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Simulation of heat and mass transfer in domain of casting made from binary alloy

B. Mochnacki[a,*], E. Majchrzak[a,b], R. Szopa[a]
[a] Częstochowa University of Technology, Dąbrowskiego 73, 42-200 Częstochowa, Poland
[b] Silesian University of Technology, Akademicka 2a, 44-100 Gliwice, Poland
*Corresponding author. E-mail address: moch@imi.pcz.pl

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Abstract

In the paper the mathematical model, numerical algorithm and example of cylindrical casting solidification are presented. In particular the casting made from Cu-Zn alloy is considered. It is assumed that the temperature corresponding to the beginning of solidification is time-dependent and it is a function of temporary alloy component concentration. The course of macrosegregation has been modelled using the mass balances in the set of control volumes resulting from a domain discretization. The balances have been constructed in different ways, in particular under the assumption of instant equalization of alloy chemical constitution (a lever arm rule), next the Scheil model (e.g. [1]) has been used and finally the broken line model [2] has been taken into account. On a stage of numerical algorithm construction the boundary element method has been used in the variant called BEM using discretization in time [3, 4, 5] supplemented by the alternating phase truncation procedure [6, 7].

Keywords: Application of information technology to the foundry industry, Solidification process, Numerical techniques

1. Governing equations

In a casting domain, two changing with time sub-domains are distinguished. They correspond to liquid and solid phases. The moving boundary is identified by a temporary position of liquidus temperature $T^*(z_L)$, where z_L is a temporary concentration of alloy component of liquid state near a border surface (in a case of lever arm and Scheil models z_L corresponds to concentration in the whole liquid part of casting domain). In the model proposed a presence of mushy zone is neglected and in a place of T^* one can introduce the so-called equivalent solidification point [7].

A transient temperature field in domain considered (taking into account the cylindrical geometry of casting - 1D task) is determined by the following system of partial differential equations

$$\begin{aligned} c_L\,\rho_L\,\frac{\partial T_L(r,t)}{\partial t} &= \frac{\lambda_L}{r}\frac{\partial}{\partial r}\left[r\,\frac{\partial T_L(r,t)}{\partial r}\right], \\ c_S\,\rho_S\,\frac{\partial T_S(r,t)}{\partial t} &= \frac{\lambda_S}{r}\frac{\partial}{\partial r}\left[r\,\frac{\partial T_S(r,t)}{\partial r}\right] \end{aligned} \tag{1}$$

In equations (1) c, ρ, λ denote the specific heats, mass densities and thermal conductivities, T, r, t - are the temperature, geometrical co-ordinates and time.
On a border surface the Stefan condition is given:

$$r=\eta(t):\quad \begin{cases} \lambda_S\,\dfrac{\partial T_S(r,t)}{\partial r}-\lambda_L\,\dfrac{\partial T_L(r,t)}{\partial r}=L_V\,\dfrac{\mathrm{d}r}{\mathrm{d}t} \\ T_S(r,t)=T_L(r,t)=T^*(z_L) \end{cases} \tag{2}$$

where L_V is a volumetric latent heat.

On an external surface the following continuity condition is assumed

$$r = R: \quad q(r,t) = \alpha \left[T(r,t) - T_a \right] \tag{3}$$

where α is a substitute heat transfer coefficient, T_a is an ambient temperature. At the moment $t = 0: T_L(r,0) = T_0,\ z_L(r,0) = z_0$, at the same time T_0 is the pouring temperature, z_0 - initial concentration of alloy component.

The algorithm of numerical simulation bases on the alternating phase truncation procedure. This approach requires the application of enthalpy approach on a stage of governing equations construction. So, we introduce the following definition of physical enthalpy

$$H(T) = \int_0^T c(\mu)\,\rho(\mu)\,\mathrm{d}\mu + L_V\,u(T) \tag{4}$$

where

$$u(T) = \begin{cases} 0 & T < T^*(z_L) \\ 1 & T \geq T^*(z_L) \end{cases} \tag{5}$$

The course of enthalpy function is shown in Figure 1.

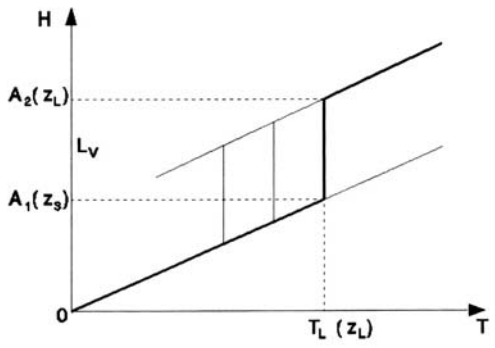

Fig. 1. Enthalpy diagram

The system of equations (1) written using the enthalpy convention takes a form

$$\begin{aligned} \frac{\partial H_L(r,t)}{\partial t} &= \frac{a_L}{r}\frac{\partial}{\partial r}\left[r\frac{\partial H_L(r,t)}{\partial r} \right], \\ \frac{\partial H_S(r,t)}{\partial t} &= \frac{a_S}{r}\frac{\partial}{\partial r}\left[r\frac{\partial H_S(r,t)}{\partial r} \right] \end{aligned} \tag{6}$$

where a_L and a_S are the heat diffusion coefficients ($a = \lambda / c\rho$).
The Stefan boundary condition can be written as follows

$$r = \eta: \quad \begin{cases} a_S \dfrac{\partial H_S(r,t)}{\partial r} - a_L \dfrac{\partial H_L(r,t)}{\partial r} = L_V \dfrac{\mathrm{d}r}{\mathrm{d}t} \\ A_L(z_L) = A_S(z_S) + L_V \end{cases} \tag{7}$$

where A_L and A_S are the right hand side and left hand side limits of enthalpy at the point T^* (see: Figure 1).
The Robin boundary condition is of the form

$$r = R: \quad q(r,t) = \beta \left[H(r,t) - H_a \right] \tag{8}$$

where $\beta = a / c\rho$ is a substitute heat transfer coefficient written using the enthalpy convention, H_a is the enthalpy corresponding to T_a. The initial condition is also given: $t = 0: H(r,0) = H_0$.

The adequate fragment of equilibrium diagram [8] of alloy considered (Zn < 30%) one can approximate by two sectors starting from the same point. In a such situation the partition coefficient $k = \text{const}$ and $z_S = k\,z_L$. The formula determining the liquidus line is of the form $T^* = T_m + m z_L$, where T_m is a solidification point of pure metal (Cu), while m - is a slope of straight line.

2. Mass balance under the assumption of lever arm model

The mass balance of component alloy in domain of casting can be written in the form

$$m_0\,z_0 = m_S(t)\,z_S(t) + m_L(t)\,z_L(t) \tag{9}$$

where m_0 denotes a mass of component.

The domain considered is divided into control volumes (cylindrical rings) which altitude can be assumed in optional way (e.g. $h = 1$). Internal radius of element V_j is denoted by r_{j-1}, while an external one by r_j - Figure 2.

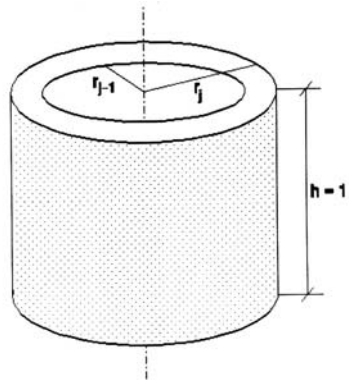

Fig. 2. Control volume V_j

Solid state fraction in volume V_j at time t equals $S_j(t)$. A mass of metal in solid and liquid state results from equations

$$m_{Sj} = S_j(t)\, V_j\, \rho_S, \quad m_{Lj} = \left[1 - S_j(t)\right] V_j\, \rho_L \tag{10}$$

Now, the time grid should be introduced

$$0 = t^0 < t^1 < \ldots < t^f < t^{f+1} < \ldots < t^F < \infty, \quad \Delta t = t^{f+1} - t^f \tag{11}$$

The local values of S_j result from the numerical model of solidification and they are defined in the following way

$$S_j\left(t^{f+1}\right) = \frac{A_L - H\left(r_j, t^{f+1}\right)}{A_L - A_S}, \quad A_S < H\left(r_j, t^{f+1}\right) < A_L \tag{12}$$

while for the others enthalpy values the function S_j equals 0 and 1, correspondingly.
Mass balance (9) written for time t^{f+1} leads to the equation

$$z_L\left(t^{f+1}\right) = \frac{m_0\, z_0}{k\, m_S\left(t^{f+1}\right) + m_L\left(t^{f+1}\right)} \tag{13}$$

In the last equation the definition of partition coefficient *k* has been introduced. Finally

$$z_L\left(t^{f+1}\right) = \frac{R^2\, \rho_L\, z_0}{k \sum_{j=1}^{n} V_j\, \rho_S\, S_j\left(t^{f+1}\right) + \sum_{j=1}^{n} V_j\, \rho_L \left[1 - S_j\left(t^{f+1}\right)\right]} \tag{14}$$

A temporary value of alloy component concentration determines a new value of solidification point T^* and border values A_L and A_S.

3. Mass balance under the assumption of Scheil model

The Scheil model results from the assumption of limiting form of macrosegregation model determining the mass diffusion in a casting domain. Because the diffusion coefficient for solid state is essentially less than the same coefficient for molten metal and, from the other hand, the convection proceeding in a molten metal causes the equalization of chemical constitution in this domain, therefore it is assumed that $D_S = 0$, while $D_L \to \infty$ (D is a diffusion coefficient). So, the mass balance resulting from Scheil's assumptions takes a form

$$\begin{aligned} m_0\, z_0 &= m_S\left(t^1\right) z_S\left(t^1\right) + m_S\left(t^2\right) z_S\left(t^2\right) + \ldots + \\ &+ m_S\left(t^f\right) z_S\left(t^f\right) + m_S\left(t^{f+1}\right) z_S\left(t^{f+1}\right) + m_L\left(t^{f+1}\right) z_L\left(t^{f+1}\right) \end{aligned} \tag{15}$$

or

$$\begin{aligned} z_L\left(t^{f+1}\right) &= \\ &= \frac{m_0\, z_0 - \left[m_S\left(t^1\right) z_S\left(t^1\right) + m_S\left(t^2\right) z_S\left(t^2\right) + \ldots + m_S\left(t^f\right) z_S\left(t^f\right)\right]}{k\, m_S\left(t^{f+1}\right) + m_L\left(t^{f+1}\right)} \end{aligned} \tag{16}$$

After mathematical manipulations one obtains

$$z_L\left(t^{f+1}\right) = \frac{R^2\, \rho_L\, z_0 - \sum_{p=1}^{f} \sum_{j=1}^{n} V_j\, \rho_S\, z_S\left(t^p\right)\left(S_j^p - S_j^{p-1}\right)}{k \sum_{j=1}^{n} V_j\, \rho_S \left(S_j^{f+1} - S_j^f\right) + \sum_{j=1}^{n} V_j\, \rho_L \left[1 - S_j^{f+1}\right]} \tag{17}$$

where $S_j^p = S_j\left(t^p\right)$ etc.

Similarly, as in a case of previous model, the calculated value of $z_L\left(t^{f+1}\right)$ determines a temporary temperature T^* and the border values A_L and A_S.

4. Broken line model

Macrosegregation process proceeding in the cylindrical casting domain is described by the system of diffusion equations in the form

$$\begin{aligned} P(r) \in \Omega_L: &\quad \frac{\partial z_L(r,t)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r}\left(D_L\, r\, \frac{\partial z_L(r,t)}{\partial r}\right) \\ P(r) \in \Omega_S: &\quad \frac{\partial z_S(r,t)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r}\left(D_S\, r\, \frac{\partial z_S(r,t)}{\partial r}\right) \end{aligned} \tag{18}$$

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, *r*, *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 [1, 5, 7]

$$r = \eta: \quad D_L \frac{\partial z_L(r,t)}{\partial r} - D_S \frac{\partial z_S(r,t)}{\partial r} = \frac{\mathrm{d}r}{\mathrm{d}t}\left[z_L(r,t) - z_S(r,t)\right] \tag{19}$$

Introducing the partition coefficient *k* one obtains the other form of condition (19)

$$r = \eta: \quad D_L \frac{\partial z_L(r,t)}{\partial r} - D_S \frac{\partial z_S(r,t)}{\partial r} = (1-k)\, z_L(r,t)\, \frac{dr}{dt} \tag{20}$$

If the mass transfer in the solid body is neglected ($D_S = 0$)

$$r = \eta: \qquad D_L \frac{\partial z_L(r,t)}{\partial r} = (1-k) v z_L \tag{21}$$

where $v = \mathrm{d}r/\mathrm{d}t$ denotes the solidification rate.
On the outer surface of the system the no-flux condition should be assumed

$$r \in \Gamma_0: \qquad \frac{\partial z_S(r,t)}{\partial r} = 0 \tag{22}$$

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

The idea of broken line model is the following. The concentration field in molten metal is assumed in the form of broken line. In particular the first segment corresponds to a certain layer δ while the second one to the other part of liquid state. The parameters of above distribution result from condition (20) and mass balance. The concentration in solid body results from partition coefficient *k* (see Fig.3). The details of this approach can be found in [9].

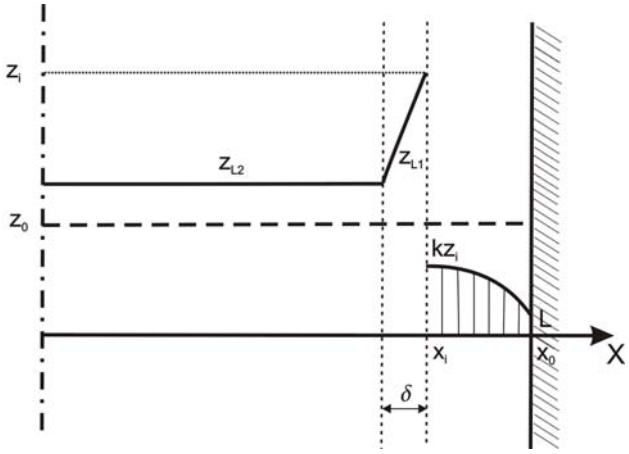

Fig. 3. The broken line model

5. Alternating phase truncation method

In this paper the classical variant of APTM presented by Rogers, Ciment and Berger (e.g. [6]) is used. Generalized form of the method can be found, among others, in [6, 7]. The algorithm of numerical solution of problem discussed (equations (6), (7) and (8)), this means the computations concerning the transition from time t^f to time t^{f+1} is the following. Let us denote by H_j^f the discrete set of enthalpy values in the casting domain at time t^f and points r_j. In the first stage of computations the casting domain is conventionally treated as a liquid one. At the points r_j for which enthalpy H_j^f is less than A_L one assumes the local value of enthalpy equal to A_L, while for the others nodes the local value of enthalpy is invariable. So, the real enthalpy distribution is substituted by the following one

$$V_1(r_j,\ t^f) = \max\ \left\{H_j^f, A_L(z_L)\right\} \tag{23}$$

For homogeneous (molten metal) casting domain the enthalpy field for time t^{f+1} is calculated (using the optional numerical method). The solution obtained we denote as $V_1'(r_j,\ t^{f+1})$ (parameter *a* in equations (6) corresponds to a_L). The first stage of algorithm goes to the end by substraction of previously added enthalpy, this means

$$V_1(r_j,\ t^{f+1}) = V_1'(r_j,\ t^{f+1}) + H_j^f - V_1(r_j,\ t^f) \tag{24}$$

The second stage of computations concerning the transition $t^f \to t^{f+1}$, starts from the homogenization of casting domain to the solid state, in other words

$$V_2(r_j,\ t^f) = \min\left\{A_S(z_L),\ V_1(r_j,\ t^{f+1})\right\} \tag{25}$$

The enthalpy field $V_2(r_j,\ t^f)$ is again calculated ($a = a_S$). The final solution concerning the time t^{f+1} results from the formula

$$H_j^{f+1} = V_2'(r_j,\ t^{f+1}) + V_1(r_j,\ t^{f+1}) - V_2(r_j, t^f) \tag{26}$$

6. Boundary element method

The numerical solution of equation

$$\frac{\partial H(r,t)}{\partial t} = a\frac{\partial^2 H(r,t)}{\partial r^2} + \frac{a}{r}\frac{\partial H(r,t)}{\partial r} \tag{27}$$

has been found using the boundary element method. Because the BEM algorithm for the objects oriented in cylindrical co-ordinate system is very complicated, the simpler approach is proposed.
Equation (22) can be written in the form

$$\frac{\partial H(r,t)}{\partial t} = a\frac{\partial^2 H(r,t)}{\partial r^2} + Q \tag{28}$$

where *Q* is the artificial source function and

$$Q(r,t) = \frac{a}{r}\frac{\partial H(r,t)}{\partial r} \tag{29}$$

In this way one obtains the energy equation corresponding to the objects oriented in cartesian co-ordinate system for which the BEM algorithm is simple and effective on a stage of numerical simulation.

In the case of variant called the BEM using discretization in time, the derivative $\partial H/\partial t$ for transition $t^f \to t^{f+1}$ is substituted by differential quotient and the equation (23) takes a form

$$\frac{H\left(r, t^{f+1}\right) - H\left(r, t^{f}\right)}{\Delta t} = a\,\frac{\partial^2 H(r,t)}{\partial r^2} + Q \tag{30}$$

A basic BEM equation for the problem (24) results from the weighted residual method application and then one obtains

$$\int_0^R \left[\frac{\partial^2 H\left(r, t^{f+1}\right)}{\partial r^2} - \frac{1}{a\Delta t} H\left(r, t^{f+1}\right) + \right. \\ \left. + \frac{1}{a\Delta t} H\left(r, t^{f}\right) + \frac{Q}{a} \right] H^*(\xi, r)\,\mathrm{d}r = 0 \tag{31}$$

where $H^*(\xi, r),\ \xi \in (0, R)$ is the fundamental solution. In the case considered it is a function of the form [3, 5]

$$H^*(\xi, r) = \frac{\sqrt{a\Delta t}}{2} \exp\left(-\frac{|r-\xi|}{\sqrt{a\Delta t}} \right) \tag{32}$$

After mathematical manipulations, the equation (28) takes a form

$$H\left(\xi, t^{f+1}\right) + \left[\frac{1}{a} H^*(\xi, r)\, q\left(r, t^{f+1}\right) \right]_0^R = \\ = \frac{1}{a} \left[q^*(\xi, r)\, H\left(r, t^{f+1}\right) \right]_0^R + p(\xi) + z(\xi) \tag{33}$$

where $q^*(\xi, r) = -a\,\partial H^*/\partial r$, while

$$p(\xi) = \frac{1}{a\Delta t} \int_0^R H^*(\xi, r)\, H\left(r, t^{f}\right) \mathrm{d}r \tag{34}$$

and

$$z(\xi) = \frac{1}{a} \int_0^R Q\, H^*(\xi, r)\, \mathrm{d}r \tag{35}$$

For $\xi \to 0^+$ i $\xi \to L^-$ one has

$$\begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \begin{bmatrix} q\left(0, t^{f+1}\right) \\ q\left(R, t^{f+1}\right) \end{bmatrix} = \\ = \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \begin{bmatrix} H\left(0, t^{f+1}\right) \\ H\left(R, t^{f+1}\right) \end{bmatrix} + \begin{bmatrix} p(0) \\ p(R) \end{bmatrix} + \begin{bmatrix} z(0) \\ z(R) \end{bmatrix} \tag{36}$$

Values of matrices **g**, **h**, **p**, **z** coefficients result from equation (33). The capacity of artificial heat source can be found by substitution of $\partial H/\partial r$ by the adequate differential quotient [2].

7. Example of computations

We consider the solidification of cylindrical casting ($R = 8$ cm) made from Cu-Zn alloy (10% Zn). The following thermophysical parameters have been assumed $\lambda_L = \lambda_S = \lambda = 0.12$ kW/mK , $c_L = c_S = c = 3354$ kJ/m^{3}K , $\rho_L = \rho_S = \rho = 8600$ kg/m^3 , $L_V = 1.634 \cdot 10^6$ kJ/m^3 , $k = 0.855$, $T^* = 1083 - 473.68 \cdot z_L$, $D_L = 3.5 \cdot 10^{-8}$ m^2/s , $\delta = 1.5$ mm , initial temperature 1070 °C. On the outer surface the Robin condition has been taken into account ($\alpha = 40$ W/m^{2}K , $T_a = 30$ °C).

In Figures 4 and 5 the kinetics of casting solidification is shown, at the same time the different models of macrosegregation have been considered. The next Figure shows the cooling curves at the points from casting domain

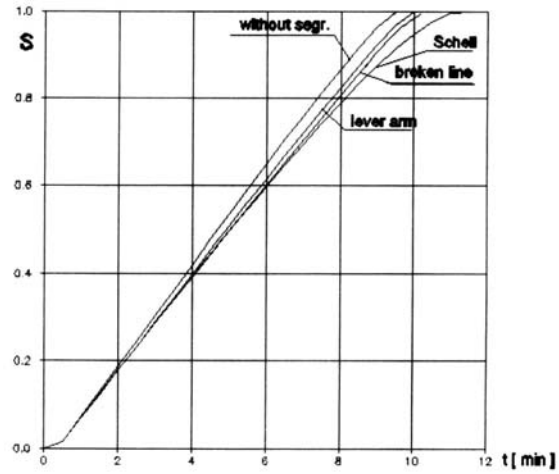

Fig. 4. Kinetics of solidification

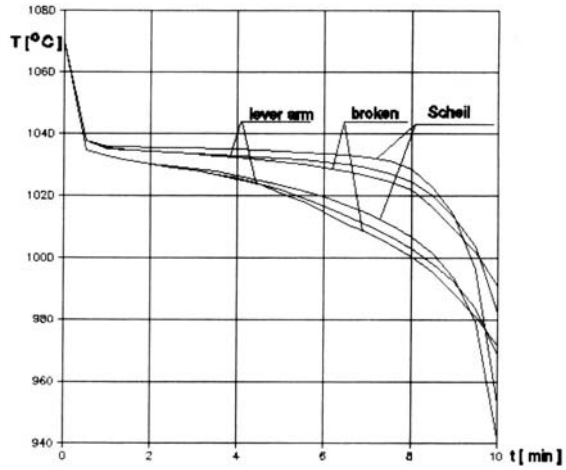

Fig. 5. Cooling curves (axis and $r = 2$ cm)

8. Final remarks

The differences between solutions are non-drastic, but visible. It seems, that the numerical algorithm of solidification supplemented by the simple procedures taking into account the changes of alloy chemical composition are closer to the real physical conditions of the process and can be used on a stage of process modelling.

Acknowledgements

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