Estimation of the thickness of boundary layer in a broken line model of binary alloy solidification

D. Słota

Institute of Mathematics, Silesian University of Technology,
Kaszubska 23, 44-100 Gliwice, Poland
Corresponding author. E-mail address: damian.slota@polsl.pl

Abstract

The solution of the inverse problem involving the designation of the thickness of boundary layer in a broken line model of binary alloy solidification for known temperature measurements at a selected point of the cast is presented. In the discussed model the temperature distribution is described by means of the Stefan problem with varying in time temperature corresponding to the beginning of solidification, depending on the concentration of the alloy component; whereas to describe the concentration, a broken line model was used..

1. Formulation of the problem

In the discussed model temperature distribution is described by the Stefan problem [1] with varying in time temperature corresponding to the beginning of solidification, depending on the concentration of the alloy component; whereas, to describe the concentration a broken line model is used [2-5]. The task involves the designation of the thickness of the boundary layer, where temperature measurements are known at a selected point of the cast.

In domain Ω, occupied by a solidifying material, two sub-domains changing with time are considered: Ω_1 occupied by the liquid phase and Ω_2 occupied by the solid phase (Fig. 1). These domains are separated by the phase change boundary Γ_g (moving boundary), which is determined by varying in time liquidus temperature (or, the so called equivalent solidification point [1]). Temperature distribution in each of the phases is determined by the following heat conduction equation ($i=1, 2$):

$$c_i \, \rho_i \, \frac{\partial T_i}{\partial t}(x,t) = \lambda_i \, \frac{\partial^2 T_i}{\partial x^2}(x,t),$$

(1)

for $x \in \Omega_i$, $t \in (0, t^*)$, where c_i, ρ_i and λ_i are the specific heat, the mass density and the thermal conductivity, in the liquid phase ($i=1$) and solid phase ($i=2$), and t and x refer to time and spatial location, respectively. On the boundary Γ_0 the following initial condition is given ($T_0 > T^*(Z_0)$):

$$T_1(x,0) = T_0 \, ,$$

(2)

where T_0 is the initial temperature, T^* is the temperature of solidification, Z_0 is the initial concentration of alloy component. On the boundaries Γ_{1i} ($i=1,2$) the following homogeneous boundary conditions of the second kind are given

$$\frac{\partial T_i}{\partial x}(x,t) = 0 \, ,$$

(3)

whereas on the boundaries Γ_{2i} ($i=1,2$) the boundary conditions of the third kind are given

$$-\lambda_i \frac{\partial T_i}{\partial x}(x,t) = \alpha\left(T_i(x,t) - T_\infty\right),$$
(4)

where α is the heat transfer coefficient, T_∞ is the ambient temperature. On the phase change boundary Γ_g the temperature continuity condition and the Stefan condition are given

$$T_1(\xi(t),t) = T_2(\xi(t),t) = T^*(Z_L(t)),$$
(5)

$$L\,\rho_2 \frac{d\xi(t)}{dt} = -\lambda_1 \left.\frac{\partial T_1(x,t)}{\partial x}\right|_{x=\xi(t)} + \lambda_2 \left.\frac{\partial T_2(x,t)}{\partial x}\right|_{x=\xi(t)},$$
(6)

where T^* is the temperature of solidification, $Z_L(t)$ is the concentration of the alloy component on the phase change boundary at the liquid side, L is the latent heat of fusion, $\xi(t)$ is a function describing the location of the phase change boundary.
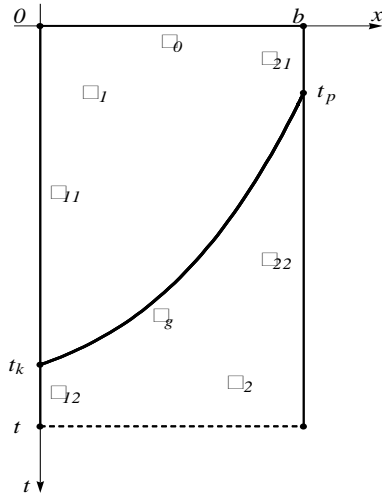

Fig. 1. Domain of the problem

The process of macrosegregation, occurring in the alloy, is described by the diffusion equation ($i=1,2$):

$$\frac{\partial Z_i}{\partial t}(x,t) = D_i \frac{\partial^2 Z_i}{\partial x^2}(x,t),$$
(7)

for $x \in \Omega_i$, $t \in (0,t^*)$, where Z_i and D_i are the concentration of the alloy component and the diffusion coefficient in the liquid phase ($i=1$) and solid phase ($i=2$), respectively. On the boundary Γ_0 the following initial condition is given

$$Z_1(x,0) = Z_0,$$
(8)

where Z_0 is the initial concentration of the alloy component. On the boundaries Γ_{1i} and Γ_{2i} ($i=1,2$) of the investigated domain homogeneous boundary conditions of the second kind are given

$$\frac{\partial Z_i}{\partial x}(x,t) = 0.$$
(9)

On the phase change boundary Γ_g the condition inferred from the mass balance is given

$$\frac{d\xi(t)}{dt}\left(Z_1(x,t) - Z_2(x,t)\right)\big|_{x=\xi(t)} =$$
$$= -D_1 \left.\frac{\partial Z_1(x,t)}{\partial x}\right|_{x=\xi(t)} + D_2 \left.\frac{\partial Z_2(x,t)}{\partial x}\right|_{x=\xi(t)}.$$
(10)

If the partition coefficient $k = \dfrac{Z_S(t)}{Z_L(t)}$ is introduced, the above condition may be expressed in the following form

$$-D_1 \left.\frac{\partial Z_1(x,t)}{\partial x}\right|_{x=\xi(t)} + D_2 \left.\frac{\partial Z_2(x,t)}{\partial x}\right|_{x=\xi(t)} = (1-k)Z_L(t)\frac{d\xi(t)}{dt},$$
(11)

where $Z_L(t)=Z_1(\xi(t),t)$ and $Z_S(t)=Z_2(\xi(t),t)$ are concentrations of the alloy component on the phase change boundary at the liquid and solid phases, respectively.
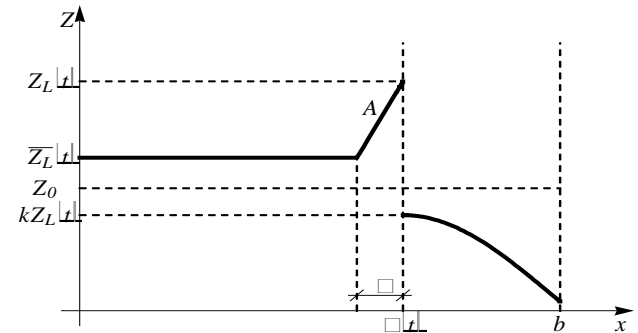

Fig. 2. Distribution of the concentration of the alloy component in broken line model

The broken line model [2-5] assumes that the concentration of the alloy component in the liquid phase may be approximated by a broken line (Fig. 2). Thus, in the layer (of the thickness of δ) close to the phase boundary (boundary layer) the concentration distribution is described by an increasing (or decreasing) linear function. However, in the remaining part of the liquid phase the concentration distribution of the alloy component is steady. For the solid phase it is assumed that $D_2=0$ (the diffusion process in the solid phase is neglected), meaning that the concentration of the alloy component is an outcome of the partition coefficient. The concentration distribution of the alloy component in the liquid phase is an outcome of the mass balance and of condition (11), where $D_2=0$. The equation of straight line A (Fig. 2) at moment t may be expressed as

$$Z_1(x,t) = m(t)(x - \xi(t)) + Z_L(t).$$

(12)

Using condition (11) it is possible to determine the slope of straight line A:

$$m(t) = \left.\frac{\partial Z_1(x,t)}{\partial x}\right|_{x=\xi(t)} = \frac{k-1}{D_1} Z_L(t) v(t),$$

(13)

where $\quad v(t) = \dfrac{d\xi(t)}{dt}\quad$ is the velocity of the phase change boundary; whereas, the values of $Z_L(t)$ may be derived from the mass balance, leading to the following equation

$$\int_0^b Z_1(x,0)dx = \int_0^{\xi(t)} Z_1(x,t)dx + \int_{\xi(t)}^b Z_2(x,t)dx,$$

(14)

i.e.,

$$Z_0 b = \int_0^{\xi(t)-\delta} \overline{Z}_L(t)dx + \\ + \int_{\xi(t)-\delta}^{\xi(t)} (m(t)(x-\xi(t)) + Z_L(t))dx + \int_{\xi(t)}^b Z_2(x,t)dx.$$

(15)

Because $\overline{Z}_L(t) = Z_L(t) - \delta\, m(t)$, in consequence, we get

$$Z_0 b = (\xi(t) - \delta)(Z_L(t) - \delta\, m(t)) + \\ + \delta Z_L(t) - \frac{1}{2}\delta^2 m(t) + \int_{\xi(t)}^b Z_2(x,t)dx.$$

(16)

Now, a time grid t_i, $i=0,1,\dots n$, of interval $[0,t^*]$ is introduced. If the values of the concentrations at moments t_i, $i=0,1,\dots p$, are known, then, on the grounds on the above equation approximated value $Z_L(t_{p+1})$ may be designated

$$Z_L(t_{p+1}) = \frac{1}{\xi_{p+1} + \frac{1}{2}h_p k}\left(Z_0 b + \delta\, m_{p+1} \xi_{p+1} - \right. \\ \left. - \frac{1}{2}\delta^2 m_{p+1} - \sum_{i=1}^{p-1}\left(\frac{Z_S(t_i) - Z_S(t_{i+1})}{2}h_i\right) - \frac{Z_S(t_p)}{2}h_p \right),$$

(17)

where $m_i = m(t_i)$, $\xi_i = \xi(t_i)$, $h_i = \xi(t_{i+1}) - \xi(t_i)$, and the values of integral in equation (16) is approximated by means of the trapezoid method.

In the discussed inverse problem for given temperature values:

$$T(x_i, t_j) = U_{ij},$$

(18)

for $i=1,2,\dots,N_1$, $j=1,2,\dots,N_2$, where N_1 denotes the number of sensors, and N_2 the number of measurements taken from each sensor, the task is to designate the thickness δ of the boundary

layer (Fig. 2). For known values of the thickness of the boundary layer the discussed problem becomes a direct problem, the solution of which will make it possible to derive temperatures $T_{ij} = T(x_i, t_j)$. Using the calculated temperatures T_{ij} and given temperatures U_{ij}, a functional determining the error of the approximate solution may be constructed

$$J(\delta) = \sum_{i=1}^{N_1}\sum_{j=1}^{N_2}(T_{ij} - U_{ij})^2.$$

(19)

2. Method of solution

The direct Stefan problem (equations (1)-(6) for given thickness of the boundary layer) was solved by means of the alternating phase truncation method [6,7]. The approximate location of the phase change boundary at moment t_{p+1} was designated in such a manner that, at first, the last point of the liquid phase was determined, i.e. such point x_i at which $T(x_i, t_{p+1}) > T^*(Z_L(t_p))$, and the first point of the solid phase, i.e. such point x_j at which $T(x_j, t_{p+1}) \le T^*(Z_L(t_p))$. In the next step, the location of the phase change boundary ξ_{p+1} was designated by linear interpolation of points $(x_i, T(x_i, t_{p+1}))$ and $(x_j, T(x_j, t_{p+1}))$ and by designating the value of the argument for which the interpolation function takes the value: $T^*(Z_L(t_p))$. The velocity of the phase change boundary was determined on the grounds of the Stefan condition (6). Next, on the basis of equation (17) the value of the concentration of the alloy component $Z_L(t_{p+1})$ was calculated for moment t_{p+1}, designating a new value of solidification temperature $T^*(Z_L(t_{p+1}))$.

To find the minimum of the functional (19) a genetic algorithm was used. The calculations involved the use of real number representations of the chromosome and tournament selection. The algorithm also included an elitist model in which the best specimen of the previous population is remembered and, if in the current population all specimens are worse, the worst specimen of the current population is replaced by the remembered best specimen of the previous population. The study also used arithmetical crossover operator and non-uniform mutation operator [7,8]. The calculation were based on the following values of the genetic algorithm: population size $n_{pop}=100$, number of generations $N=100$, crossover probability $p_c=0,7$ and mutation probability $p_m=0,1$.

3. Example of computations

In the example the considered alloy was Cu-Zn (10% Zn) [6]: b=0,08 [m], $\lambda_1=\lambda_2=120$ [W/(m K)], $c_1=c_2=390$ [J/(kg K)], $\rho_1=\rho_2=8600$ [kg/m³], $L=190000$ [J/kg], $\delta=0,0015$ [m], $D_1=3,5\cdot10^{-8}$ [m²/s], $k=0,855$, $Z_0=0,1$, temperature of solidification $T^*(Z_L)=1356–473,68\,Z_L$ [K], the ambient temperature $T_\infty=298$ [K] and initial temperature $T_0=1323$ [K].

It was assumed that in the tested domain there is one thermocouple placed at the distance of 40 mm from the domain boundary (in the middle of the investigated domain). From thermocouple 100 temperature measurements were used (taken at

the time intervals of 1 s). The calculations were based on the exact values of temperature and on the values disturbed by random error with normal distribution and values 1%, 2% as well as 5%. The designated thickness of the boundary layer were: 0.00149917, 0.00150817, 0.00151699 and 0.00154380, respectively for the exact data and for 1%, 2% and 5% errors. The reconstruction errors were: 0.055%, 0.545%, 1.132% and 2.920%.

Table 1.
Errors in the reconstruction of temperature at measurement point (Δ_{sre} - mean value of the absolute error, Δ_{max} - maximum value of the absolute error, δ_{sre} - mean value of the relative error, δ_{max} - maximum value of the relative error)

Per.	0%	1%
Δ_{sre} [K]	$1.388\ 10^{-4}$	$1.517\ 10^{-4}$
Δ_{max} [K]	$4.857\ 10^{-3}$	$5.470\ 10^{-3}$
δ_{sre} [%]	$1.068\ 10^{-5}$	$1.167\ 10^{-5}$
δ_{max} [%]	$3.727\ 10^{-4}$	$4.200\ 10^{-4}$
Zab.	2%	5%
Δ_{sre} [K]	$1.758\ 10^{-4}$	$1.702\ 10^{-4}$
Δ_{max} [K]	$6.932\ 10^{-3}$	$4.054\ 10^{-3}$
δ_{sre} [%]	$1.354\ 10^{-5}$	$1.310\ 10^{-5}$
δ_{max} [%]	$5.322\ 10^{-4}$	$3.111\ 10^{-4}$

In Fig. 3 the exact and reconstructed temperature distribution at the measurement point is shown for the disturbance of 5%. However in Table 1 the reconstruction errors of temperature values at the measurement point were compiled for the exact input data and for the input data burdened with errors 1%, 2% and 5%. It may be inferred from the presented results that in each case the reconstruction of the temperature distribution is very good, and the maximum absolute error does not exceed 0.007 K. Accordingly, the differences in the thickness of the boundary layer do not exert a big impact on the temperature distribution at the measurement point.
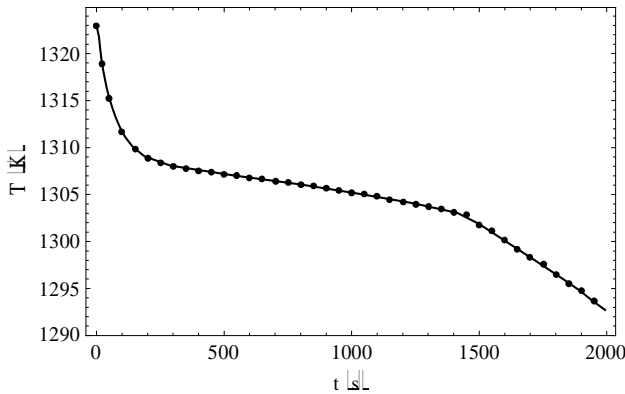

Fig. 3. Exact (solid line) and reconstructed (dots) distributions of the temperature at measurement point for perturbation equals 5%

4. Conclusions

The discussed algorithm makes it possible to designate the thickness of the boundary layer rendering very good reconstruction of temperature distribution. The results indicate, that small differences in the thickness of the boundary layer do not have a significant impact on the temperature distribution. The results are a follow up of [5], where on the grounds of a direct problem with the constant value of solidification rate it was concluded, that small differences in the thickness of the boundary layer do not significantly influence the concentration distribution in the cast.

References

[1] B. Mochnacki, J.S. Suchy, Numerical Methods in Computations of Foundry Processes, PFTA, Cracow 1995.
[2] J.S. Suchy, B. Mochnacki, Analysis of segregation process using the broken line model. Theoretical base, Archives of Foundry, vol. 3, no. 10 (2003), 229-234.
[3] J.S. Suchy, B. Mochnacki, M. Prażmowski, Analysis of segregation process using the broken line model. Numerical realization, Archives of Foundry, vol. 3, no. 10 (2003), 235-240.
[4] J.S. Suchy, B. Mochnacki, M. Prażmowski, Control volume method in numerical modelling of macrosegregation, Zeszyty Naukowe Politechniki Opolskiej ser. Mechanika, vol. 76 (2003), 275-278.
[5] B. Mochnacki, E. Majchrzak, R. Szopa, Simulation of heat and mass transfer in domain of casting made from binary alloy, Archives of Foundry Engineering, vol. 8 (4) (2008), 121-126.
[6] E. Majchrzak, B. Mochnacki, Application of the BEM in the thermal theory of foundry, Engineering Analysis with Boundary Elements, vol. 16 (1995), 99-121.
[7] D. Słota, Solving the inverse Stefan design problem using genetic algorithms, Inverse Problems in Science and Engineering, vol. 16 (2008), 829-846.
[8] D. Słota, Identification of the cooling condition in 2-D and 3-D continuous casting processes, Numerical Heat Transfer Part B, vol. 55 (2009), 155-176.