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Multiscale model of segregation process

B. Mochnacki, S. Lara, E. Pawlak

Czestochowa University of Technology, 42-200 Czestochowa, Dabrowskiego 68, Poland,
email: moch@imi.pcz.pl

Abstract: The microsegregation process proceeding in the single grain volume is analyzed. The distribution of alloy component in the domain considered is described by the broken line (boundary layer and the remaining part of liquid subdomain). The temporary solidification rate of grain results from the macro model of thermal processes proceeding in the casting domain (the temperature in the casting volume is assumed to be equalized and only time-dependent). In the final part of the paper the example of computations is shown.

Keywords: Numerical modelling, Solidification, Broken line model

1. MODEL OF CASTING SOLIDIFICATION

We consider the solidification process proceeding in the casting volume assuming that the temperature field in domain considered is only time-dependent and equalized. Such assumption quite good corresponds to conditions of volumetric solidification proceeding in typical sand mould.

The casting volume equals V, while this part of the boundary from which the heat is flowing away equals ΔS. The ratio $V/\Delta S$ corresponds to the solidification modulus. In the paper [1] is shown that the final form of differential equation describing the thermal processes in the system considered is of the form

$$M\, c(T)\frac{\mathrm{d}T(t)}{\mathrm{d}t} = M\, L_V\,\frac{\mathrm{d}\, f_S(t)}{\mathrm{d}t} + \alpha\left[T_a - T(t)\right] \tag{1}$$

where $c(T)$ is a volumetric specific heat, f_S is the volumetric solid state fraction, α is a substitute heat transfer coefficient, L_V is a latent heat per unit of volume, T_a is an ambient temperature. The value of f_S results from the Mehl-Johnson-Avrami-Kolmogorov theory, namely

$$f_S(t) = 1 - \exp\left[-\omega(t)\right] \tag{2}$$

where

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

In the last equation the constant density N of nuclei is assumed - it results from the assumption concerning the equalized temperature in casting domain. Let us

$$u(t)=\frac{\mathrm{d}R(t)}{\mathrm{d}t}=\mu\Delta T^2(t) \tag{4}$$

where $R(t)$ is a grain radius, μ is a growth coefficient, ΔT undercooling below the temporary liquidus temperature T_L. Taking into account the equation (2) we obtain

$$M\,c(T)\frac{\mathrm{d}T(t)}{\mathrm{d}t}=M\,L_V\exp(-\omega)\frac{\mathrm{d}\omega}{\mathrm{d}t}+\alpha\left[T_a-T(t)\right] \tag{5}$$

In numerical realization the last equation can be solved using the Euler method

$$T(t+\Delta t)=T(t)+\exp(-\omega)\left[\omega(t+\Delta t)-\omega(t)\right]+\frac{\alpha\Delta t}{M\,c\left[T(t)\right]}\left[T_a-T(t)\right] \tag{6}$$

At the same time the value of $\omega(t+\Delta t)$ equals

$$\omega(t+\Delta t)=\frac{4}{3}\pi N\left[R(t)+\mu\Delta T^2(t)\Delta t\right]^3 \tag{7}$$

For $t=0: T(0)=T_p$, where T_p is the pouring temperature. For $T(t)>T_L$ the capacity of internal heat sources is equal to 0 (because $f_S=0=\mathrm{const}$).

2. MODEL OF MACROSEGREGATION

The changing with time temperature T_L can be determined on the basis of the microsegregation model concerning the single grain. We consider the spherical control volume which external radius L results from the nuclei density N. Additionally we assume that the mass transfer takes place only in the liquid state subdomain [2]. The concentration of alloy component in this subdomain is described by the broken line [3] - Figure1. On the contact surface between liquid and solid we have [4]

$$x=\xi(t): \qquad -D_L\frac{\partial z_L(x,t)}{\partial x}=(1-k)\,u\,z_L(x,t) \tag{8}$$

where z_L is the concentration of alloy component in the liquid subdomain, k is the partition coefficient, D_L is the diffusion coefficient, u is the solidification rate.
On the external surface of spherical control volume we have

$$x = L: \qquad \frac{\partial z_L(x, t)}{\partial x} = 0 \tag{9}$$

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

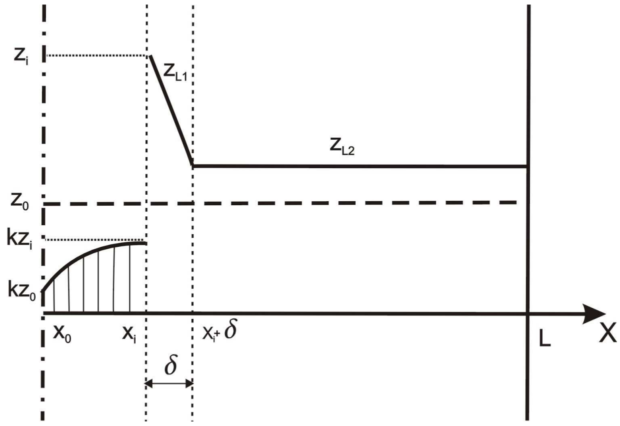

Figure 1. The broken line model (spherical geometry)

The parameters of broken line can be found as follows [3].
The slope of the sector corresponding to boundary layer is defined

$$m_i = \frac{(k-1) v_{i-1} z_{Li-1}}{D_L} \tag{10}$$

and the following function describes the first and the second part of broken line

$$\begin{cases} z_{L1}(x) = z_i + m_i (x - x_i) & x \in [x_i, x_i + \delta] \\ z_{L2}(x) = z_i + m_i \delta & x \in [x_i + \delta, L] \end{cases} \tag{11}$$

where δ is the boundary layer.
Using the balance

$$z_0 V_0 = \iiint_{V_L} z_L \, \mathrm{d}V + \iiint_{V_S} z_S \, \mathrm{d}V \tag{12}$$

we obtain

$$z_i = \frac{z_0 \left[L^3 + x_i^3 (k-1) \right] + m_i \, \delta \left(4x_i^3 + 6x_i^2 \delta + 4x_i \delta^2 - L^3 + \delta^3 \right) - k \sum_{j=0}^{i-1} z_j \left(x_{j+1}^3 - x_j^3 \right)}{L^3 - x_i^3} \tag{13}$$

Above equation allows to find the boundary value z_i.

3. EXAMPLE OF COMPUTATIONS

As an example the casting made from Al-Si alloy ($z_0 = 0.05$) which modulus is equal to $M = 0.01\,[\mathrm{m}]$ is considered. The thermophysical parameters of the material considered are collected in [5]. The different densities of nuclei ($N = 10^{10}$, 10^{11} and 10^{12}) are taken into account. The thickness of boundary layer was assumed on the basis of 'exact' solution presented in [6] (the distribution of z_L has been found using the approximate solution of adequate boundary-initial problem). In Figure 2 the distribution of alloy component concentration found in [6] is shown, while in the next Figure the solution obtained on the basis of broken line model is presented. One can notice that the proposed simple model gives the results close to the essentially complex one. Summing up, it seems that the proposed method of microsegregation modelling is sufficiently exact from the practical point of view. The model presented concerns the case of volumetric solidification and it is the limitation of its application. From the other hand, however, this type of solidification is very typical, especially for the technologies in which the typical sand molds are used. The numerical solution of the problem discussed gives a lot of essential information concerning the course of the process but in this paper we show only the small part of the results.

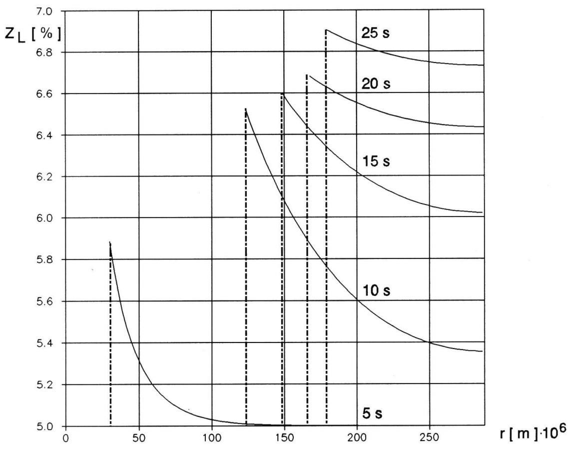

Figure 2. Concentration of z_L ($N = 10^{10}$ - [6])

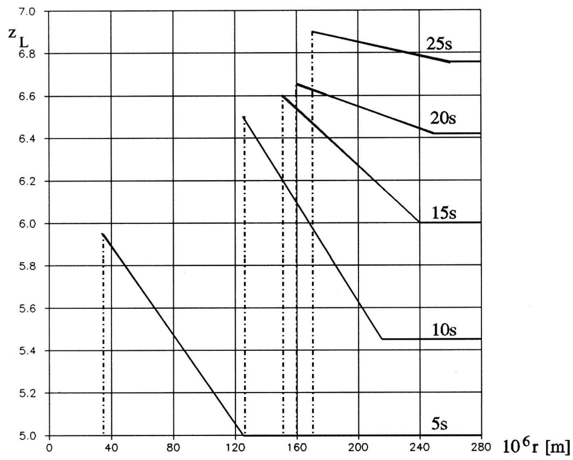

Figure 3. Broken line solution ($N = 10^{10}$)

REFERENCES

1. B. Mochnacki, J.S. Suchy, M. Prażmowski, Modelling of segregation in the process of Al-Si alloy solidification, Solidification of Metals and Alloys, Vol. 2, Book No 44, 229-234, 2000.
2. E. Fras, Crystalization of metals and alloys, PWN, Warshaw, 1992.
3. S. Lara, E. Pawlak, M. Prażmowski, Simplified model of macrosegregation, Archives of Foundary, Vol. 4, No 14, 259-266, 2004.
4. N.A. Avdonin, Matematiceskoje opisanie kristalizacji, Zinatne, Riga, 1980.
5. B. Mochnacki, J.S. Suchy, Numerical methods in computations of foundry processes, PFTA, Cracow, 1995.
6. B. Mochnacki, E. Majchrzak, J.S. Suchy, Boundary element model of coupled heat and mass transfer in solidifying casting, International Journal of Cast Metals Research, Vol. 12, No 4, 227-232, 1999.