ANALYSIS OF SEGREGATION PROCESS USING THE BROKEN LINE MODEL. THEORETICAL BASE

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SUMMARY

In the paper the mathematical description of the macrosegregation process proceeding in the 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 and the Scheil assumption and also the model worked out by the authors of this paper called 'a broken line model'. The considerations presented concern the problems for which the solidification rate is assumed to be known (the mutual connections between solidification model and segregation one are omitted).

Key words: macrosegregation, numerical modelling, broken line model

1. GOVERNING EQUATIONS

The macrosegregation process proceeding in the casting domain is described by the system of partial differential equations in the form [1]

\[
P(x) \in \Omega : \frac{\partial z_e(x, t)}{\partial t} = \nabla \left[ D_e \nabla z_e(x, t) \right]
\]

where \( e = 1, 2 \) (liquid and solid states), \( z_e(x, t) \) is an alloy component concentration, \( D_e \) is a diffusion coefficient, \( x, t \) denote spatial co-ordinates and time.

On the moving boundary between liquid and solid sub-domains the condition resulting from the mass balance is given [1, 2, 3]

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\[ D_1 \frac{\partial z_1(x,t)}{\partial n} \bigg|_{x=\xi} - D_1 \frac{\partial z_1(x,t)}{\partial n} \bigg|_{x=\xi} = \frac{d\xi}{dt} \left[ z_1(\xi, t) - z_1(\xi, t) \right] \]  

or

\[ D_2 \frac{\partial z_2(x,t)}{\partial n} \bigg|_{x=\xi} - D_1 \frac{\partial z_1(x,t)}{\partial n} \bigg|_{x=\xi} = (1-k) \frac{d\xi}{dt} z_1(\xi, t) \]  

where \( \partial/\partial n \) is a normal derivative, \( x = \xi \) corresponds to the solid-liquid interface, \( k \) is a partition coefficient.

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

\[ x \in \Gamma_0 : \frac{\partial z_2(x,t)}{\partial n} = 0 \]  

For time \( t=0: z_1(x, 0) = z_{10} \).

It should be pointed out that the solidification rate \( d\xi/dt \) results, as a rule, from the model of thermal processes proceeding in the casting domain. The co-ordinate \( \xi \) corresponds to the liquidus border temperature or to the substitute solidification point defined as follows [4]

\[ T^* = \frac{\int_{T_l}^{T_s} C(T)T \,dT}{\int_{T_l}^{T_s} C(T) \,dT} \]  

where \( T_s \) and \( T_l \) are the border temperatures, \( C(T) \) is the substitute thermal capacity of the casting material [4].

For instance, if one assumes the constant value of substitute thermal capacity then the temperature \( T \) corresponds to the arithmetic mean between the border temperatures.

### 2. Simplified Segregation Models

Below the consideration done by the authors of this paper concerning the simplification of the macrosegregation model will be presented.

We assume the constant value of the mass density and then in place of the mass balances we can analyze the volume ones. Let \( t \) and \( t + \Delta t \) denote two successive levels of time. Then
Using the Taylor formula one obtains
\[ V_2(t + \Delta t) = V_2(t) + \frac{dV_2(t)}{dt} \Delta t \]  
\[ V_1(t + \Delta t) = V_1(t) + \frac{dV_1(t)}{dt} \Delta t \]  
\[ z_2(t + \Delta t) = z_2(t) + \frac{dz_2(t)}{dt} \Delta t \]  
\[ z_1(t + \Delta t) = z_1(t) + \frac{dz_1(t)}{dt} \Delta t \]

Introducing above formulas to equation (6) and neglecting the components containing \( \Delta t^2 \) one has
\[ V_2 \frac{d z_2}{dt} + \frac{dV_2}{dt} z_2 + V_1 \frac{d z_1}{dt} + \frac{dV_1}{dt} z_1 = 0 \]  
\[ f_2(t) = \frac{V_2(t)}{V}, \quad f_1(t) = \frac{V_1(t)}{V}, \quad f_2(t) = 1 - f_1(t) \]

we obtain
\[ f_2 \frac{d z_2}{dt} + \frac{d f_2}{dt} z_2 + f_1 \frac{d z_1}{dt} + \frac{d f_1}{dt} z_1 = 0 \]

Next, introducing the partition coefficient and using the dependence \( f_2 = 1 - f_1 \) we have the final form of balance equation
\[ \frac{d f_1}{dt} + \frac{f_1}{z_1} = -\frac{k}{1-k} \frac{1}{z_i} \]

This linear differential equation should be solved for the initial condition in the form: \( z = z_0; f_1 = 1 \). Assuming the constant value of \( k \) we find
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 \( \frac{dz}{dt} = 0 \) and then

\[
\frac{df_1}{dt} z_2 + f_1 \frac{dz_1}{dt} + \frac{df_1}{dt} z_1 = 0
\]  

or

\[
\frac{df_1}{f_1} = - \frac{dz_1}{[1-k(z_1)]z_1}
\]  

For \( k = \text{const} \) and the initial condition in the form \( z = z_0 : f_1 = 1 \) one obtains

\[
f_1 = \left( \frac{z_0}{z_1} \right)^{1/z}
\]  

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

In this chapter we propose the approximation of the alloy concentration in the molten metal sub-domain by the broken line - Figure 1. The first part of this function corresponds to boundary layer \( \delta \) [5], while the second one corresponds to the sub-domain in which the convectional mass flow causes the equalization of function \( z \).

Assuming, as previously, the same values of solid and liquid mass densities, the mass balance can be substituted by the volume one. Additionally, the diffusion process in the solidified part of casting is neglected (\( D_2 = 0 \)). So, the boundary condition given on the solidification front takes a form

\[
x = x_1 : -D \left( \frac{\partial z}{\partial x} \right) \bigg|_{x=x_1} = (1-k)vz
\]  

where (c.f. chapter 2) \( D = D_1, \ z = z_1 (x, t) \), at the same time we assume that the solidification rate \( v \) or \( v(t) \) and the thickness of boundary layer \( \delta \) are known.
Using the condition (19) we can determine the slope of the sector corresponding to boundary layer

\[ x = x_i : \left( \frac{\partial z}{\partial x} \right)_{x = x_i} = \frac{k - 1}{D} v_{i-1} z_{i-1} = m_i \]  \hspace{1cm} (20)

and then the first part of broken line is described by the function

\[ x \in [x_i, x_i + \delta] : \quad z(x) = z_i + m_i (x - x_i) \]  \hspace{1cm} (21)

One can notice that

\[ z(x_i + \delta) = z_i + m_i \delta \]  \hspace{1cm} (22)

therefore the second part of broken corresponds to the constant value

\[ x \in [x_i + \delta, L] : \quad z(x) = z_i + m_i \delta \]  \hspace{1cm} (23)

After the mathematical manipulations the volume balance takes a form

\[ L z_{i+1} = kh \left( \frac{z_i + z_{i+1}}{2} + \sum_{j=1}^{i-1} z_j \right) + (z_i + 0.5m_i \delta) \delta + (z_i + m_i \delta)(L - ih - \delta) \]  \hspace{1cm} (24)

where \( h = x_i - x_{i-1} = \text{const} \). In the case of constant value of solidification rate the step \( h \) can be determined immediately, while for the variable value of \( v \) the constant step \( h \) corresponds to the different time interval \( \Delta t \). Equation (24) allows to find the boundary value \( z_i \) and next to start with the new loop of computations.
The numerical aspects of the algorithm discussed will be presented in the second part of the paper.

REFERENCES


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**OPIS PROCESU SEGREGACJI ZA POMOCĄ MODELU LINII ŁAMANEJ. PODSTAWY TEORETYCZNE**

**STRESZCZENIE**

W pracy przedstawiono opis matematyczny procesu makrosegregacji w obszarze krzepnącego odlewu. Ponieważ konstrukcja efektywnego algorytmu numerycznego na bazie takiego opisu jest raczej skomplikowana, więc rozpatruje się również modele uproszczone. Autorzy prezentują własne podejście do modelu wynikającego z reguły dźwigni oraz modelu wynikającego z założeń Scheila. W dalszej części artykułu omówiony jest nowy sposób opisu procesu segregacji, w którym rozkład stężenia w fazie ciekłej przybliża się linią łamanej. Prezentowane w tej części rozważania dotyczą przypadku, gdy szybkość narastania warstwy zakrzepłej jest znana, co umożliwia rozprężenie modelu krzepnięcia z modelem ruchu masy.

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