ANALYSIS OF SEGREGATION PROCESS USING THE BROKEN LINE MODEL FOR AN INFINITE CYLINDER

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Abstract. In the paper the mathematical description of the macrosegregation process proceeding in the cylindrical casting domain is discussed. Because the solution of the task formulated in such way is rather complicated we present the simplified models in particular the considerations resulting from the lever arm rule, the Scheil assumption and next the solution resulting from 'a broken line model' [1].

1. Governing equations

The macrosegregation process proceeding in the casting domain is described by the system of partial differential equations in the form [2]:

$$\begin{aligned} P(x)\in\Omega_L: \quad & \frac{\partial z_L(x,t)}{\partial t}=\frac{1}{x}\frac{\partial}{\partial x}\left(D_L x\frac{\partial z_L(x,t)}{\partial x}\right) \\ P(x)\in\Omega_S: \quad & \frac{\partial z_S(x,t)}{\partial t}=\frac{1}{x}\frac{\partial}{\partial x}\left(D_S x\frac{\partial z_S(x,t)}{\partial x}\right) \end{aligned} \tag{1}$$

where z_L, z_S are the concentrations of alloy component for liquid and solid state sub-domains, D_L, D_S are the diffusion coefficients, x, t denote spatial co-ordinates and time. It is assumed that the diffusion coefficients of liquid and solid sub--domains are the constant values.
On the moving boundary between liquid and solid sub-domains the condition resulting from the mass balance is given [2-4]

$$D_L\left.\frac{\partial z_L(x,t)}{\partial x}\right|_{x=\xi}-D_S\left.\frac{\partial z_S(x,t)}{\partial x}\right|_{x=\xi}=\frac{d\xi}{dt}\left[z_L(\xi,t)-z_S(\xi,t)\right] \tag{2}$$

On the outer surface of the system the no-flux condition should be assumed

$$x\in\Gamma_0: \quad \frac{\partial z_S(x,t)}{\partial x}=0 \tag{3}$$

For time $t=0$: $z_L(x,0)=z_0$.

It should be pointed out that the solidification rate $\mathrm{d}\xi/\mathrm{d}t$ results, as a rule, from the model of thermal processes proceeding in the casting domain. The co-ordinate ξ corresponds to the liquidus border temperature or to the substitute solidification point defined as follows [5]

$$T^{*}=\frac{\int_{T_S}^{T_L} C(T)\,T\,\mathrm{d}T}{\int_{T_S}^{T_L} C(T)\,\mathrm{d}T} \tag{4}$$

where T_S and T_L are the border temperatures, $C(T)$ is the substitute thermal capacity of the casting material [5].

2. Simplified segregation models

Below the basic idea of simplified model of macrosegregation [1] process will be presented.
We assume the constant value of the mass density, but different for the liquid and solid state, and the mass balances will be analyzed.
Let t and $t+\Delta t$ denote two successive levels of time. Then

$$\begin{gathered}\rho_L V_L(t)\,z_L(t)+\rho_S V_S(t)\,z_S(t)=\\ \rho_L V_L(t+\Delta t)\,z_L(t+\Delta t)+\rho_S V_S(t+\Delta t)\,z_S(t+\Delta t)\end{gathered} \tag{5}$$

Using the Taylor formula one obtains:

$$V_L(t+\Delta t)=V_L(t)+\frac{\mathrm{d}V_L(t)}{\mathrm{d}t}\Delta t \tag{6}$$

$$V_S(t+\Delta t)=V_S(t)+\frac{\mathrm{d}V_S(t)}{\mathrm{d}t}\Delta t \tag{7}$$

$$z_L(t+\Delta t)=z_L(t)+\frac{\mathrm{d}z_L(t)}{\mathrm{d}t}\Delta t \tag{8}$$

$$z_S(t+\Delta t)=z_S(t)+\frac{\mathrm{d}z_S(t)}{\mathrm{d}t}\Delta t \tag{9}$$

Introducing above formulas to equation (5), neglecting the components containing Δt^2 and denoting

$$f_L(t)=\frac{V_L(t)}{V},\quad f_S(t)=\frac{V_S(t)}{V},\quad f_S(t)=1-f_L(t) \tag{10}$$

we have

$$\rho_L f_L\frac{\mathrm{d}z_L}{\mathrm{d}t}+\rho_L z_L\frac{\mathrm{d}f_L}{\mathrm{d}t}+\rho_S\left(1-f_L\right)\frac{\mathrm{d}z_S}{\mathrm{d}t}-\rho_S z_S\frac{\mathrm{d}f_L}{\mathrm{d}t}=0 \tag{11}$$

Introducing the partition coefficients

$$z_S=k\,z_L,\quad \rho_S=w\,\rho_L \tag{12}$$

we obtain the final form of balance equation

$$\frac{\mathrm{d}f_L}{\mathrm{d}z_L}+\frac{f_L}{z_L}=-\frac{wk}{1-wk}\cdot\frac{1}{z_L} \tag{13}$$

This linear differential equation should be solved for the initial condition in the form: $z_L=z_0:\ f_L=1$. Assuming the constant values of *k* and *w* we find

$$f_L=\frac{z_0-wk\,z_L}{\left(1-wk\right)z_L} \tag{14}$$

Above solution correspond to the solution resulting from the well-known lever-arm principle. The same equation can be used in order to find the solution of the so-called Scheil model (diffusion if the solid state is neglected). Let us assume that $\mathrm{d}z_S/\mathrm{d}t=0$ and then

$$\left(1-wk\right)\frac{\mathrm{d}f_L}{\mathrm{d}z_L}+\rho_L f_L=0 \tag{15}$$

or

$$\frac{\mathrm{d}f_L}{f_L}=-\frac{\mathrm{d}z_L}{\left(1-wk\right)z_L} \tag{16}$$

For $k=\text{const},\ w=\text{const}$ and the initial condition in the form $z_L=z_0:\ f_L=1$ one obtains

$$f_L=\left(\frac{z_0}{z_L}\right)^{\frac{1}{1-wk}} \tag{17}$$

The other possibility of simplified analysis of macrosegregation process result from the assumption determining a'priori the function describing the concentration of alloy component in the molten part of the casting domain.

3. 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 moving boundary leads to the following condition [4, 5]

$$D_L \frac{\partial z_L(x, t)}{\partial x}\bigg|_{x=\xi} - D_S \frac{\partial z_S(x, t)}{\partial x}\bigg|_{x=\xi} = (1-k) z_L(\xi, t) \frac{\mathrm{d}\xi}{\mathrm{d}t} \tag{18}$$

If the mass transfer in the solid body is neglected ($D_S = 0$) and the 1D problem is considered then

$$x = \xi = x_i: \quad D_L \frac{\partial z_L(x,t)}{\partial x}\bigg|_{x=x_i} = (1-k) v z_L \tag{19}$$

where $v = \mathrm{d}\xi/\mathrm{d}t$ denotes the solidification rate. Additionally we assume that the thickness of boundary layer δ [6] are known.

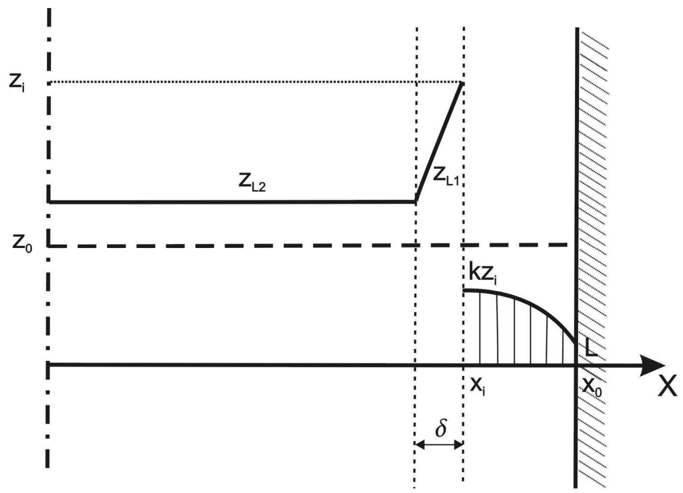

Fig. 1. The broken line model

Using the condition (19) and denoting $m_i = \partial z_L(x,t)/\partial x$ we can determine the slope of the sector corresponding to boundary layer

$$\frac{(1-k) v_{i-1} z_{Li-1}}{D_L} = m_i \tag{20}$$

The first and the second part of broken line is described by the function

$$\begin{cases} z_{L2}(x) = z_i - m_i\,\delta & x \in [0,\, x_i - \delta] \\ z_{L1}(x) = z_i + m_i(x - x_i) & x \in [x_i - \delta,\, x_i] \end{cases} \tag{21}$$

Next on the basis of balance for time t corresponding to $x = x_i$ we have

$$z_0 V_0 = \int_{V_L} z_L \,\mathrm{d}V + \int_{V_S} z_S \,\mathrm{d}V \tag{22}$$

where the first integral in equation (22) is in the form

$$\int_{V_L} z_L \,\mathrm{d}V = 2\pi \left[\int_0^{x_i - \delta} x\left(z_i - m_i\,\delta\right)\mathrm{d}x + \int_{x_i - \delta}^{x_i} x\left[z_i + m_i\left(x - x_i\right)\right]\mathrm{d}x \right] \tag{23}$$

The second one denotes volume of solid state in the casting domain, so

$$\int_{V_S} z_S \,\mathrm{d}V = \sum_{j=1}^{i} V_j \tag{24}$$

where (using the trapezoids formula)

$$V_j = h\,k\,\pi\left(x_j + \frac{h}{2}\right)\left(z_{j-1} + z_j\right) \tag{25}$$

The integral (25) corresponds to the sum of the following volumes:

$$\begin{aligned} V_1 &= h\,k\,\pi\left(x_1 + \frac{h}{2}\right)\left(z_0 + z_1\right) \\ V_2 &= h\,k\,\pi\left(x_2 + \frac{h}{2}\right)\left(z_1 + z_2\right) \\ V_3 &= h\,k\,\pi\left(x_3 + \frac{h}{2}\right)\left(z_2 + z_3\right) \\ &\vdots \\ V_i &= h\,k\,\pi\left(x_i + \frac{h}{2}\right)\left(z_{i-1} + z_i\right) \end{aligned} \tag{26}$$

Introducing (23), (24) and (25) to the equation (22) and next after the mathematical calculations the mass balance takes a form

$$z_0 \pi L^2 = 2\pi \left[\frac{1}{2}(z_i - m_i\,\delta)(x_i - \delta)^2 + \frac{1}{2} z_i \left(2x_i\,\delta - \delta^2\right) + m_i \left(\frac{1}{3}\delta^3 - \frac{1}{2} x_i \delta^2 \right) \right] + \\ + hk\pi \sum_{j=1}^{i} \left(x_j + \frac{h}{2} \right) \left(z_{j-1} + z_j \right) \tag{27}$$

or

$$z_0 L^2 = m_i\,\delta^2 \left(x_i - \frac{1}{3}\delta \right) + (z_i - m_i\,\delta) x_i^2 + hk \sum_{j=1}^{i} \left(x_j + \frac{h}{2} \right) \left(z_{j-1} + z_j \right) \tag{28}$$

Equation (28) allows to find the boundary value z_i, namely

$$z_i = \begin{cases} \dfrac{z_0 L^2 + m_i\,\delta \left(x_i^2 - x_i \delta + \frac{1}{3}\delta^2 \right) - hk \left(x_i + \frac{h}{2} \right) z_{i-1}}{x_i^2 + hk \left(x_i + \frac{h}{2} \right)} & i = 1 \\[2ex] \dfrac{z_0 L^2 + m_i\,\delta \left(x_i^2 - x_i \delta + \frac{1}{3}\delta^2 \right) - hk \left[\left(x_i + \frac{h}{2} \right) z_{i-1} + \sum_{j=1}^{i-1} \left(x_j + \frac{h}{2} \right) \left(z_{j-1} + z_j \right) \right]}{x_i^2 + hk \left(x_i + \frac{h}{2} \right)} & i > 1 \end{cases} \tag{29}$$

The first stage of calculation allows to find the value z_1, from the upper component of formula (29), we also obtain V_1. Next computations are realised from the below part of this equation. In this way we can find the successive values of z_i.

4. The example of computation

We consider the cylindrical casting (R = 1.5 cm) made from Al-Si alloy (z_0 = = 0.05). The following parameters of the process have been assumed: k = 0.4, $D_L = 3.5 \cdot 10^{-8}$ m^2/s, δ = 1 and next 1.5 mm, v = const = $2 \cdot 10^{-4}$ cm/s. In Figures 2 and 3 the solutions obtained are presented.

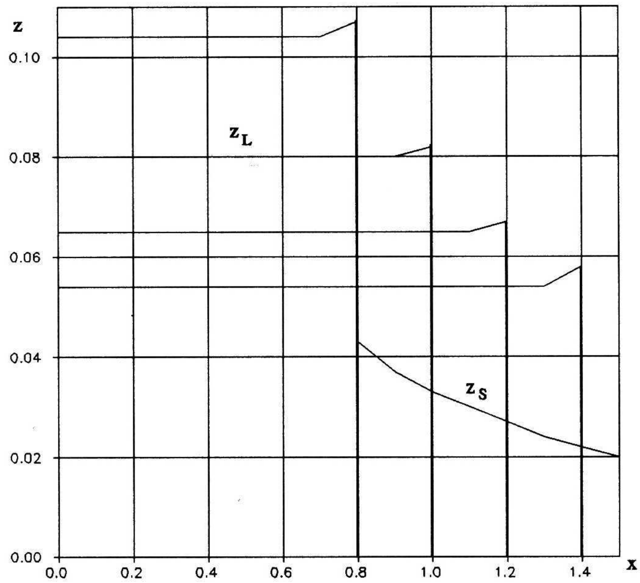

Fig. 2. The distribution of z for $\delta = 1$ mm

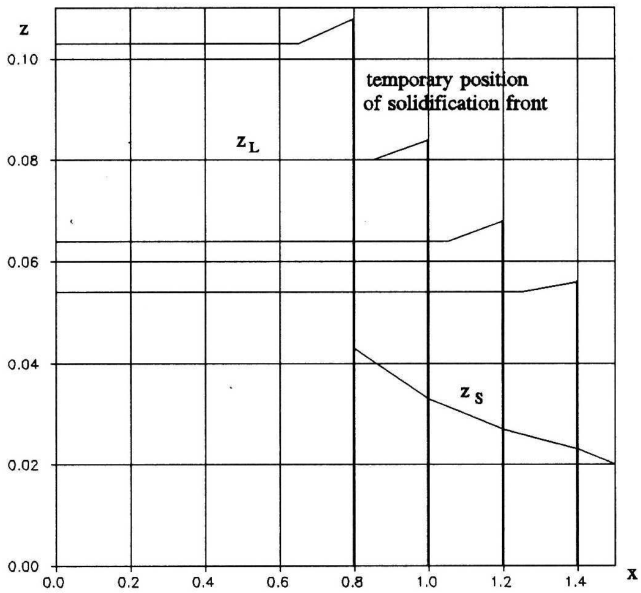

Fig. 3. The distribution of z for $\delta = 1.5$ mm

The results of numerical computations show that the assumption concerning the thickness of boundary layer δ is not very essential and the curses of function z are similar (in particular the boundary values of concentration in liquid state). We can also see that the solution is close to the solution resulting from the Scheil model.

The differences between $z(\xi)$ and $z(\xi - \delta)$ are rather small. Summing up, the broken line model is not complicated, easy on the stage of numerical realization and can be efficiently used for simplified computations of macrosegregation process.

References

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