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SIMPLIFIED MODELS OF MACROSEGREGATION

Bohdan Mochnacki

Institute of Mathematics and Computer Science, Technical University of Częstochowa
e-mail: moch@imi.pcz.pl

Józef S. Suchy

Department of Foundry Processes Modelling, AGH, Cracow
e-mail: jsuchy@agh.edu.pl

The macrosegregation process takes place during typical solidification of alloys. Fractions of alloy components in a liquid and solid sub-domains are time-dependent and determined by the course of border lines on the equilibrium diagram. From the mathematical point of view, the process is described by a system of partial differential equations (diffusion equations) and boundary-initial conditions. The process is coupled with the solidification one. In this paper, simplified models of macrosegregation are discussed. The volumetric solidification and the 'sharp' solid-liquid interface are considered. Examples of computations are also shown. It seems that for practical applications, the methods proposed are sufficiently exact. Additionally, they are very simple for numerical realization.

Key words: macrosegregation, solidification, numerical simulation

1. Introduction

The proceeding of a macrosegregation process in the casting domain is described by a system of equations in the form (Crank, 1984)

$$x \in \Omega_m \ : \qquad \frac{\partial z_m(x,t)}{\partial t} = \nabla[D_m \nabla z_m(x,t)] \tag{1.1}$$

where $m = 1, 2$ correspond to the liquid and solid sub-domains, $z_m(x,t)$ is the alloy component concentration, D_m – diffusion coefficient, x, t – spatial co-ordinate and time.

On the moving boundary Γ_{12} limiting the liquid and solid sub-domains, the following boundary condition is given (Fraś, 1992; Majchrzak *et al.*, 1998)

$$D_2 \frac{\partial z_2(x,t)}{\partial n}\Big|_{x=\xi} - D_1 \frac{\partial z_1(x,t)}{\partial n}\Big|_{x=\xi} = (1-k)\frac{d\xi}{dt} z_1(\xi,t) \tag{1.2}$$

where $\partial/\partial n$ denotes the normal derivative, $x = \xi$ is the solid-liquid interface, $k = z_2/z_1$ is the partition coefficient. It should be pointed out that the solidification rate $d\xi/dt$ results from the solution of the solidification model. The position of ξ corresponds to the liquid border temperature T_L or to the equivalent solidification point defined as follows

$$T^* = \frac{\int\limits_{T_S}^{T_L} C(T)T\, dT}{\int\limits_{T_S}^{T_L} C(T)\, dT} \tag{1.3}$$

where T_S is the temperature corresponding to the end of solidification, $C(T)$ is the substitute thermal capacity of the alloy (Mochnacki and Majchrzak, 1995; Mochnacki and Suchy, 1997).

On the outer surface of the system, the no-flux condition is accepted. This means

$$x \in \Gamma_0 \; : \qquad \frac{\partial z_2(x,t)}{\partial n} = 0 \tag{1.4}$$

Additionally, for time $t = 0$: $z_1(x,0) = z_0$.

The model presented can be useful if we describe the alloy solidification using the classical Stefan approach (Mochnacki and Suchy, 1995) because the position of solid-liquid interface and solidification rate must be known (see: Crank, 1984; Mochnacki and Suchy, 1995). On the other hand, however, the solidification proceeds in an interval of temperature and the Stefan model concerning pure metals is not entirely acceptable.

The obtainment of numerical solution to the problem presented is possible, of course, but taking into account mutual connections between the solidification and macrosegregation models, the task is rather complex. Additionally, as was mentioned, the temporary position of the solid-liquid interface must be known, in other words we can consider the process in which the 'sharp' solidification front is generated. In the case of volumetric solidification, such an approach to the macrosegregation modelling is useless.

2. The macrosegregation during volumetric solidification

The simplest and the well known criterion determining the type of the solidification is based on the ratio $K = \Delta T/(T_L - T_S)$, where ΔT is the maximum change of temperature in the casting domain. If $K \leqslant 1$ then the 'sharp' front appears, if $K \approx 1$ then the volumetric solidification takes place.

Below the approach based on the lever arm rule and the Scheil models for such a situation will be presented. At first, we assume a constant value of the mass density and then, in the place of mass balances, we can analyze the volume ones.

Let t and $t + \Delta t$ denote two successive levels of time. Then

$$V_2(t)z_2(t) + V_1(t)z_1(t) = V_2(t + \Delta t)z_2(t + \Delta t) + V_1(t + \Delta t)z_1(t + \Delta t) \quad (2.1)$$

Using the Taylor formula, one obtains $(m = 1, 2)$

$$\begin{aligned} V_m(t + \Delta t) &= V_m(t) + \frac{dV_m(t)}{dt}\Delta t \\ z_m(t + \Delta t) &= z_m(t) + \frac{dz_m(t)}{dt}\Delta t \end{aligned} \quad (2.2)$$

Introducing the above formulas to balance (2.1) and neglecting the components containing Δt^2, one arrives at

$$f_2\frac{dz_2}{dt} + \frac{df_2}{dt}z_2 + f_1\frac{dz_1}{dt} + \frac{df_1}{dt}z_1 = 0 \quad (2.3)$$

where

$$f_2(t) = \frac{V_2(t)}{V} \qquad f_1(t) = \frac{V_1(t)}{V} \qquad f_2(t) = 1 - f_1(t) \quad (2.4)$$

Next, introducing the partition coefficient and using the dependence $f_2 = 1 - f_1$, we obtain the final form of the balance equation. It should be solved for the initial condition in the form: $z = z_0$: $f_1 = 1$. Assuming the constant value of the partition coefficient k, we find

$$f_1 = \frac{z_0 - kz_1}{(1 - k)z_1} \quad (2.5)$$

The above solution corresponds to the solution resulting from the well known lever-arm principle, in other words in equations (2.1) $D_1 \to \infty$, $D_2 \to \infty$. The same equation can be used in order to find the solution to the so-called Scheil

model (diffusion in the solid state is neglected, $D_2 = 0$, $D_1 \to \infty$). Let us assume that $dz_2/dt = 0$ and then

$$f_1 = \left(\frac{z_0}{z_1}\right)^{\frac{1}{1-k}} \tag{2.6}$$

The knowledge of temporary $f_1(t)$ in the casting domain (this value results from the solidification model) allows one to determine $z_1(t)$ and next to correct the values of border temperatures T_L and T_S. Solutions (2.5) and (2.6) have been obtained an the assumption that the functions $f_1(t)$ and $f_2(t)$ are uniform in the whole casting domain. In reality, the local values of solid or liquid volumetric fractions can change from 0 to 1. So, a better approach to the mass balances results from the introduction of the control volume approach. The casting domain is divided into n control volumes and then one obtains the following formulas determining temporary values of $z_1(t)$

$$z_1(t) = \frac{V\rho_1 z_0}{k\sum_{i=1}^{n} \Delta V_i \rho_2 f_{2i}(t) + \sum_{i=1}^{n} \Delta V_i \rho_1 [1 - f_{2i}(t)]} \tag{2.7}$$

or

$$z_1(t^p) = \frac{V\rho_L z_0 - \sum_{s=1}^{p-1}\sum_{i=1}^{n} \Delta V_i \rho_2 z_2(t^s)(f_{2i}^s - f_{2i}^{s-1})}{k\sum_{i=1}^{n} \Delta V_i \rho_2 (f_{2i}^p - f_{2i}^{p-1}) + \sum_{i=1}^{n} \Delta V_i \rho_1 (1 - f_{2i}^p)} \tag{2.8}$$

where V is the casting domain, ΔV_i are the control volumes. Additionally, it is assumed that the mass densities of solid and liquid phases are different. Formula (2.7) concerns the lever-arm model, while formula (2.8) concerns the Scheil one. In the case of Scheil approach, we must remember the 'history' of the solidification process and $t^0 = 0, t^1, t^2, \ldots, t^p, \ldots$ denote the points forming the time grid (Majchrzak and Szopa, 1998; Mochnacki *et al.*, 1999).

In the quoted papers, the examples of numerical computations are also presented. As an example, the solidification of spherical casting ($R = 0.05\,\mathrm{m}$) made of Cu-Zn alloy (10%Zn) was considered (Mochnacki *et al.*, 1999). The following thermophysical parameters were introduced there: $\lambda_1 = \lambda_2 = \lambda = 120\,\mathrm{W/(mk)}$, $c_1 = c_2 = c = 390\,\mathrm{J/(kgK)}$, $\rho_1 = \rho_2 = \rho = 8600\,\mathrm{kg/m^3}$, $L_V = 1.63 \cdot 10^6\,\mathrm{kJ/m^3}$ (latent heat), $k = 0.855$, the function $T_L = f(z_1)$ is of the form $T_L = 1083 - 473.68 \cdot z_1$, $T_0(r) = 1080^\circ\mathrm{C}$ (initial temperature), $z_0 = 0.1$ (initial concentration of Zn). On the outer surface of the casting, the Robin condition was assumed (heat transfer coefficient $\alpha = 35\,\mathrm{W/(m^2K)}$, ambient temperature $T^\infty = 0^\circ\mathrm{C}$).

In Figure 1, the kinetics of solidification (the course of $f_2(t)$) is shown. The next figure illustrates the cooling curves for $r = R$ (casting surface), at the same time the numbers 1, 2, 3 correspond to the model without segregation,

lever-arm model and the Scheil one. In Fig. 3, changes of the solidification point are marked.

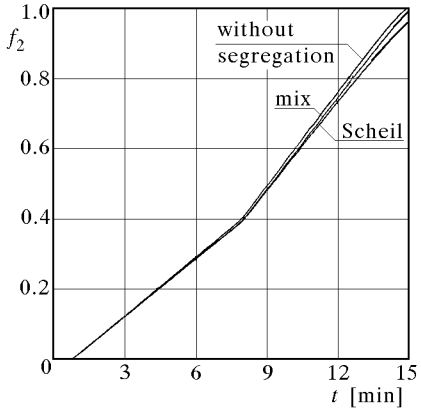

Fig. 1. Kinetics of solidification

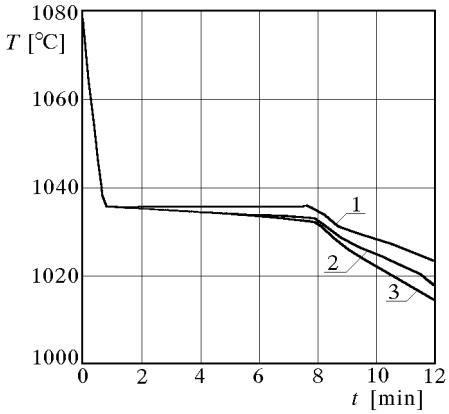

Fig. 2. Cooling curves

3. The models of macrosegregation in the case of 'sharp' interface

In the papers by Mochnacki *et al.* (2003, 2004), Suchy and Mochnacki (2003), the approximation of the alloy concentration in the molten metal subdomain by the broken line aas discussed. The first part of this function corresponds to the boundary layer δ (Suchy, 1983), while the second one corresponds

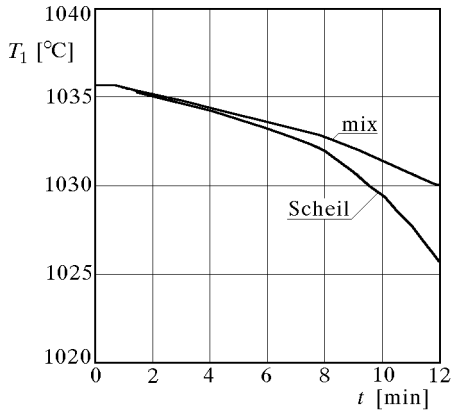

Fig. 3. Changes of the solidification point

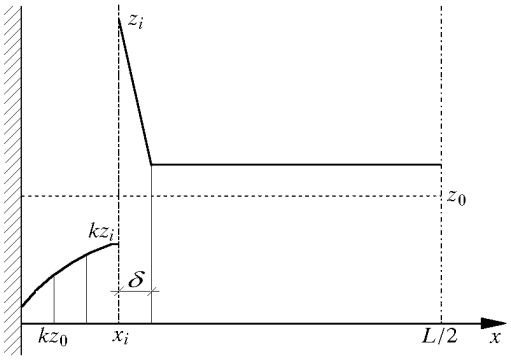

Fig. 4. The broken line model

to the sub-domain in which the convectional mass flow causes equalization of the function z_1 (Fig. 4).

The amount of information concerning the physical aspects of the process (solidification rate, thickness of the boundary layer, etc.) assures the univocal determination of the parameters of the assumed function. The starting point of the algorithm consists in computations of the direction of a sector corresponding to the boundary layer. Next, the mass balance of alloy components allows one to determine other parameters of the broken line model.

We consider the solidification problem for which the temporary position of interface and the function determining its dislocation are known. The mass balance for the neighborhood of the moving boundary leads to condition (2.2).

If the mass transfer in the solid body is neglected ($D_2 = 0$) and a 1D problem (plate of thickness $L/2$) is considered, then

$$-D_1 \frac{\partial z_1(x,t)}{\partial x}\Big|_{x=\xi} = (1-k)\frac{d\xi}{dt} z_1(\xi,t) \tag{3.1}$$

On the basis of the last formula, we determine the slope of the first section of the broken line for $x = \xi$ (ξ is a multiple of the assumed step $\Delta x = h$). Next, on the basis of the balance for time t corresponding to $x = \xi$, namely

$$\int_0^{\xi} z_2(x)\,dx + \int_{\xi}^{\xi+\delta} z_{11}(x)\,dx + z_{12}\Big(\frac{L}{2} - \xi - \delta\Big) = \frac{L}{2} z_0 \tag{3.2}$$

where z_{11} is a linear function approximating the concentration field in the domain of boundary layer, z_{12} is a constant value (see: horizontal sector in Fig. 4), we can calculate the alloy component concentration for $x = \xi$. In this way, the set of parameters determining the course of the broken line is known.

As an example, a plate ($2L = 0.018\,\mathrm{m}$) made of Al-Si alloy ($z_0 = 0.05$) has been considered. The constant solidification rate $d\xi/dt = 2 \cdot 10^{-6}\,\mathrm{m/s}$, partition coefficient: $k = 0.2$, diffusion coefficient: $D_1 = 3.5 \cdot 10^{-8}\,\mathrm{m^2/s}$, thickness of boundary layer $\delta = 0.5,\ 1,\ 1.5\,\mathrm{mm}$ have been assumed, respectively (Suchy, 1983). In Figure 5, changes of the concentration in the liquid state for $x = \xi(t)$ are shown. The solution presented in Fig. 5 shows that the assumption concerning the thickness of the boundary layer does not cause essential differences in the calculated courses of boundary and internal concentrations.

In Figure 6, the concentration profiles for different times are shown. The thickness of the boundary layer equals 1.5 mm.

The solution presented in Figure 7 has been found for variable solidification rate. The well known equation $\xi = \beta\sqrt{t}$ has been taken into account ($\beta = 6.32 \cdot 10^{-5}$) and the solidification rate resulted from differentiation of the formula discussed. From the numerical point of view, such a problem is not more complicated than the problems discussed previously.

Similar considerations can be done in the case of cylindrical or spherical geometry (Mochnacki *et al.*, 2005).

The collocation method presented in Mochnacki and Suchy (1995) can be a base for other segregation model (1D task is also considered). The mathematical description of the process bases on the Fick equation. The mass transfer process in the solidified part of the casting has been neglected, while the domain of liquid metal in which the Fick equation is obligatory corresponds to

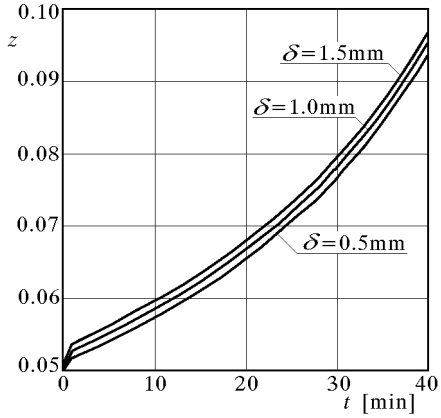

Fig. 5. Concentration for $x = \xi(t)$

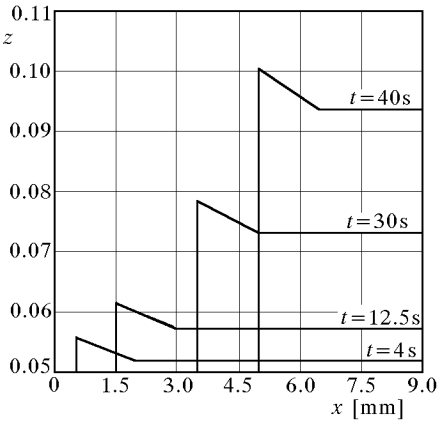

Fig. 6. Concentration ($\delta = 1.5\,\mathrm{mm}$)

a certain layer δ close to the solidification front. For the remaining part of the liquid sub-domain, we assume a constant value of the alloy component concentration. Thus, we have

$$x \in (\xi, \xi + \delta) \; : \qquad \frac{\partial z_1(x,t)}{\partial t} = D_1 \frac{\partial^2 z_1(x,t)}{\partial x^2} \tag{3.3}$$

For $x = \xi$ the condition (3.1) is given.

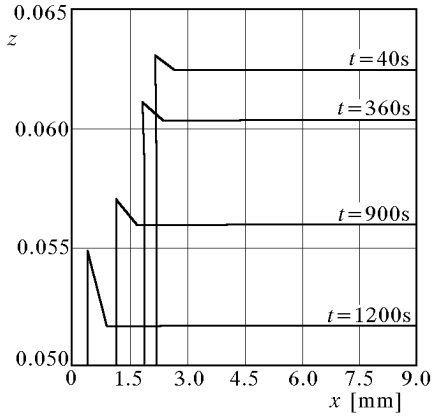

Fig. 7. Concentration field for $v(t)$

In order to assure the constant mass of alloy component, the following condition should be formulated, see (3.2)

$$z_0 \frac{L}{2} = \int_0^{\xi} z_2(x)\, dx + \int_{\xi}^{\xi+\delta} z_1(x,t)\, dx + z_1(\xi+\delta,t)\Big(\frac{L}{2} - \xi - \delta\Big) \tag{3.4}$$

In order to estimate the co-ordinate ξ and the parameter v, one should find a numerical solution to the solidification problem or assume the knowledge of solidification rate.

In this place, the model of solidification based on the control volume method (Mochnacki and Ciesielski, 2002)] can be used. Here, some remarks concerning the model of segregation will be discussed. In the layer δ, we distinguish the set of points $x_0, x_1, \ldots, x_n$. The concentration field for time $t + \Delta t$ is assumed in the form of the algebraic polynomial

$$z_1(x, t+\Delta t) = \sum_{j=0}^{n} a_j x^j \tag{3.5}$$

The first and the second derivatives of (3.5) are equal to

$$\begin{aligned} \frac{dz_1(x,t+\Delta t)}{dx} &= \sum_{j=1}^{n} j a_j x^{j-1} \\ \frac{d^2 z_1(x,t+\Delta t)}{dx^2} &= \sum_{j=2}^{n} j(j-1) a_j x^{j-2} \end{aligned} \tag{3.6}$$

The numerical approximation of the Fick equation for $x = x_2, \ldots, x_{n-1}$ takes a form

$$\sum_{j=0}^{n} a_j x_i^j = z_i(x_i, t) + D_1 \Delta t \sum_{j=2}^{n} j(j-1) a_j x_i^{j-2} \tag{3.7}$$

It should be pointed out that the course of $z_1(x,t)$ is known from the initial or pseudo-initial conditions. For $x = x_0$, we have

$$a_0 \nu (1-k) + D_1 a_1 = 0 \tag{3.8}$$

The mass balance leads to the equation

$$z_0 \frac{L}{2} = \int_0^{\xi} z_2(x)\, dx + \int_{\xi}^{\xi+\delta} \sum_{j=0}^{n} a_j x^j\, dx + z_1(x_n, t+\Delta t)\Big(\frac{L}{2} - \xi - \delta\Big) \tag{3.9}$$

Equations (3.7)-(3.9) create a linear system from which the coefficients a_k can be found. Next, we can define the continuous function $z_1(x, t+\Delta t)$.

As it was mentioned, the broken line model gives the solution in the form of C^0 type. So, the thus obtained function $z_1(t)$ is not differentiable and it is, to a certain extent, the fault of the method proposed. For the same assumptions, it is possible to construct the distribution of $z_1(t)$ in the form (a 1D task is considered)

$$\begin{aligned} &x \in [\xi, \xi+\delta] : \quad z_1(t) = a_0 + a_1 x + a_2 x^2 \\ &x \in [\xi+\delta, L] : \quad z_1(t) = A_0 = \text{const} \end{aligned} \tag{3.10}$$

The parameters of the above distribution result from the mass balance, boundary condition given on the liquid-solid interface and the assumption concerning continuity of the first derivative for $x = \xi + \delta$ $(\partial z_1 / \partial x = 0)$. The number of unknown parameters corresponds to the number of conditions, and the temporary values of a_0, a_1, a_2 can be easily found (on the assumption that the solidification rate is known).

As an example, distributions of $z_1(t)$ in the domain of a plate $(L = 2\,\text{cm})$ made of Al-Si alloy $(z_0 = 0.05)$ have been determined. In the first version, the constant solidification rate $\nu = 2 \cdot 10^{-6}\,\text{m/s}$ has been assumed. In Figure 8, the solutions for 0.5 and 1.5 mm boundary layers are shown.

In the second version of the solution, the model of solidification basing on the CVM algorithm has been introduced, while the macrosegregation one resulted from the parabolic approximation of z_1. In Figure 9, the results obtained for $\delta = 1$ and 1.5 mm and the physical parameters quoted in Mochnacki and Suchy (1995) are presented.

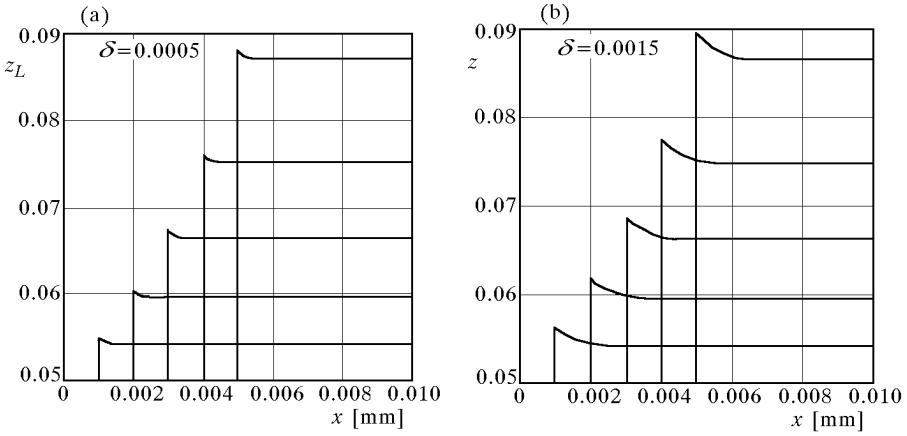

Fig. 8. Distribution of z_1, (a) – 0.5 mm, (b) – 1,5 mm

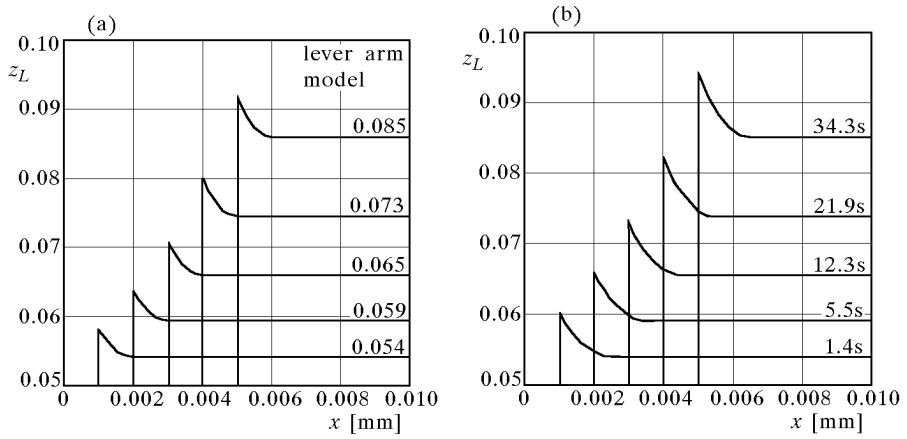

Fig. 9. Distribution of z_1 (solidification)

The testing computations show that the model incorporating the parabolic approximation gives good results for rather small solidification rates (e.g. system casting-sand mix mould).

Summing up, the numerical solutions discussed in this paper concern 1D problems. It is, of course, the self–evident limitation of their applications. On the other hand however, in the initial stages of solidification (at that time the heat and mass transfer proceed very intensively and determine the further course of the process analyzed) the real geometry of the domain is not essential, and the 1D solution is quite acceptable. So, the applications of presented models go beyond the 1D limit.

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Uproszczone modele makrosegregacji

Streszczenie

W pracy przedstawiono opis matematyczny procesu segregacji składników stopowych w objętości krzepnącego odlewu. Wskazano na trudności związane z rozwiązaniem odpowiedniego problemu brzegowo-początkowego, a w dalszej części artykułu przedstawiono propozycje rozwiązań przybliżonych. Rozpatrywano zarówno problem krzepnięcia objętościowego, jak i klasyczne zadanie Stefana. Rozważania teoretyczne zilustrowano przykładami obliczeń numerycznych.

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