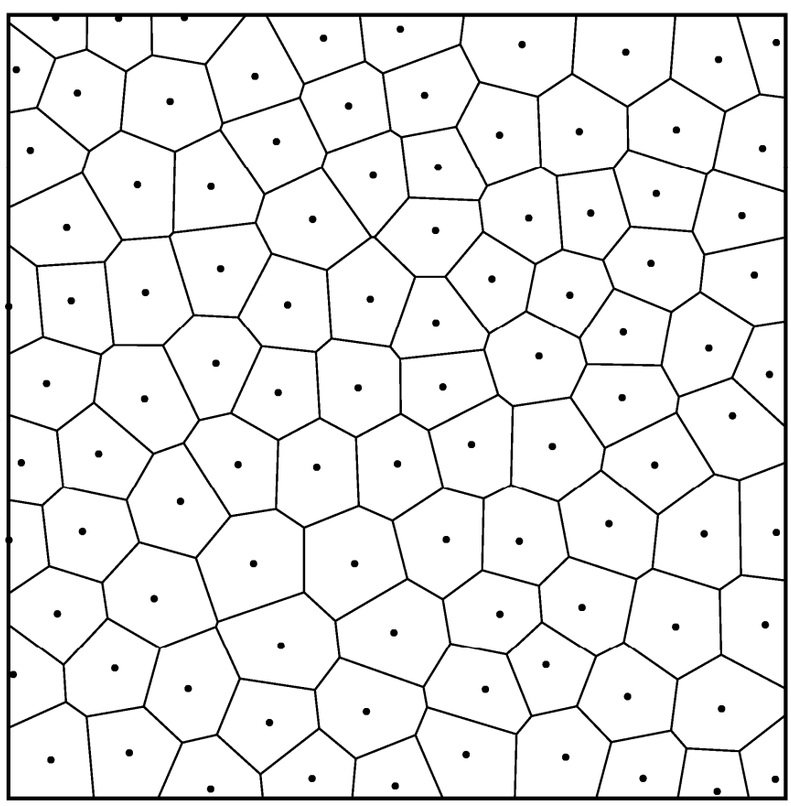

Fig. 8. The inner structure of macro control volume.

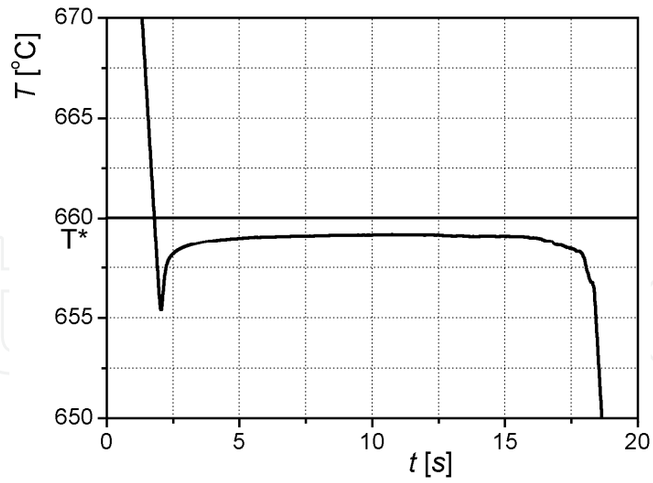

Fig. 9. Temperature history at the central point of macro control volume.

Now, the problems connected with the boundary element method (Brebbia et al., 1984; Brebbia & Dominguez, 1992; Majchrzak, 2001) application in the scope of solidification process modeling will be discussed. So, the boundary element method constitutes the effective tool for numerical simulation of solidification processes (Majchrzak & Mochnacki, 1995; Majchrzak & Mochnacki, 1996; Majchrzak & Szopa, 2001; Mochnacki & Majchrzak, 2007b). The method assures the exact approximation of real shapes of the boundaries and also the very good exactness of boundary conditions approximation (Brebbia et al., 1984; Brebbia & Dominguez, 1992). These features of the BEM are very essential in the case of solidification processes modeling because the big gradients of temperature near the boundary require the adequate exact method of temperature field computations. The main disadvantage of the method is the fact that it can be used only for linear tasks (the constant values of metal and mould thermophysical parameters) because the fundamental solutions are only available for linear equations. Nevertheless, several techniques have been developed for the numerical solution of nonlinear problems. In the case of solidification problem the basic BEM algorithm for linear Fourier's equation should be coupled with procedures correcting the temporary solutions for successive levels of time. These procedures are called the temperature field correction method (Mochnacki & Suchy, 1995; Mochnacki & Szopa, 2008), the alternating phase truncation method (Mochnacki & Suchy, 1995; Majchrzak & Mochnacki, 1995; Majchrzak & Mendakiewicz, 1993) and the artificial heat source method (Mochnacki & Majchrzak, 2010; Mochnacki & Szopa, 1998).

The basic idea of the BEM can be realized in different ways. In the case of parabolic equations the I and II scheme of the BEM, the dual reciprocity BEM, the BEM using discretization in time etc. are used. The detailed information concerning the BEM application in the scope of heat transfer problems can be found in the numerous books and papers published by Ewa Majchrzak from the Silesian University of Technology (Poland). Below, the short discussion of the BEM using discretization in time taken from (Majchrzak & Szopa, 2001; Mochnacki & Szopa, 1998; Mochnacki & Szopa, 2002) (it is not very popular but quite effective version of the BEM) will be presented.

Let us consider the following parabolic equation

$$\frac{\partial T(x,t)}{\partial t} = a \nabla^2 T(x,t) + \frac{Q(x,t)}{c} \tag{49}$$

where a is a thermal diffusivity, c is a volumetric specific heat, Q is a capacity of internal heat sources. The equation (49) is supplemented by the assumed boundary and initial conditions. At first the time grid

$$0 = t^0 < t^1 < \ldots < t^{f-2} < t^{f-1} < t^f < \ldots < t^F < \infty \tag{50}$$

with constant step $\Delta t = t^f - t^{f-1}$ is introduced.
We substitute the energy equation (10) for time $t \in [t^{f-1}, t^f]$ by the equation in which the time derivative is approximated by the differential quotient, in particular

$$\frac{T(x, t^f) - T(x, t^{f-1})}{\Delta t} = a \nabla^2 T(x, t^f) + \frac{Q(x, t^f)}{c} \tag{51}$$

The last equation can be written in the form

$$\begin{aligned} &\nabla^2 T(x, t^f) - \frac{1}{a \Delta t} T(x, t^f) + \\ &\frac{1}{a \Delta t} T(x, t^{f-1}) + \frac{Q(x, t^f)}{\lambda} = 0 \end{aligned} \tag{52}$$

Using the weighted residual method criterion (WRM) (Stefanescu, 1999; Szopa, 1999) one obtains

$$\begin{aligned} &\int_\Omega \left[\nabla^2 T(x, t^f) - \frac{1}{a \Delta t} T(x, t^f) + \right. \\ &\left. \frac{1}{a \Delta t} T(x, t^{f-1}) + \frac{Q(x, t^f)}{\lambda} \right] T^*(\xi, x)\, \mathrm{d}\Omega = 0 \end{aligned} \tag{53}$$

where $T^*(\xi, x)$ is the fundamental solution and for the objects oriented in rectangular co-ordinate system it is a function of the form

$$T^*(\xi, x) = \begin{cases} \dfrac{\sqrt{a \Delta t}}{2} \exp\left(-\dfrac{r}{\sqrt{a \Delta t}} \right), & \text{for 1 D problem} \\ \dfrac{1}{2\pi} \mathrm{K}_0 \left(\dfrac{r}{\sqrt{a \Delta t}} \right), & \text{for 2 D problem} \\ \dfrac{1}{4\pi r} \exp\left(-\dfrac{r}{\sqrt{a \Delta t}} \right), & \text{for 3 D problem} \end{cases} \tag{54}$$

where $\mathrm{K}_0(\cdot)$ is the modified Bessel function of zero order, r is the distance between the points x and ξ.
The fundamental solution fulfills the following equation

$$\nabla^2 T^*(\xi, x) - \frac{1}{a \Delta t} T^*(\xi, x) = -\delta(\xi, x) \tag{55}$$

Additionally, on a basis of formula (54) the heat flux resulting from the fundamental solution

$$q^*(\xi, x) = -\lambda\, n \cdot \nabla T^*(\xi, x) \tag{56}$$

can be calculated in analytical way.
Applying the second Green formula to the first component of criterion (53) and taking into account the property (55) of fundamental solution one obtains the following boundary integral equation ($\xi \in \Gamma$)

$$\begin{aligned} T(\xi, t^f) + \frac{1}{\lambda}\int_\Gamma T^*(\xi, x)\, q(x, t^f)\, \mathrm{d}\Gamma = \\ \frac{1}{\lambda}\int_\Gamma q^*(\xi, x)\, T(x, t^f)\, \mathrm{d}\Gamma + \\ \frac{1}{a\Delta t}\int_\Omega T(x, t^{f-1})\, T^*(\xi, x)\, \mathrm{d}\Omega + \\ \frac{1}{\lambda}\int_\Omega Q(x, t^f)\, T^*(\xi, x)\, \mathrm{d}\Omega \end{aligned} \tag{57}$$

For example, in a case of 1D problem (plate of thickness L) the last equation takes a form

$$\begin{aligned} T(\xi, t^f) + \left[\frac{1}{\lambda} T^*(\xi, x) q(x, t^f)\right]_0^L = \\ \left[\frac{1}{\lambda} q^*(\xi, x) T(x, t^f)\right]_0^L + p(\xi) + z(\xi) \end{aligned} \tag{58}$$

where

$$p(\xi) = \frac{1}{a\Delta t}\int_0^L T^*(\xi, x)\, T(x, t^{f-1})\, \mathrm{d}x \tag{59}$$

and

$$z(\xi) = \frac{1}{\lambda}\int_0^L Q(x, t^f)\, T^*(\xi, x)\, \mathrm{d}x \tag{60}$$

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

$$\begin{aligned} \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \begin{bmatrix} q(0, t^f) \\ q(L, t^f) \end{bmatrix} = \\ \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} T(0, t^f) \\ T(L, t^f) \end{bmatrix} + \begin{bmatrix} p(0) \\ p(L) \end{bmatrix} + \begin{bmatrix} z(0) \\ z(L) \end{bmatrix} \end{aligned} \tag{61}$$

where

$$g_{11} = -g_{22} = -\frac{\sqrt{\Delta t}}{2\sqrt{\lambda c}} \qquad g_{12} = -g_{21} = \frac{\sqrt{\Delta t}}{2\sqrt{\lambda c}} exp\left(-\frac{L}{\sqrt{a\Delta t}}\right) \tag{62}$$

while

$$h_{11} = h_{22} = -\frac{1}{2} \qquad h_{12} = h_{21} = \frac{1}{2} exp\left(-\frac{L}{\sqrt{a\Delta t}}\right) \tag{63}$$

Equation (61) allows to determine the 'missing' boundary values (temperatures and heat fluxes for $x = 0$ and $x = L$), while in the second step of computations the temporary temperatures in the set of internal points $\xi \in (0, L)$ can be found on the basis of equation (58).

As the example of 1D solution concerning the solidification process (micro/macro approach) a problem of heat transfer in domain of aluminium plate ($L = 0.02$ [m]) is discussed. 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}], exponent $n = 1.5$ (equation (31)). Pouring temperature: $T_0 = 700$°C, solidification point: $T_c = 660$°C. The thermophysical parameters of Al are assumed to be constant. The solidification model corresponds to description previously presented (see: formulas (38), (39), (40)). In domain of plate 20 internal points has been distinguished and in Figure 10 the cooling curves at points 10, 14 and 18 are presented, while in Figure 11 the evolution of source function at the same points are shown.

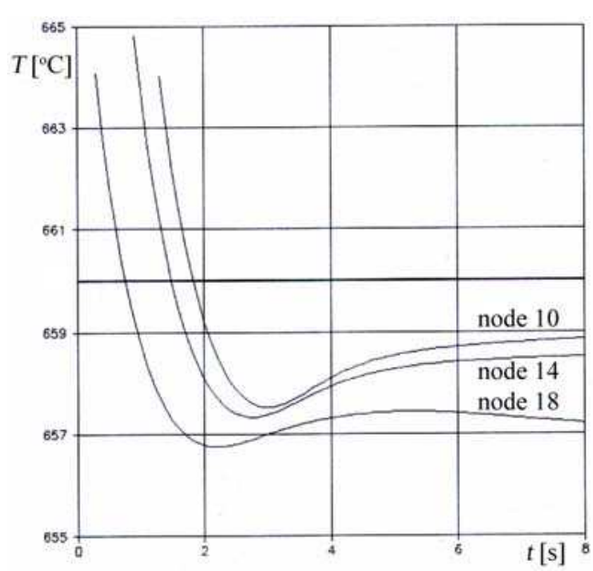

Fig. 10. Cooling curves.

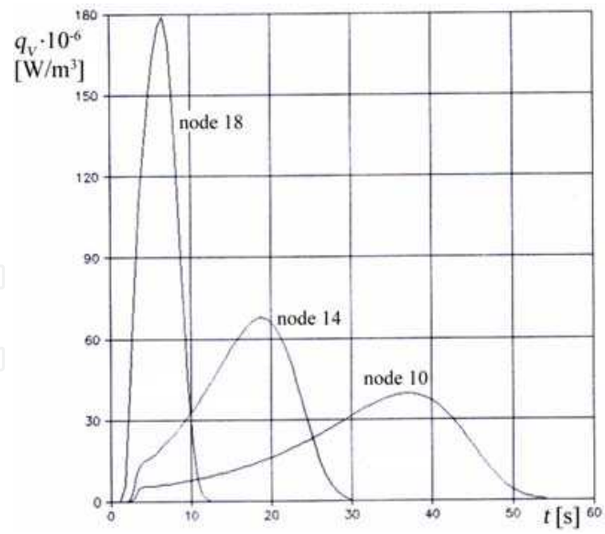

Fig. 11. Source function evolution.

The second example concerns the 3D problem solution (Szopa, 1999). Figure 12 shows the shape of considered steel casting domain (dimensions are marked in mm).
The boundary surface was divided into constant boundary elements (squares), whereas the interior was divided into constant internal cells (cubes). The boundary condition of the form $x \in \Gamma$: $T(x, t) = 1465°C$ was assumed (this value results from well known Schwarz's solution and was treated as a constant one). The initial temperature $T(x, 0) = 1550°C$ whereas the thermophysical parameters correspond to the cast steel 0.35%C. The solidification process was taken into account by the correction of temperature field for successive levels of time (Temperature Field Correction Method). In Figure 13 the temporary temperature field for $t = 180s$ and two selected vertical sections is shown.

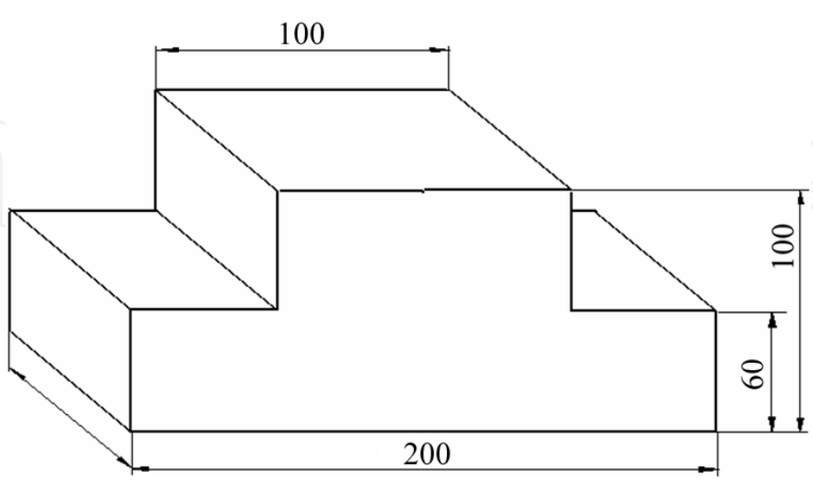

Fig. 12. Temperature field in domain considered.

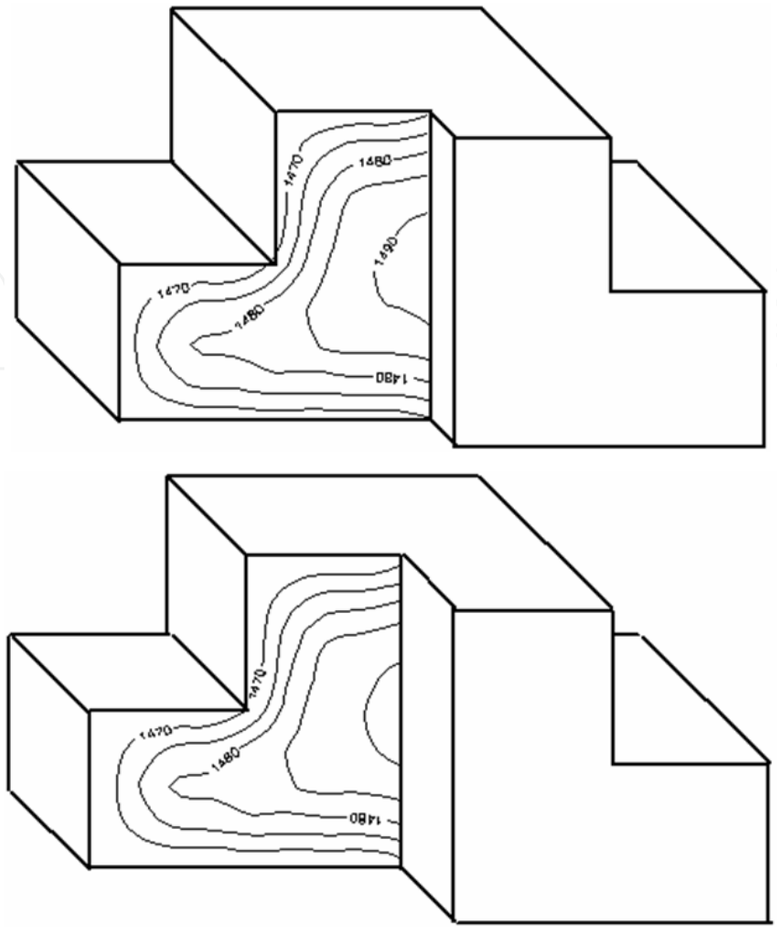

Fig. 13. Temperature field in domain considered.

5. Sensitivity analysis

In this sub-chapter the selected problems from the scope of sensitivity analysis application in the thermal theory of solidification processes are discussed. It should be pointed out that the sensitivity models are the essential part of inverse problems solutions, they allow to rebuilt the solution obtained for assumed input data on the other one (see: considerations and examples presented below), sensitivity methods can be also used on a stage of measurements in order to determine the optimum positions of sensors.

The examples of applications here discussed concern the sensitivity of temperature field in a system solidifying metal-mould with respect to perturbations of external, boundary and initial parameters appearing in the mathematical model of process discussed, at the same time the approach called 'a direct sensitivity analysis' is presented. Both the macro models and macro/micro ones are considered

Let us assume that the searched solution of boundary-initial problem (e.g. transient temperature field in the system metal - mould), is the function of parameters z_1 , z_2 ,..., z_n . They can correspond, among others, to thermophysical parameters of sub-domains, heat transfer coefficient on the outer surface of the system, pouring temperature, initial temperature of mould, geometrical parameters etc. The sensitivity U_k of boundary-initial

problem solution with respect to parameter z_k is defined as a partial derivative $U_k(x,t) = \partial T(x,t,z_1,\dots z_n)/\partial z_k$ (Kleiber, 1997; Dems & Rousselet, 1999). As it was mentioned below the methods of sensitivity analysis allows one 'to rebuilt' the solution of problem considered to the solution concerning the other value of parameter z_k. So, the set of parameters introduced to the computer program as the input data we denote by z_1^0, z_2^0, ..., z_n^0. Additionally we are interested in the others solutions corresponding to changed input data (e.g. new pouring temperature). The methods of sensitivity analysis give the possibilities to transform the basic solution on the solution for disturbed initial parameters. The transformation results from the Taylor formula, namely

$$\begin{gathered} T(x,\ t,\ z_1^0, z_2^0, \dots, z_k^0 \pm \Delta z_k, \dots, z_n^0) = \\ T(x,\ t,\ z_1^0, z_2^0, \dots, z_k^0, \dots, z_n^0) \pm U_k^0 \Delta z_k + V_k^0 \frac{\Delta z_k^0}{2} + \dots \end{gathered} \tag{64}$$

where T is a searched function (e.g. temperature), x is a spatial coordinate, t is a time, U_k^0 denotes the derivative $\partial T/\partial z_k$ at the start point 0, whereas V_k^0 is the second derivative with respect to z_k at the same point. The equations determining the values of U_i^0 (the first order sensitivity) and V_i^0 (the second order sensitivity) result from the differentiation of equations and conditions describing the physical process considered with respect to parameter z_k (direct approach) We can notice that formula (64) concerns to the disturbance of distinguished parameter, but one can analyze also the disturbance of the certain set of parameters z_k, simultaneously.

5.1 Sensitivity analysis of macro models

Sensitivity analysis with respect to boundary and initial conditions (e.g. heat transfer coefficient α, ambient temperature T_a , initial temperatures T_0, T_{m0}) or mould parameters (c_m, λ_m) will be discussed, at the same time the direct approach will be applied. The problem is more complicated in comparison with the others ones, because the mathematical model of solidification is strongly non-linear (Szopa, 2005; Szopa & Wojciechowska, 2003; Szopa et al., 2004; Mochnacki & Szopa, 2009).

At first, the energy equation (8) should be differentiated with respect to parameter z_k, this means

$$\frac{\partial}{\partial z_k}\left[C(T)\frac{\partial T(x,t)}{\partial t}\right] = \nabla\left[\frac{\partial}{\partial z_k}\left[\lambda(T)\nabla T(x,t)\right]\right] \tag{65}$$

Because

$$\frac{\partial C(T)}{\partial z_k} = \frac{\mathrm{d}C(T)}{\mathrm{d}T}\frac{\partial T}{\partial z_k}, \qquad \frac{\partial \lambda(T)}{\partial z_k} = \frac{\mathrm{d}\lambda(T)}{\mathrm{d}T}\frac{\partial T}{\partial z_k} \tag{66}$$

therefore (using additionally Schwarz theorem)

$$\begin{gathered} C(T)\frac{\partial U(x,t)}{\partial t} = \nabla[\lambda(T)\nabla U(x,t)] + \\ \nabla[\lambda'(T)U(x,t)\nabla T(x,t)] - C'(T)U(x,t)\frac{\partial T(x,t)}{\partial t} \end{gathered} \tag{67}$$

where $U = \partial T/\partial z_k$ is the sensitivity of temperature field in a solidifying metal domain with respect to perturbations of parameter z_k.
Now, the equation concerning a mould sub-domain is differentiated with respect to z_k under the assumption that c_m and λ_m are the constant values (this assumption is not necessary)

$$\frac{\partial c_m}{\partial z_k}\frac{\partial T_m(x,t)}{\partial t} + c_m \frac{\partial U_m(x,t)}{\partial t} = \frac{\partial \lambda_m}{\partial z_k}\nabla^2 T_m(x,t) + \lambda_m \nabla^2 U_m(x,t) \tag{68}$$

where $U_m = \partial T_m/\partial z_k$. Taking into account the equation (2) one can write

$$c_m \frac{\partial U_m(x,t)}{\partial t} = \lambda_m \nabla^2 U_m(x,t) + \left(\frac{\partial \lambda_m}{\partial z_k}\frac{c_m}{\lambda_m} - \frac{\partial c_m}{\partial z_k} \right) \frac{\partial T_m(x,t)}{\partial t} \tag{69}$$

The sensitivity equations become simpler when in place of z_k the actual parameters (e.g. initial casting temperature, initial mould temperature, heat transfer coefficient or ambient temperature) are introduced.
The following boundary conditions should be considered

- Robin condition (e.g. external surface of mould):

$$-\frac{\partial \lambda_m}{\partial z_k}\frac{\partial T_m(x,t)}{\partial n} - \lambda_m \frac{\partial U_m(x,t)}{\partial n} = \frac{\partial \alpha}{\partial z_k}\left[T_m(x,t) - T_a \right] + \alpha \left[U_m(x,t) - \frac{\partial T_a}{\partial z_k} \right] \tag{70}$$

- metal-mould contact surface:

$$\begin{cases} -\lambda'(T)U(x,t)\dfrac{\partial T(x,t)}{\partial n} - \lambda(T)\dfrac{\partial U(x,t)}{\partial n} = \\ -\dfrac{\partial \lambda_m}{\partial z_k}\dfrac{\partial T_m(x,t)}{\partial n} - \lambda_m \dfrac{\partial U_m(x,t)}{\partial n} \\ U(x,t) = U_m(x,t) \end{cases} \tag{71}$$

One can see that for the constant values of metal and mould thermal conductivities the conditions (70) and (71) are similar to conditions (3) and (5).
The initial conditions takes a form

$$t = 0: \quad U = \frac{\partial T_0}{\partial z_k} = U_0, \quad U_m = \frac{\partial T_{m\,0}}{\partial z_k} = U_{m\,0} \tag{72}$$

If the sensitivity analysis does not concern the initial temperatures then the initial conditions are uniform

$$t=0: \quad U=\frac{\partial T_0}{\partial z_k}=0, \quad U_m=\frac{\partial T_{m\,0}}{\partial z_k}=0 \tag{73}$$

Below, as an example, the sensitivity method is applied to the analysis of dependence between the pouring temperature and the course of solidification and cooling proceeding in the casting domain. The equation describing the heat diffusion in the casting is non-linear one, whereas the thermophysical parameters of mould are assumed to be the constant.

The equation describing the thermal processes proceeding in the metal domain oriented in rectangular co-ordinate system $\{x, y\}$ (2D problem) is of the form (c.f. equation (1))

$$C(T)\frac{\partial T(x,y,t)}{\partial t}= \frac{\partial}{\partial x}\left[\lambda(T)\frac{\partial T(x,y,t)}{\partial x}\right]+\frac{\partial}{\partial y}\left[\lambda(T)\frac{\partial T(x,y,t)}{\partial y}\right] \tag{74}$$

The energy equation for the mould domain is the following

$$c_m\frac{\partial T_m(x,y,t)}{\partial t}=\lambda_m\left(\frac{\partial^2 T_m(x,y,t)}{\partial x^2}+\frac{\partial^2 T_m(x,y,t)}{\partial y^2}\right) \tag{75}$$

The boundary conditions on the outer surface of the mould determine the continuity of heat flux between the mould and the environment (the Robin condition), but in practice one can assume in this place the no-flux condition (especially in the case of sand mould). On the contact surface between casting and the condition (5) is given.

The mathematical model is supplemented by the initial conditions:

$$t=0: \quad T=T_0, \quad T_m=T_{m0} \tag{76}$$

In order to analyze the influence of the pouring temperature on the course of casting solidification the direct variant of sensitivity analysis has been used and the solidification model is differentiated with respect to pouring temperature T_0. So, for $(x, y) \in \Omega$

$$C_T\,U\frac{\partial T}{\partial t}+C\frac{\partial U}{\partial t}=\frac{\partial}{\partial x}\left(\lambda\frac{\partial U}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda\frac{\partial U}{\partial y}\right)+ \frac{\partial}{\partial x}\left(\lambda_T\,U\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda_T\,U\frac{\partial T}{\partial y}\right) \tag{77}$$

where $U = \partial T/\partial T_0$, $C_T = \mathrm{d}C/\mathrm{d}T$, $\lambda_T = \mathrm{d}\lambda/\mathrm{d}T$. Next

$$(x, y) \in \Omega_m: \quad c_m\frac{\partial U_m}{\partial t}=\lambda_m\left(\frac{\partial^2 U_m}{\partial x^2}+\frac{\partial^2 U_m}{\partial y^2}\right) \tag{78}$$

where $U_m = \partial T_m/\partial T_0$.

If on the outer surface Γ_0 of the system we assume the no-flux condition then the adequate boundary condition takes a form, $\partial U_m/\partial n = 0$. On the contact surface (for λ = const) one has

$$(x, y) \in \Gamma_m: \quad \begin{cases} -\lambda \dfrac{\partial U}{\partial n} = -\lambda_m \dfrac{\partial U_m}{\partial n} \\ U = U_m \end{cases} \tag{79}$$

The problem is supplemented by the initial condition for $t = 0$: $U = 1$, $U_m = 0$.
As an example the bar of rectangular section (10×14 cm) made from Cu-Sn alloy (10% Sn) is considered. The casting is produced in the sand mix which parameters are equal $\lambda_m = 2.28$ [W/mK], $c_m = 2.320 \cdot 10^6$ [J/m^{3}K]. The thermal conductivity of the casting material equals $\lambda = 50$ [W/mK]. According to literature (e.g. [3]) the substitute thermal capacity can be approximated by the piece-wise constant function $T > 990$°C: $C = 3.678 \cdot 10^6$ [J/m^{3}K], $T < 825$°C: $C = 3.678 \cdot 10^6$ [J/m^{3}K], $T \in [825, 990]$: $C = 14.558 \cdot 10^6$ [J/m^{3}K]. In order to assure the differentiation of function C, the smoothing procedure has been applied (Mochnacki & Suchy, 1995). The initial temperatures are equal to $T(0) = 1000$°C, $T_m(0) = 30$°C. The quarter of domain is taken into account and its shape is marked in Figure14. In this Figure the temperature field for time $t = 6$ minutes is shown.
The sensitivity analysis shows that the influence of pouring temperature on the temperature field is the most essential in the metal sub-domain (in particular at the initial stages of cooling process) and sand mix layer close to contact surface. In other words, the change of $T_0 = 1000$°C to the value from interval $[T_0 - \Delta T_0,\ T_0 + \Delta T_0]$ determines the essential fluctuations of temporary temperature field in these sub-domains.

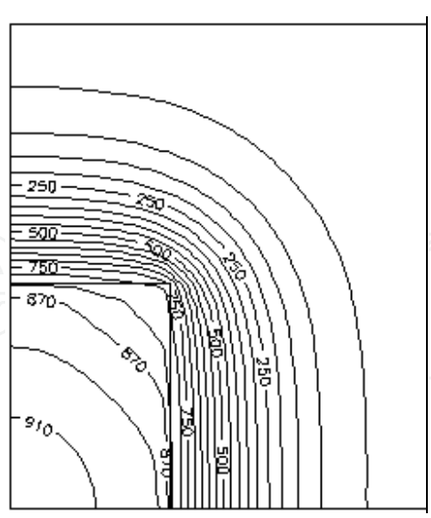

Fig. 14. Temperature field.

Figure 15 illustrates the isolines of function U for the same time.

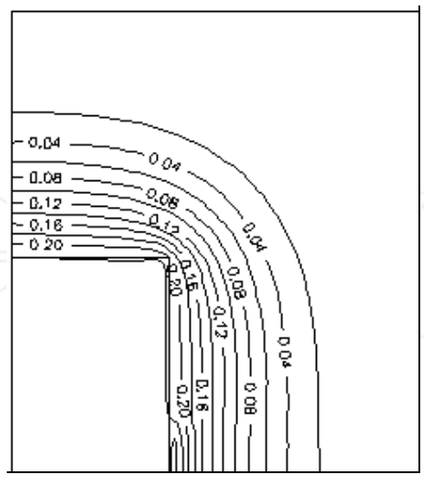

Fig. 15. Distribution of function U for time 6 minutes.

Now, the considerations concerning the continuous casting process will be presented. The goal of work is to apply the sensitivity analysis tool in order to observe the perturbations of casting solidification due to the perturbations of substitute heat transfer coefficient in primary cooling zone of CCT installation. The basic energy equation describing the thermal processes in the domain of vertical, rectangular cast slab can be written in the form

$$C(T)\left[\frac{\partial T}{\partial t}+w\frac{\partial T}{\partial z}\right]=\frac{\partial}{\partial x}\left[\lambda(T)\frac{\partial T}{\partial x}\right]+\frac{\partial}{\partial y}\left[\lambda(T)\frac{\partial T}{\partial y}\right]+\frac{\partial}{\partial z}\left[\lambda(T)\frac{\partial T}{\partial z}\right] \tag{80}$$

where $T = T(x, y, z, t)$, w is the pulling rate – the cast slab shifts in z direction (see: Figure 16).

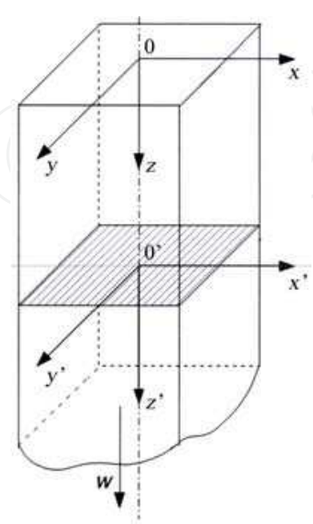

Fig. 16. Vertical continuous casting.

The boundary conditions on the lateral surface of cast slab (the continuous casting mould region) are assumed in the form

$$-\lambda(T)\frac{\partial T}{\partial n}=\alpha(T-T_w) \tag{81}$$

where α is the substitute heat transfer coefficient, T_w is the cooling water temperature. On the upper surface of the casting (free surface of molten metal) the boundary condition of the 1st type (pouring temperature) can be taken into account. On the conventionally assumed bottom surface limiting the domain considered we can put $\partial T/\partial n = 0$, this means the adiabatic condition.

The initial condition resolves itself into the assumption, that a certain layer of molten metal directly over the starter bar has a pouring temperature T_p. The starter bar allows to shut the continuous casting mould during the plant starting.

The numerous experiments show that conductional component of heat transfer corresponding to the direction of cast strand displacement is very small (in the case of steel castings this component constitutes about 5% of the heat conducted from the axis to the lateral surfaces). So, the equation (80) can be simplified to the 2D one. Let we rewrite this equation using the coordinate system 'tied' to a certain section of shifting casting, namely $x'=x,\ y'=y,\ z'=z-wt$. It is easy to check up that we 'lose' in energy equation the component $\partial T/\partial z$ and we obtain

$$C(T)\ \frac{\partial T}{\partial t}\ =\ \frac{\partial}{\partial x'}\left[\lambda(T)\frac{\partial T}{\partial x'}\right]+\ \frac{\partial}{\partial y'}\left[\lambda(T)\ \frac{\partial T}{\partial y'}\right] \tag{82}$$

This approach is called 'a wandering cross section method' (Mochnacki & Suchy, 1995). We consider the lateral section of the cast strand which position at the moment $t = 0$ corresponds to $z = 0$ (the initial condition has a form $T(0) = T_p$), while the boundary conditions on the periphery of this section are the functions of time. If Δt_1 corresponds to the 'hold time' of the section in the continuous casting mould region, then for $0 \le t \le \Delta t_1$ on the casting periphery the boundary condition for the primary cooling zone (e.g., heat flux) is assumed. For the next interval Δt_2 we consider the boundary condition characterizing the heat transfer in the 1st sector of the secondary cooling zone etc.

In order to construct the sensitivity model respect to α we differentiate the governing equations over this parameter (a direct approach is applied)

$$\begin{gathered}\frac{\mathrm{d}C(T)}{\mathrm{d}T}U\frac{\partial T}{\partial t}+C(T)\frac{\partial U}{\partial t}=\\ \frac{\partial}{\partial x}\left[\frac{\mathrm{d}\lambda(T)}{\mathrm{d}T}U\frac{\partial T}{\partial x}+\lambda(T)\frac{\partial U}{\partial x}\right]+\frac{\partial}{\partial y}\left[\frac{\mathrm{d}\lambda(T)}{\mathrm{d}T}U\frac{\partial T}{\partial x}+\lambda(T)\frac{\partial U}{\partial x}\right]+\end{gathered} \tag{83}$$

In equation (83) one substitutes again $x' = x$, $y' = y$, symbol $\partial T/\partial\alpha = U$ denotes the sensitivity function.

Differentiating the condition (81) one has

$$-\lambda\frac{\partial U}{\partial n}=T-T_w+\alpha U \tag{84}$$

The initial condition takes a form: $U(x, y, 0) = 0$.
As an example the following task is presented. The rectangular steel slab (0.44%C) with dimensions 0.6×0.2 m is considered. The pouring temperature equals 1550°C, pulling rate: $w = 0.017$ m/s] The basic heat transfer coefficient in the primary cooling zone equals $\alpha = 1500$ [W/m²K]. The temperature field at the distance 0.6 m from upper surface of the slab has been observed. The precise results will be shown below. For the nodes located near the corner of cast slab the nodal temperatures for $\alpha = 1500$ are collected on the left side of the page. The temperatures found directly for $\alpha = 1700$ are written in the middle of this page, while on the right side one can find the temperatures for $\alpha = 1700$ obtained on the basis of the sensitivity analysis and Taylor series:

925 883 812 812	858 815 741 741	855 814 740 740
1259 1201 1046 812	1216 1155 986 741	1214 1155 987 740
1496 1478 1201 883	1492 1468 1155 816	1493 1471 1155 814
1512 1496 1259 925	1510 1492 1216 858	1510 1493 1215 855

The sensitivity analysis constitutes also the essential tool of inverse problems solution, in particular when the minimum of functional (corresponding to the least squares criterion) is searched using the gradient methods. The problems connected with the inverse methods applications in the thermal theory of foundry processes can be found, among others, in (Majchrzak et al., 2007; Majchrzak et al., 2008a; Majchrzak & Mendakiewicz 2009; Mochnacki & Majchrzak, 2006; Mendakiewicz, 2008; Majchrzak & Mendakiewicz, 2007; Majchrzak et al., 2008b; Majchrzak et al., 2008c).
In this chapter only the part of problems connected with the solidification process modeling has been presented because the subject-matter discussed is very extensive. It also the reason that the references contain mainly the papers prepared by the author of this chapter and his co-workers.

6. References

Stefanescu, D.M. (1999). Critical review of the second generation of solidification models for casting, *Modelling of Casting, Welding and Advanced Solidification Processes VI*. The Minerals, Metals and Materials Society 1999, pp. 3-20.

Mochnacki, B. & Majchrzak, E. (2007a). Identification of macro and micro parameters in solidification model, *Bulletin of the Polish Academy of Sciences, Technical Sciences*, Vol. 55, No. 1, 2007, pp. 107-113.

Mochnacki, B. & Suchy, J. S. (1995). *Numerical methods in computations of foundry processes*, PFTA, Cracow, Poland.

Szopa, R. (1999). Modelling of solidification using the combined variant of the BEM, *Metallurgy, Publ. of the Silesian Univ. of Technology*, Gliwice, Poland.

Mochnacki, B., Majchrzak, E., Szopa, R. & Suchy, J.S. (2006). Inverse problems in the thermal theory of foundry, *Scientific Research of the Institute of Mathematics and Computer Science*, Czestochowa, 1(5), pp. 154-179.

Majchrzak, E. & Mochnacki, B. (2007). Identification of thermal properties of the system casting - mould, *Materials Science Forum*, Vols. 539-543, pp. 2491-2496.

Majchrzak, E. & Mochnacki, B. (1995). Application of the BEM in the thermal theory of foundry, *Engineering Analysis with Boundary Elements*, Vol. 16, pp. 99-121.

Majchrzak, E. & Mendakiewicz, J. (1993). Application of the generalized alternating phase truncation method for numerical modelling of cast iron solidification, *Solidification of Metals and Alloys*, Vol. 18, pp. 103-112.

Majchrzak, E., Suchy, J. S. & Szopa, R. (2006). Linear model of crystallization. Identification of nuclei density, *Giessereiforschung, International Foundry Research*, Vol. 2, pp. 29-32.

Mochnacki, B. & Szopa, R. (2007) Model of pure metal solidification using the power-type function, *Journal of Achievements in Materials and Manufacturing Engineering*, Vol. 22, pp. 65-71.

Fraś, E., Kapturkiewicz, W. & Lopez, H.F. (1993). Macro and micro modelling of the solidification kinetics of casting, *AFS Transactions*, Vol. 48-92, pp. 583-591.

Lupa, M., Szopa, R. & Wojciechowska, W. (2004). Sensitivity analysis of crystallization with respect internal parameters, *Scientific Research of the Institute of Mathematics and Computer Science*, 1(3), pp. 91-98.

Mochnacki, B. & Szopa, R. (2010). Generalized micro/macro model of crystallization and its numerical realization, *Journal for Multiscale Computational Engineering*, 8(3), pp. 259-266.

Majchrzak, E. & Piasecka, A. (1997). Numerical micro/macro model of solidification process, *Journal of Materials Processing Technology*, Vol. 64, pp. 267-276.

Domański, Z., Ciesielski, M. & Mochnacki, B. (2009a). Voronoi tessellations description of cast composite solidification process, *World Congress on Engineering 2009, Lecture Notes in Engineering and Computer Science*, Vol. 2, pp. 1197-1201.

Domański, Z., Ciesielski, M. & Mochnacki, B. (2009b). Applicatiom of CVM using the Voronoi tesselation in numerical modelling of solidification process, *Current Themes in Engineering Science 2009*. Ed. M. Korsunsky, American Institute of Physics, Melville, New York, pp. 17-27.

Mochnacki, B. & Ciesielski, M. (2007). Micro/macro model of solidification. Numerical simulation using the control volume method, *17th International Conference on Computer Methods in Mechanics CMM-2007*, CD ROM Proceedings, ISBN-978-83-923982-3-3.

Brebbia, C.A., Telles, J.C.F. & Wrobel, L.C. (1984). *Boundary Element Techniques*, Springer-Verlag.

Brebbia, C.A. & Dominguez, J. (1992). *Boundary elements, an introductory course*, Computational Mechanics Publications, McGraw-Hill Book Company, London.

Majchrzak, E. (2001). *Boundary element method in heat transfer*, Publication of the Czestochowa University of Technology, Czestochowa, Poland (in Polish).

Majchrzak, E. & Mochnacki, B. (1996). The BEM application for numerical solution of non-steady and non-linear thermal diffusion problems, *Computer Assisted Mechanics and Engineering Sciences*, Vol. 3, No. 4, pp. 327-346.

Majchrzak, E. & Szopa, R. (2001). Analysis of thermal processes in solidifying casting using the combined variant of the BEM, *Journal of Materials Processing Technology*, Vol. 109, pp. 126-132.

Mochnacki, B. & Majchrzak, E. (2007b). Application of the shape sensitivity analysis in numerical modelling of solidification process, *Materials Science Forum*, Vols. 539-543, pp. 2524-2529.

Mochnacki, B. & Szopa, R. (2008). Generalization of temporary temperature field correction method in numerical modelling of solidification, *Archives of Foundry Engineering*, Vol. 8, No. 1, pp. 219-222.

Mochnacki, B. & Majchrzak, E. (2010). Numerical modeling of casting solidification using generalized finite difference method, *Materials Science Forum*, Vols. 638-642, pp. 2676-2681.

Mochnacki, B. & Szopa, R. (1998). Application of the boundary element method in numerical modelling of solidification – Part I. The One Domain Approach, *Journal of Theoretical and Applied Mechanics*, Vol. 2, No. 36, pp. 457-468.

Mochnacki, B. & Szopa, R. (2002). Numerical modelling of heat transfer in spherical domains by mean of the BEM using discretization on time, *Journal of Theoretical and Applied Mechanics*, Vol. 2, No. 40, pp. 357-370.

Kleiber, M. (1997). *Parameter Sensitivity in Nonlinear Mechanics*, J. Wiley & Sons Ltd., Chichester, England.

Dems, K. & Rousselet, B. (1999). *Structural Optimization*, Vol. 17, pp. 36-45.

Szopa, R. (2005). The parametric sensitivity analysis of solidification process, *Archives of Foundry*, Vol. 5, No. 15, pp. 395-404.

Szopa, R. & Wojciechowska, W. (2003). Sensitivity analysis of solidification process with respect to grains geometry, *Archives of Foundry*, Vol. 3, No 10, pp. 255-260.

Szopa, R., Siedlecki, J. & Wojciechowska, W. (2004). The influence of initial conditions on the course of solidification process, *Scientific Research of the Institute of Mathematics and Computer Science*, 1(3), pp. 201-208.

Mochnacki, B. & Szopa, R. (2009). Application of sensitivity analysis in numerical simulation of solidification process, In: *Progress of Foundry Theory and Practice*, Pol. Ac. of Sciences, pp. 271-286.

Majchrzak, E., Dziewonski, M. & Kaluza, G. (2007). Identification of cast steel latent heat by means of gradient method, *Int. J. Computational Materials Science and Surface Engineering*, Vol. 1, No. 5, pp. 555-570.

Majchrzak, E., Mochnacki, B. & Suchy, J.S. (2008a). Identification of substitute thermal capacity of solidifying alloy, *Journal of Theoretical and Applied Mechanics*, Vol. 46, No. 2, pp. 257-268.

Majchrzak, E. & Mendakiewicz, J. (2009). Identification of cast steel latent heat on a basis of thermal and difference analysis, *Computer Methods in Material Science*, Vol. 9, No. 2, pp. 195-199.

Mochnacki, B. & Majchrzak, E. (2006). The methods of inverse problems solution in the thermal theory of foundry processes, In: *Research in Polish Metallurgy at the beginning of XXI century*, Ed. K. Świątkowski, Committee of Metallurgy of the Polish Academy of Sciences, pp. 239-254.

Mendakiewicz, J. (2008). Application of identification methods in solidification process modelling, *Archives of Foundry Engineering*, Vol. 8, No. 1, pp. 203-210.

Majchrzak, E. & Mendakiewicz, J. (2007). Gradient method of cast iron latent heat identification, *Archives of Foundry Engineering*, Vol. 7, No. 4, pp. 121-126.

Majchrzak, E., Mochnacki, B. & Suchy, J.S. (2008b). Estimation of boundary heat flux between casting and mould using the global function specification method, *Archives of Foundry Engineering*, Vol. 8, No. 1, pp. 193-198.

Majchrzak, E., Mochnacki, B., Dziewoński, M. & Jasiński, M. (2008c). Identification of boundary heat flux on the continuous casting surface, *Archives of Foundry Engineering*, Vol. 8, No. 4, pp. 105-110.

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Computational Simulations and Applications

Edited by Dr. Jianping Zhu

ISBN 978-953-307-430-6

Hard cover, 560 pages

Publisher InTech

Published online 26, October, 2011

Published in print edition October, 2011

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