NUMERICAL SIMULATION OF SOLIDIFICATION PROCESS USING THE SCHEIL MODEL

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Abstract. In the paper the macro model of volumetric solidification is discussed. The mathematical description of the process bases on a one domain approach, this means in order to take into account the evolution of latent heat, the substitute thermal capacity is introduced to the energy equation. This parameter is determined using the well known Scheil model of macrosegregation. In the first part of paper the theoretical considerations are presented, while in the second one the example of simulation are presented (solidification of Al-Si alloy is considered). The numerical algorithm bases on the finite differences method.

1. Mathematical description of the problems

At first the mass balance of alloy component of solidifying material Ω will be presented. Considering two successive time levels t and $t + \Delta t$ one obtains the following form of balance discussed

$$m_S(t)z_S(t) + m_L(t)z_L(t) = m_S(t + \Delta t)z_S(t + \Delta t) + m_L(t + \Delta t)z_L(t + \Delta t) \qquad (1)$$

where z_S, z_L are the concentrations of alloy component in solid and liquid phases, m_S is a mass of solidified part of domain considered, m_L is a mass of molten metal. Assuming that the mass densities $\rho_S = \rho_L$ one can transform the balance (1) to the form

$$V_S(t)z_S(t) + V_L(t)z_L(t) = V_S(t + \Delta t)z_S(t + \Delta t) + V_L(t + \Delta t)z_L(t + \Delta t) \qquad (2)$$

where V_S, V_L are the volumes of liquid and solid in domain Ω.
The change of $V_S(t+\Delta t) - V_S(t)$ (volumetric solidification) is conventionally shown in Figure 1. The values of V_S, V_L and z_S, z_L at the moment $t+\Delta t$ can be found using the Taylor formula

$$V_S(t + \Delta t) \approx V_S(t) + \frac{\mathrm{d}V_S(t)}{\mathrm{d}t}\Delta t \qquad (3)$$

$$V_L(t + \Delta t) \approx V_L(t) + \frac{dV_L(t)}{dt} \Delta t \tag{4}$$

$$z_L(t + \Delta t) \approx z_L(t) + \frac{dz_L(t)}{dt} \Delta t \tag{5}$$

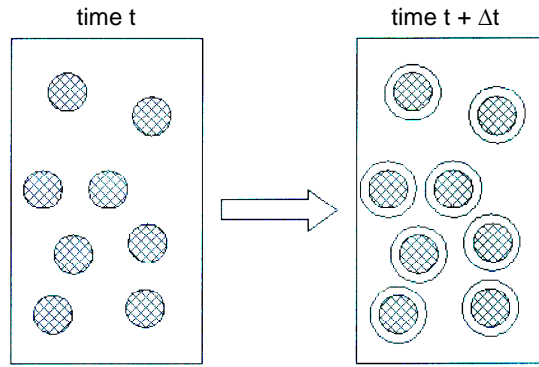$$z_S(t + \Delta t) \approx z_S(t) + \frac{dz_S(t)}{dt} \Delta t \tag{6}$$

time t   time t + Δt

Fig. 1. Change of global V_S

Neglecting the second order terms (Δt^2) one obtains the mass balance in the form

$$V_S \frac{dz_S}{dt} + \frac{dV_S}{dt} z_S + V_L \frac{dz_L}{dt} + \frac{dV_L}{dt} z_L = 0 \tag{7}$$

or

$$f_S \frac{dz_S}{dt} + \frac{df_S}{dt} z_S + f_L \frac{dz_L}{dt} + \frac{df_L}{dt} z_L = 0 \tag{8}$$

where $f_S = V_S/V$, $f_L = V_L/V$ are the volumetric fractions of solid and liquid phases in domain Ω (V is a volume of Ω)

We introduce the partition coefficient $k = z_S/z_L$ [1] (this parameter is assumed to be a constant value), and apply the obvious dependence $f_S = 1 - f_L$. So

$$\frac{df_L}{dz_L} + \frac{f_L}{z_L} = -\frac{k}{1-k} \cdot \frac{1}{z_L} \tag{9}$$

The Scheil model is constructed under the assumption that diffusion of alloy component in a liquid phase proceeds immediately (diffusion coefficient $D_L \rightarrow \infty$), while diffusion in a solid phase can be neglected ($D_S = 0$). From the point of mass

balance presented previously it corresponds to the assumption $dz_S/dt = 0$ and then the equation (9) takes a form

$$\frac{df_L}{f_L} = -\frac{dz_L}{[1-k]z_L}$$

(10)

This simple differential equation must be solved using the condition $z = z_0 : f_L = 1$ (z_0 is an initial concentration of alloy component). In this place it should be pointed out that the constant value of k correspond to equilibrium diagram created by two straight lines with common point $(0, T_p)$, T_p is a solidification point of pure metal - Figure 2.
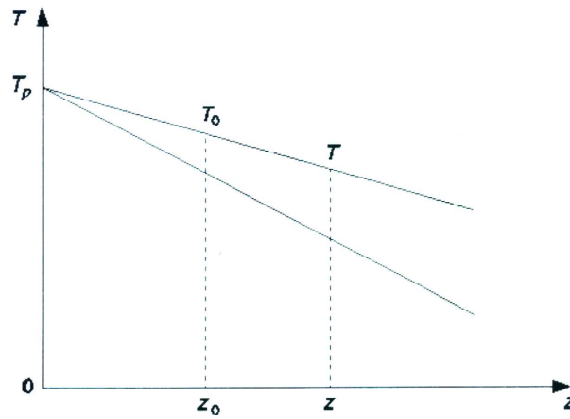

Fig. 2. A fragment of equilibrium diagram

A situation close to this assumption takes place (among others) in the case of Al-Si alloy (for the small concentrations of Si).
The solution of equation (10) is the following

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

(11)

The equation determining the course of upper border line $T = T_L$ (Fig. 2) can be written in the form

$$T = T_p + m\, z_L$$

(12)

where m is a slope of line $T(z_L)$. So, the equation (11) can be transformed to the form

$$f_L = \left(\frac{T_p - T_0}{T_p - T}\right)^{\frac{1}{1-k}}$$

(13)

Now, the basic energy equation determining the solidification and cooling processes in domain Ω will be discussed. It is the parabolic equation known as the Fourier-Kirchhoff one [2, 3]

$$c(T)\frac{\partial T(x,t)}{\partial t} = \nabla[\lambda(T)\nabla T(x,t)] - L\frac{\partial f_L(x,t)}{\partial t} \tag{14}$$

where $c(T)$ is a volumetric specific heat, $\lambda(T)$ is a thermal conductivity, L is a volumetric latent heat, T, x, t denote the temperature, geometrical co-ordinates and time. The form of equation (14) shows that only conductional heat transfer is considered and the convection in the molten metal is neglected.

Let us assume that the function f_S is temperature-dependent one. Because

$$\frac{\partial f_L(x,t)}{\partial t} = \frac{\mathrm{d}f_L(T)}{\mathrm{d}T}\frac{\partial T(x,t)}{\partial t} \tag{15}$$

(this transformation is typical in the case of fixed domain approach application) therefore the equation (14) takes a form [2, 3]

$$\left[c(T) + L\frac{\mathrm{d}f_L(T)}{\mathrm{d}T}\right]\frac{\partial T(x,t)}{\partial t} = \nabla[\lambda(T)\nabla T(x,t)] \tag{16}$$

or

$$c(T)\frac{\partial T(x,t)}{\partial t} = \nabla[\lambda(T)\nabla T(x,t)] \tag{17}$$

Parameter

$$C(T) = c(T) + L\frac{\mathrm{d}f_L(T)}{\mathrm{d}T} \tag{18}$$

is called a substitute thermal capacity and in the case considered it is given by the formula

$$C(T) = c(T) + \frac{L}{(1-k)(T_p - T_0)}\left(\frac{T_p - T_0}{T_p - T}\right)^{\frac{2-k}{1-k}} \tag{19}$$

The details concerning above equation will be discussed in the next chapter.

2. Results of computations

The 2D object being a composition of casting, core and mould sub-domains is shown in Figure 1. It corresponds to the symmetrical fragment of frame with different walls thicknesses. The casting is made from Al-Si alloy (2% Si).
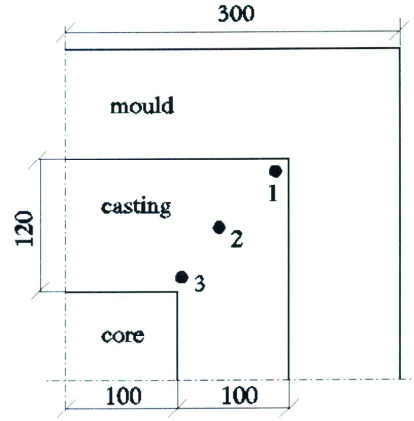
Fig. 3. Domain considered

The following input data have been introduced: $c_S = 2.96 \, \text{MJ/m}^3 \, \text{K}$, $c_L = 3.07$, $\lambda_S = 250 \, \text{W/mK}$, $\lambda_L = 104$, $L = 990.6 \, \text{MJ/m}^3$, $k = 0.25$, $T_p = 660^\circ \text{C}$.

The equations determining the heating processes proceeding in the core and mould sub-domains have a form

$$c_m(T) \frac{\partial T_m(x,t)}{\partial t} = \nabla [\lambda_m(T) \nabla T_m(x,t)] \tag{20}$$

where $c_m(T)$ is a volumetric specific heat of core and mould (these values have been assumed as the same and the constant ones), $\lambda_m(T)$ is a thermal conductivity of core and mould (as previously $\lambda_m = \lambda_c = \text{const.}$). So, $c_m = 1.750 \, \text{MJ/m}^3\text{K}$, while thermal conductivity $\lambda_m = 1.0$.

On the contact surfaces casting-mould and casting-core the continuity of temperature and heat flux is assumed

$$\begin{cases} -\lambda \dfrac{\partial T(x,t)}{\partial n} = -\lambda_m \dfrac{\partial T_m(x,t)}{\partial n} \\ T(x,t) = T_m(x,t) \end{cases} \tag{21}$$

where $\partial/\partial n$ denotes a normal derivative.

Taking into account the symmetry of frame geometry on the external surface of the system the no-flux condition in a form

$$\frac{\partial T(x,t)}{\partial n} = 0 \tag{22}$$

is given. Additionally the initial temperature field in the system is known, in particular

$$t = 0 \quad : \quad T(x,0) = 660, \qquad T_m(x,0) = 20 \tag{23}$$

The definition of $C(T)$ - equation (19) is correct from the mathematical point of view, but in practice the certain difficulties appear. In order to assure the continuity of (19) at the temperature corresponding to $f_S = 1$ ($f_L = 0$) in a place of $c(T)$ one should introduce the value of c_S. Because of the fact that function (13) does not tends towards 0 for temperature characteristic for solid state and the shape of equilibrium diagram of Al-Si alloy (e.g. [4]) only in rather small fragment fulfills the conditions resulting from Figure 2, the value of $c(T)$ must be assumed in an artificial way. It turned out that the continuity of substitute thermal capacity at the border temperature between mushy zone and solid state on obtains for $c(T) = 1.5$ MJ/m^3 K (Fig. 4). For the others concentrations of Si this value should be changed.
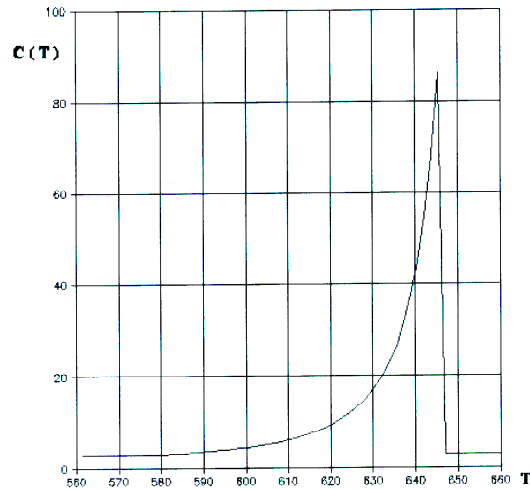

Fig. 4. Course of substitute thermal capacity

Summing up, it seems, that the better variant reduces to the assumption of function $C(T)$ in the form

$$C(T) = c_S + a[T(x,t) - T_S]^p \tag{24}$$

The physical condition resulting from a change of physical enthalpy

$$\int_{T_S}^{T_0} C(T)\mathrm{d}T = c_S(T_0 - T_S) + L \tag{25}$$

must be also fulfilled and additionally the parameter p should be chosen in this way in order to obtain the course of $C(T)$ close to the shape shown in Figure 4.
In Figure 5 the cooling curves at points 1, 2, 3 from costing domain obtained for collected above input data are shown. On a stage of numerical modelling the finite

differences method (FDM) has been used. The casting-core-mould domain has been divided into 900 control volumes, time step $\Delta t = 0.001$ s.
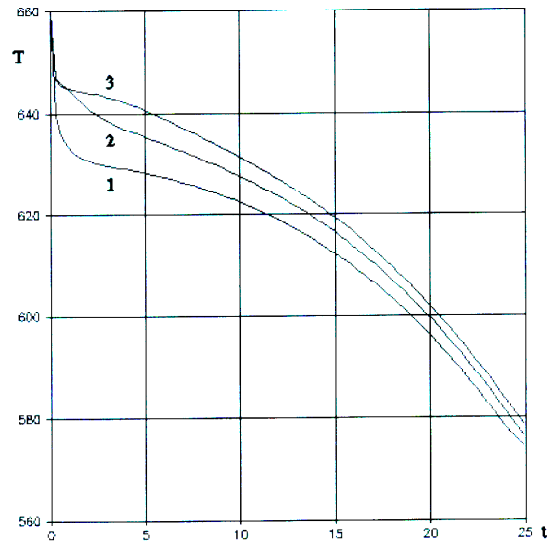

Fig. 5. Cooling curves

It should be pointed out that the formulas (11) and (19) are known in literature, but the aim of authors was to show how these equations can be educed. Additionally we wanted to test the effectiveness of approach basing on the Scheil theory in numerical simulation of solidification process.

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