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NUMERICAL MODEL OF BINARY ALLOYS SOLIDIFICATION BASING ON THE ONE DOMAIN APPROACH AND THE SIMPLE MACROSEGREGATION MODELS

MODEL NUMERYCZNY KRZEPNIĘCIA STOPÓW DWUSKŁADNIKOWYCH Z WYKORZYSTANIEM METODY JEDNEGO OBSZARU I PROSTYCH MODELI MAKROSEGREGACJI

In the paper the thermal processes proceeding in the domain of solidifying binary alloy are considered. The mathematical model of solidification and cooling processes bases on the one domain method (or fixed domain method). In such a model the parameter called a substitute thermal capacity (STC) appears. At the stage of STC construction the macrosegregation process described by the lever arm rule or the Scheil model is taken into account. In this way one obtains the formulas determining the course of STC resulting from the certain physical considerations and this approach seems to be closer to the real course of thermal processes proceeding in domain of solidifying alloy. In the final part the examples of numerical solutions basing on the finite difference method are presented.

Keywords: alloys solidification, one domain approach, macrosegregation process, substitute thermal capacity, numerical modeling.

W pracy rozpatruje się procesy cieplne zachodzące w obszarze krzepnącego i stygnącego stopu dwuskładnikowego. Model matematyczny tych procesów bazuje na podejściu nazywanym metodą jednego obszaru. W modelach tego typu pojawia się parametr nazywany zastępczą pojemnością cieplną. Na etapie jej definiowania autorzy uwzględnili proste modele makrosegregacji wynikające z reguły dźwigni i znanego modelu Scheila. Otrzymane zależności determinujące przebiegi pojemności zastępczej na podstawie pewnych rozważań fizycznych wydają się lepiej przybliżać rzeczywisty przebieg procesów cieplnych zachodzących w obszarze krzepnącego stopu. W końcowej części pracy pokazano wyniki rozwiązań numerycznych uzyskanych przy wykorzystaniu metody różnic skończonych.

1. Introduction

Numerical computations of macroscopic thermal processes proceeding in the domain of solidifying casting are based on the different mathematical models. In the case of alloys, however, the most effective approach is connected with the introduction of the model called the one domain method (e.g. [1]). The governing equation corresponding to the one domain method contains the parameter called a substitute thermal capacity (STC). The function describing STC is connected with the function determining the local volumetric fraction f_S of solid state between border temperatures corresponding to the beginning and the end of solidification process. So, the capacity of source function controlling the solidification process is proportional to the time derivative of f_S and if one assumes the knowledge of the function $f_S = f_S(T)$ (T denotes a temperature) then after the mathematical manipulations the STC can be defined. Such approach is, among others, presented in [2,3].

Substitute thermal capacity can be also defined directly omitting the function f_S (or f_L). The general form of STC is assumed arbitrary, while the parameters appearing in this function can be found using the required conditions, among others, the integration of STC between border temperatures should correspond to the change of physical enthalpy due to the cooling and solidification processes proceeding in the mushy zone domain [4,5,6].

The alloy solidification process is accompanied by the changes in the chemical composition of the molten and solidified

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parts of the casting (macrosegregation).The macro model of this phenomenon is based on the system of two partial differential equations (the diffusion equations) supplemented by the boundary condition on the moving boundary and the remaining boundary and initial conditions [7]. Different simplifications are often accepted at the stage of segregation process modelling. For example, the diffusion process in the solid state is neglected, while the changes in concentration of alloying component in the molten metal takes place only in the layer close to the solidification front, in the remaining liquid sub-domain the concentration is aligned [8,9]. The further simplification of this model is the assumption that the concentration field in domain of molten metal can be approximated by the broken line (a broken line model [10]). The other approach to the macrosegregation modeling results from the assumption that the diffusion coefficients for the liquid and solid state are infinitely large (the lever arm model) or that the diffusion coefficient of solid is equal to zero, while the same coefficient of liquid is almost limitless (the Scheil model). The models above discussed concern the segregation process proceeding in the macroscale. In literature one can also find the models basing on some different approach and concerning the microscale processes. As an example one can mention the papers [11-15].

2. One domain method

Let us consider the following energy equation

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

where $c(T)$ is a volumetric specific heat of casting material, $\lambda(T)$ is a thermal conductivity, L is a volumetric latent heat, $T = T(x,t)$, $f_S = f_S(x,t)$ are the temperature and the local volumetric fraction of solid state, x, t are the spatial co-ordinates and time.

We denote the temperatures corresponding to the beginning and the end of solidification process by T_L and T_S. The energy equation corresponding to the one domain approach results from the assumption that the temperature-dependent function $f_S(T)$ in the interval $[T_S, T_L]$ is known. Then

$$\frac{\partial f_S(x,t)}{\partial t} = \frac{d f_S(T)}{d T}\frac{\partial T(x,t)}{\partial t} \qquad (2)$$

Introducing this formula to energy equation (1) one obtains

$$C(T)\frac{\partial T(x,t)}{\partial t} = \nabla\left[\lambda(T)\nabla T(x,t)\right] \qquad (3)$$

where the parameter

$$C(T) = c(T) - L\frac{d f_S(T)}{d T} = c(T) + L\frac{d f_L(T)}{d T} \qquad (4)$$

is called 'a substitute thermal capacity', while $f_L = 1 - f_S$ is the local liquid state fraction in the neighborhood of the point considered. One can see that for $T < T_S: f_S = 0$, while for $T > T_L: f_S = 1$ and then the derivatives $d f_S / d T = 0$. Summing up, the following definition of substitute thermal capacity can be accepted [2,3]

$$C(T) = \begin{cases} c_L & T > T_L \\ c_P - L\dfrac{d f_S(T)}{d T} & T_S \leq T \leq T_L \\ c_S & T < T_S \end{cases} \qquad (5)$$

or

$$C(T) = \begin{cases} c_L & T > T_L \\ c_P + L\dfrac{d f_L(T)}{d T} & T_S \leq T \leq T_L \\ c_S & T < T_S \end{cases} \qquad (6)$$

where c_L, c_P, c_S are the volumetric specific heats of molten metal, mushy zone and solid state sub-domains. One can see, that the equation (3) can be used as the model of thermal processes proceeding in the whole, conventionally homogeneous, casting domain. The function $f_S(T)$ in the interval $[T_S, T_L]$ should be monotonic, decreasing and from the scope from 1 to 0. One can construct the large number of such functions, of course, and this approach leads to the purely mathematical hypotheses concerning the course of function f_S (see: [16]). For example the following function

$$f_S(T) = \left(\frac{T_L - T}{T_L - T_S}\right)^n \qquad (7)$$

can be considered. The formula (7) fulfils all necessary conditions imposed on the course of function $f_S(T)$ and then

$$C(T) = c_P + \frac{L}{T_L - T_S}\,n\left(\frac{T_L - T}{T_L - T_S}\right)^{n-1} \qquad (8)$$

The quotient $L/(T_L - T_S) = c_{sp}$ is called 'a spectral latent heat'. Above formula is very often used for the case $n = 1$ (e.g. [3]), then

$$C(T) = c_P + \frac{L}{T_L - T_S} = c_P + c_{sp}, \quad T \in [T_S, T_L] \qquad (9)$$

In literature one can find also the other way of $C(T)$ construction. The mathematical form of substitute thermal capacity is assumed a'priori and the function proposed must fulfill the condition resulting from the change of physical enthalpy in the interval $[T_S, T_L]$, namely

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

As an example the 'bell type' function describing the substitute thermal capacity for $[T_S, T_L]$ is considered [5,6]. The adequate fourth-degree polynomial fulfils the condition (10), additionally $C(T_S) = c_S$, $C(T_L) = c_L$ and the derivatives of $C(T)$ at the points T_S and T_L are equal to 0. In Figure 1 the course of STC for carbon steel (0.44%C) is shown [5].

One can see, that the function shown in Figure 1 is continuous and differentiable which is important in the case of considerations requiring the knowledge of derivative $d C(T)/d T$ (e.g. sensitivity analysis).
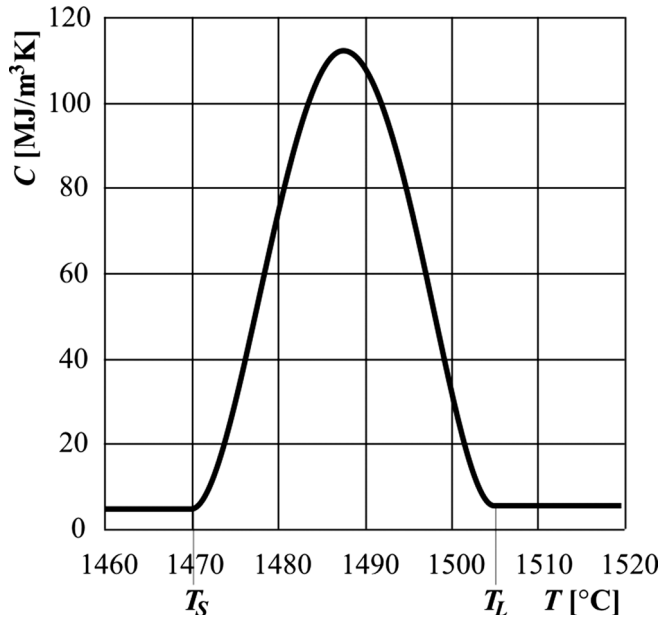
Fig. 1. Bell type approximation of STC

The typical mathematical model of the real foundry technology requires the supplement of equation (3) by the equation determining the course of thermal processes in a mould sub-domain, in particular

$$c_m(T)\frac{\partial T_m(x,t)}{\partial t} = \nabla\left[\lambda_m(T)\,\nabla T_m(x,t)\right] \qquad (11)$$

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

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

$$-\lambda_m\frac{\partial T_m(x,t)}{\partial n} = \alpha\left[T_m(x,t) - T_a\right] \qquad (12)$$

is, as a rule, accepted. In formula (12) 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

$$-\lambda\frac{\partial T(x,t)}{\partial n} = \frac{T(x,t) - T_m(x,t)}{R(x,t)} = -\lambda_m\frac{\partial T_m(x,t)}{\partial n} \qquad (13)$$

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

$$\begin{cases} -\lambda\dfrac{\partial T(x,t)}{\partial n} = -\lambda_m\dfrac{\partial T_m(x,t)}{\partial n} \\ T(x,t) = T_m(x,t) \end{cases} \qquad (14)$$

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

$$t = 0: \quad T(x,0) = T_{p0}(x), \quad T_m(x,0) = T_{pm0}(x) \qquad (15)$$

The mathematical model presented above can be more complicated. One can consider the convectional component of heat transfer which appears in the molten metal sub-domain. The phase changes occurring in the solid state, the segregation effects etc. can be also taken into account. Generally speaking, the model above presented belongs to the group of macro models of solidification.

3. Simplified macrosegregation models and definitions of STC

The macrosegregation models discussed in this chapter correspond to the assumptions leading to the formulas determining the values $f_L(z_L)$ when the diffusion coefficients of solid and liquid tend to infinity (the lever arm model) or the diffusion coefficient for liquid also tends to infinity, while the diffusion coefficient of solid is equal to zero (the Scheil model). Both models constitute the quite good aproximation of the macrosegregation processes proceeding in the conditions of volumetric solidification. Presented below considerations are based on the mass balances of alloy component. For two successive time levels t and $t + \Delta t$ one has the following form of mass balance

$$\begin{aligned} &\rho_S V_S(t)\,z_S(t) + \rho_L V_L(t)\,z_L(t) = \\ &\rho_S V_S(t+\Delta t)\,z_S(t+\Delta t) + \rho_L V_L(t+\Delta t)\,z_L(t+\Delta t) \end{aligned} \qquad (16)$$

where z_S, z_L are the concentrations of alloy component in the solid and liquid phases, ρ_S, ρ_L are the mass densities.

The values of V_S, V_L and z_S, z_L for time $t + \Delta t$ one can find using the Taylor series (only the first derivatives are taken into account)

$$V_S(t+\Delta t) = V_S(t) + \frac{dV_S}{dt}\Delta t \qquad (17)$$

$$V_L(t+\Delta t) = V_L(t) + \frac{dV_L}{dt}\Delta t \qquad (18)$$

and

$$z_S(t+\Delta t) = z_S(t) + \frac{dz_S}{dt}\Delta t \qquad (19)$$

$$z_L(t+\Delta t) = z_L(t) + \frac{dz_L}{dt}\Delta t \qquad (20)$$

Introducing formulas (17) – (20) to (16) and neglecting the terms containing Δt^2 one obtains

$$\rho_S V_S\frac{dz_S}{dt} + \frac{dV_S}{dt}\rho_S z_S + \rho_L V_L\frac{dz_L}{dt} + \frac{dV_L}{dt}\rho_L z_L = 0 \qquad (21)$$

or, taking into account the definitions of f_S and f_L

$$\rho_S f_S\frac{dz_S}{dt} + \frac{df_S}{dt}\rho_S z_S + \rho_L f_L\frac{dz_L}{dt} + \frac{df_L}{dt}\rho_L z_L = 0 \qquad (22)$$

We multiply the equation (22) by Δt. Next we introduce the definition of partition coefficient $k = z_S/z_L$ and the dependence $f_S = 1 - f_L$. Then

$$\rho_S(1-f_L)k - \frac{df_L}{dz_L}\rho_S k z_L + \rho_L f_L + \frac{df_L}{dz_L}\rho_L z_L = 0 \qquad (23)$$

Finally after not very complex mathematical manipulations one obtains

$$\frac{df_L}{dz_L} + \frac{f_L}{z_L} = -\frac{k\rho_S}{\rho_L - k\rho_S} \cdot \frac{1}{z_L} \tag{24}$$

The analytical solution of equation (24) is found under the assumption that the partition coefficient is a constant value (the lines T_S and T_L on the equilibrium diagram are the straight ones and they start from the same point T_P, see: considerations presented below). The equation (24) is a linear one and it should be solved for the condition $z = z_0 : f_L = 1$. Finally

$$f_L = \frac{\rho_L z_0 - \rho_S k z_L}{(\rho_L - \rho_S k) z_L} \tag{25}$$

For the same values of mass densities the last equation takes a form

$$f_L = \frac{z_0 - k z_L}{(1-k) z_L} \tag{26}$$

Knowledge of the function $f_L(z_L)$ allows one to determine the course of STC. So, the straight lines determining the dependencies $T_S(z_S)$ and $T_L(z_L)$ are of the form

$$\begin{aligned} T_L &= T_P + a_L z_L \\ T_S &= T_P + a_S z_S \end{aligned} \tag{27}$$

where T_p is a solidification point of pure metal, a_L and a_S are the slopes of appropriate border lines. Then

$$\begin{aligned} z_L &= \frac{T_L - T_P}{a_L} \\ z_0 &= \frac{T_0 - T_P}{a_L} \end{aligned} \tag{28}$$

where T_0 is the temperature corresponding to the concentration z_0. Because

$$\frac{df_L}{dT} = \frac{df_L}{dz_L}\frac{dz_L}{dT} = -\frac{\rho_L z_0}{(\rho_L - \rho_S k)z_L^2}\frac{1}{a_L} \tag{29}$$

consequently

$$C(T) = c_P - \frac{\rho_L z_0}{(\rho_L - \rho_S k)z_L^2}\frac{L}{a_L} \tag{30}$$

or introducing in a place of concentration the dependencies (28) and assuming $\rho_L = \rho_S$ one obtains

$$C(T) = c_P + \frac{L(T_P - T_0)}{(1-k)(T_P - T_L)^2} \tag{31}$$

We can also assume that in equation (22) the derivative $\frac{dz_S}{dt} = 0$ and then the considerations similar as previously lead to the differential equation corresponding to the Scheil model. The solution of this equation for $\rho_L = \rho_S$ is the following

$$f_L = \left(\frac{z_0}{z_L}\right)^{\frac{1}{1-k}} \tag{32}$$

while

$$C(T) = c_p + \frac{L}{(1-k)(T_p - T_0)}\left(\frac{T_p - T_0}{T_p - T_L}\right)^{\frac{2-k}{1-k}} \tag{33}$$

4. Examples of computations

The cylindrical casting (cast carbon steel – 0.44%C, $H = 0.08$ m, $R = 0.02$ m) made in the typical sand mould is considered – Figure 2. Thermophysical parameters of casting and mould materials are the following: $c_S = 4.875$ MJ/(m³K), $c_L = 5.904$ MJ/(m³K), $c_P = 5.39$ MJ/(m³K), $L = 1985$ MJ/m³, $\lambda_S = 35$ W/(mK), $\lambda_L = 20$ W/(mK), $\lambda_P = 27.5$ W/(mK), $T_P = 1535$°C, $T_L = 1505$°C, $k = 0.465$, $c_m = 1.75$ MJ/m³, $\lambda_m = 1$ W/(mK). Initial temperature of casting domain equals 1550°C, while the initial temperature of mould equals 30°C. The thickness of mould is large enough that on the external boundary one can assume the no-flux condition, in other words the coefficient α in equation (12) is equal to zero.
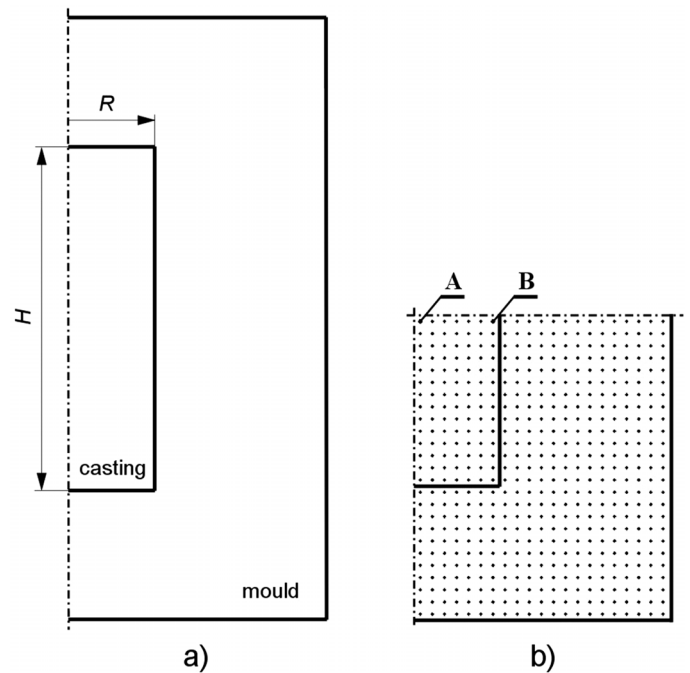

Fig. 2. Casting and mould, differential mesh

At the stage of numerical modeling the variant of finite difference method discussed in [16,17] has been used. The uniform differential mesh was created by 900 nodes (30×30), $h = 0.002$ m, time step was equal to 0.05 s.

In Figure 3 the cooling curves at the points A, B, C selected from the casting domain are shown. Both the solutions corresponding to the lever arm model and the Scheil one are shown. At the final stages of solidification process the differences are visible. This problem will be discussed in the next chapter.
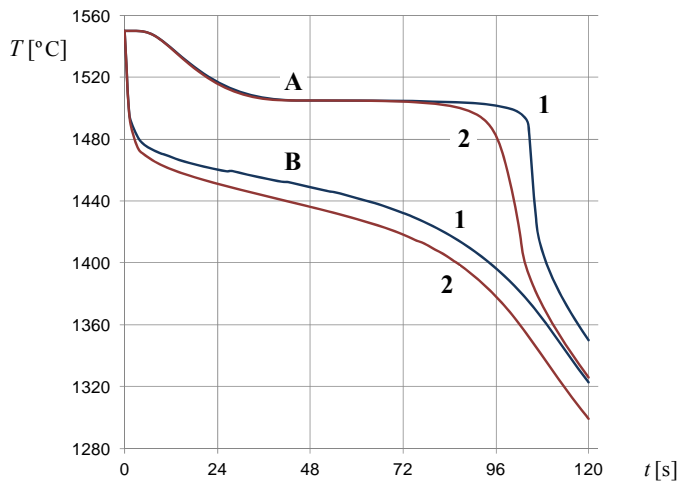
Fig. 3. Cooling curves at the points A and B, 1 – lever-arm model, 2 – Scheil model

5. Final remarks

The subject of the paper is connected with the application of numerical methods for the analysis of thermal processes proceeding in the solidifying binary alloy. The mathematical model is based on the one domain method, while the substitute thermal capacities result from the simple macrosegregation models (the lever arm rule and the Scheil model). The results obtained are somewhat different. It results, first of all, from the fact that in the case of Scheil model the value of the function f_L has never reach 0. So, the authors assumed that the end of solidification process takes place when $f_L < 0.05$. This assumption allows one to find the temperature assuring the fulfillment of integral condition (10). Despite the fact that this condition was satisfied, however, non-zero final value of f_L may cause the disturbances in the final stages of solidification modeling. Such problems did not occur in the case of complete mixing model. At the stage of numerical computations the FDM has been used, in the case of more complex shape of casting the generalized version of the FDM [18] can be also applied.

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