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MODEL OF THERMAL PROCESSES PROCEEDING IN DOMAIN OF CAST COMPOSITE WITH PARTICLES

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Abstract. The solidification of cast composite with particles is considered, in particular the single lead particle and its spherical surroundings (metal matrix) are analyzed. The dimension of particle-metal matrix sub-domain results from the mean particles radius and the fraction of particles. On a stage of numerical modelling the finite difference method (FDM) is applied. The additional procedures simulating the course of solidification and melting are also introduced. In the final part of the paper the examples of computations are presented.

1. Mathematical formulation of the problem

Thermal interactions between a single particle of lead and metal matrix (Al-Si alloy) are analyzed. In the domain of a cast composite, the control volume corresponding to the lead particle (a central part of this volume) and its surroundings are distinguished - as in Figure 1.

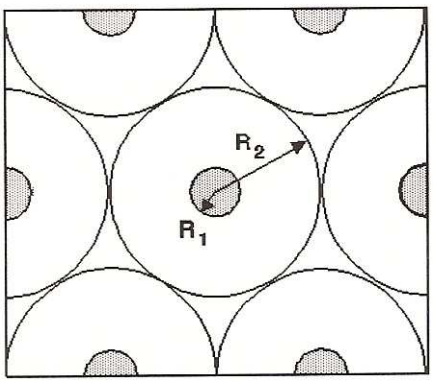

Fig. 1. Set of control volumes

On the external surface of the system, the non-flux condition is assumed. So, the model discussed corresponds to the situation directly after the insertation of particles into the molten metal matrix.

The heat transfer processes proceeding in the heterogeneous system particle - metal matrix are described by a system of Fourier equations and boundary-initial conditions. The solidification and melting processes are taken into account using the one domain method (metal matrix) [1-3] and the temperature recovery method (lead particle) [4, 5].
The different parameters (dimension of particle, volumetric fractions of particles, initial temperature of metal matrix etc.) have been considered and the examples of results are presented in the final part of the paper.
The energy equation describing the solidification and cooling processes in a metal matrix sub-domain Ω_2 can be written in the form (1D problem is considered)

$$c_2(T)\frac{\partial T_2(r,t)}{\partial t}=\frac{1}{r^2}\frac{\partial}{\partial r}\left[\lambda_2(T)\,r^2\frac{\partial T_2(r,t)}{\partial r}\right]+L_2\frac{\partial S_2(r,t)}{\partial t} \tag{1}$$

where c_2, L_2 are the specific heat and latent heat per unit of volume, λ_2 is the thermal conductivity, S_2 is the solid state fraction at the neighborhood of point considered, T_2, r, t denote temperature, spatial co-ordinate and time. Assuming that volumetric solid state fraction S_2 is a known function of temperature one can write

$$\frac{\partial S_2(r,t)}{\partial t}=\frac{\mathrm{d}S_2}{\mathrm{d}T}\frac{\partial T(r,t)}{\partial t} \tag{2}$$

and after the simple mathematical manipulations one obtains

$$\left[c_2(T)-L_2\frac{dS_2}{dT}\right]\frac{\partial T_2(r,t)}{\partial t}=\frac{1}{r^2}\frac{\partial}{\partial r}\left[\lambda_2(T)\,r^2\frac{\partial T_2(r,t)}{\partial r}\right] \tag{3}$$

or

$$C_2(T)\frac{\partial T_2(r,t)}{\partial t}=\frac{1}{r^2}\frac{\partial}{\partial r}\left[\lambda_2(T)\,r^2\frac{\partial T_2(r,t)}{\partial r}\right] \tag{4}$$

The parameter $C_2(T)$ is called a substitute thermal capacity, while this approach especially convenient in the case of alloy solidification modelling is called 'a one domain method'. The solidification of alloys proceeds in an interval of temperatures $T_2\in[T_S,T_L]$ corresponding to mushy zone sub-domain, at the same time $S_2(T_S)=1$, $S_2(T_L)=0$, in the interval considered $S_2\in[0,1]$. One of the possibilities of $C_2(T)$ construction results from the assumption that this function (e.g. polynomial) fulfills the condition resulting from a change of mushy zone physical enthalpy, namely

$$\int_{T_S}^{T_L} C_2(T)\,\mathrm{d}T = c_p(T_L - T_S) + L_2 \tag{5}$$

where c_p is a mushy zone volumetric specific heat. Additionally one assumes the C^1 class continuity of $C_2(T)$ at the points T_S and T_L. Finally the approximation of substitute thermal capacity (STC) can be found.
The course of STC for Al-Si alloy is shown in Figure 2.

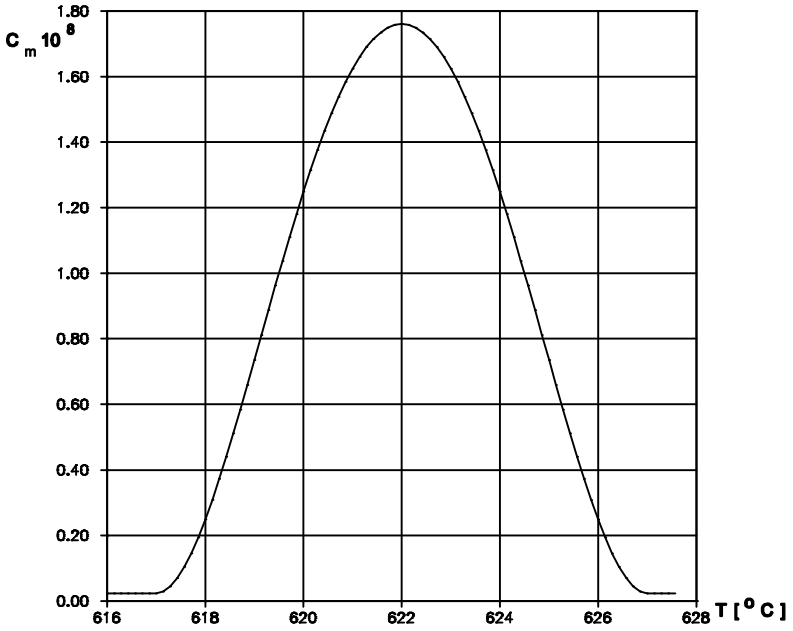

Fig. 2. STC of Al-Si [J/m^3 K]

Thermal processes proceeding in the lead particle sub-domain (pure metal) should be described using the Stefan model (e.g. [6]). In numerical realization the approach called 'a temperature recovery method' is here used, and then the course of thermal processes in the particle volume Ω_1 can be analyzed on the basis of equation

$$c_1(T)\frac{\partial T_1(r,t)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left[\lambda_1(T)\,r^2\,\frac{\partial T_1(r,t)}{\partial r}\right] \tag{6}$$

where c_1 is a volumetric specific heat of solid metal. The results obtained under this assumption can be in a special way 'rebuilt' in order to take into account the real course of the process. In other words, the particle sub-domain is treated as a homogeneous one, while the temperature field found from this equation for time t is corrected using the temperature recovery procedure.

On the contact surface $r = R_1$ the continuity condition in the following form

$$r = R_1: \quad \begin{cases} -\lambda_1 \dfrac{\partial T_1(r,t)}{\partial r} = -\lambda_2 \dfrac{\partial T_2(r,t)}{\partial r} \\ T_1(r,t) = T_2(r,t) \end{cases} \tag{7}$$

is assumed, while for $r = R_2$:

$$q(r,t) = -\lambda_2 \frac{\partial T_2(r,t)}{\partial r} = 0 \tag{8}$$

The initial condition

$$t = 0: \; T_1(r,0) = T_{10}, \; T_2(r,0) = T_{20} \tag{9}$$

is also known.

2. Temperature recovery method

Let us assume that the thermophysical parameters of liquid and solid part of particle sub-domain are constant and equal. The 'reserve' of temperature θ is defined as follows [6]

$$\theta = \frac{L_1}{c_1} \tag{10}$$

where L_1 as a lead volumetric latent heat.

If the point x_i belongs to the particle domain then at the moment $t = 0$ the temperature at this point corresponds to the initial temperature T_{10} whereas the temperature reserve results from (10). On the basis of numerical methods one can find a discrete temperature field at the set of points x_i for successive levels of time. If during the interval $\Delta t = t^f - t^{f-1}$ the temperature $T_1(x_i, t^f)$ increases above the melting point T^*, then it is assumed that the temperature at this point is equal to T^* and the reserve of temperature must be decreased, namely $\theta(x_i, t^f) = \theta(x_i, t^{f-1}) - \Delta\theta(x_i, t^f)$, where $\Delta\theta(x_i, t^f) = T_1(x_i, t^f) - T^*$. So, the temperature field obtained at time t^f is corrected in following way:

- For the nodes in which $T_1(x_i, t^f) < T^*$, the temperature reserve $\theta(x_i, t^f)$ is untouched and equal to its initial value. The calculated temperature $T_1(x_i, t^f)$ is, of course, accepted.

– For the nodes in which $T_1(x_i,t^f)>T^*$ and $T_1(x_i,t^{f-1})<T^*$ it is assumed that $T_1(x_i,t^f)=T^*$ and the TRM procedure is initiated.
– For the nodes fulfilling the conditions $T_1(x_i,t^{f-1})=T^*$, $T_1(x_i,t^f)>T^*$ and $\theta(x_i,t^{f-1})>0$ it is assumed that $T_1(x_i,t^f)=T^*$ and the temperature reserve is decreased according to the formula $\theta(x_i,t^f)=\theta(x_i,t^{f-1})-\Delta\theta(x_i,t^f)$.
– For the nodes in which $T_1(x_i,t^f)\geq T^*$ and $\theta(x_i,t^f)\leq 0$ the obtained value of temperature is accepted.

3. Finite difference method

The following differential operator is considered [6]

$$F(x)=\frac{1}{x^m}\frac{\partial}{\partial x}\left[\lambda x^m\frac{\partial T}{\partial x}\right] \tag{11}$$

This is a typical component of a 1D energy equation, while $m=0,1,2$ corresponds to the geometry of plate, cylinder and sphere.

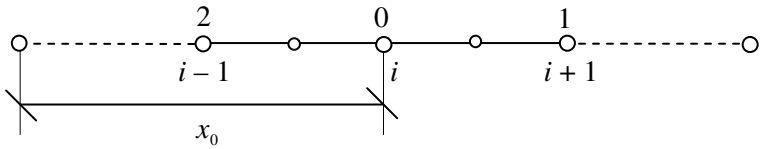

Fig. 3. The star

In Figure 3a 1D three-points star with two auxiliary points and double numeration (global and local) is shown.
We shall use the mean differential quotient

$$\left(x^m\lambda\frac{\partial T}{\partial x}\right)_{i+0.5}=x_{i+0.5}^m\,\lambda_{i+0.5}\frac{T_{i+1}-T_i}{h}=\left(x_0+\frac{h}{2}\right)^m\frac{T_1-T_0}{R_{01}} \tag{12}$$

$$\left(x^m\lambda\frac{\partial T}{\partial x}\right)_{i-0.5}=x_{i-0.5}^m\,\lambda_{i-0.5}\frac{T_i-T_{i-1}}{h}=\left(x_0-\frac{h}{2}\right)^m\frac{T_0-T_2}{R_{02}} \tag{13}$$

Let us the thermal conductivities at the auxiliary points are defined as a harmonic means of λ_{i-1}, λ_i and λ_i, λ_{i+1}. Then it can be shown that

$$R_{01} = \frac{0.5h}{\lambda_{i+1}} + \frac{0.5h}{\lambda_i} \tag{14}$$

and

$$R_{02} = \frac{0.5h}{\lambda_{i-1}} + \frac{0.5h}{\lambda_i} \tag{15}$$

at the same time, the points $i-1,\ i,\ i+1$ can belong to the different sub-domains (see [6]). Using the mean quotient again one obtains

$$\frac{1}{x^m}\frac{\partial}{\partial x}\left(\lambda x^m \frac{\partial T}{\partial x}\right)_i = \frac{1}{x_0^m}\frac{1}{h}\left[\left(x_0 + \frac{h}{2}\right)^m \frac{T_1 - T_0}{R_{01}} + \left(x_0 - \frac{h}{2}\right)^m \frac{T_2 - T_0}{R_{02}}\right] \tag{16}$$

or

$$\frac{1}{x^m}\frac{\partial}{\partial x}\left(\lambda x^m \frac{\partial T}{\partial x}\right)_i = \sum_{e=1}^{2} \frac{T_e - T_0}{R_{0e}} \Phi_e \tag{17}$$

where

$$\Phi_1 = \frac{1}{h}\left(\frac{x_0 + 0.5h}{x_0}\right)^m,\ \Phi_2 = \frac{1}{h}\left(\frac{x_0 - 0.5h}{x_0}\right)^m \tag{18}$$

It should be pointed out, that in the case considered $m = 2$.
Because the non-steady state problem is considered the time grid with step $\Delta t = t^f - t^{f-1}$ must be introduced (t^{f-1}, t^f denote two successive levels of time). Using the explicit scheme, the following FDM equation can be taken into account

$$c_0^{f-1} \frac{T_0^f - T_0^{f-1}}{\Delta t} = \sum_{e=1}^{2} \frac{T_e^{f-1} - T_0^{f-1}}{R_{0e}^{f-1}} \Phi_e \tag{19}$$

from which the values of T_0^f can be found. The FDM equation for the boundary node close to external surface of the system is the same as (19), but the thermal resistance R_{01} should be assumed as a very big value (e.g. 10^{10}). Because the explicit scheme is considered, the well known stability conditions determine the border value of time interval in equations (19).

4. Examples of computations

The particles of diameters from 0.1 to 1 mm have been considered. The external radius of control volume results from the assumption concerning the volumetric

fraction of particles and metal matrix in the domain of cast composite. Various pouring temperatures have been also taken into account.

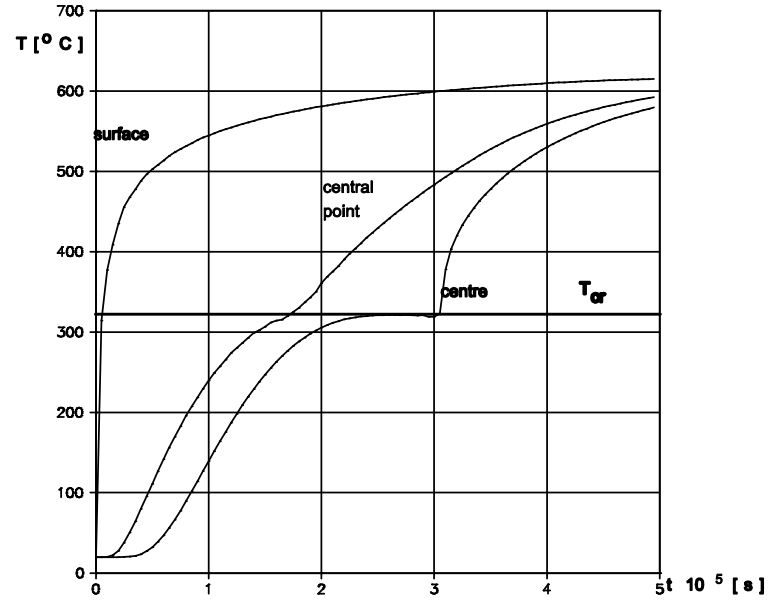

Fig. 4. Temperature history (particle)

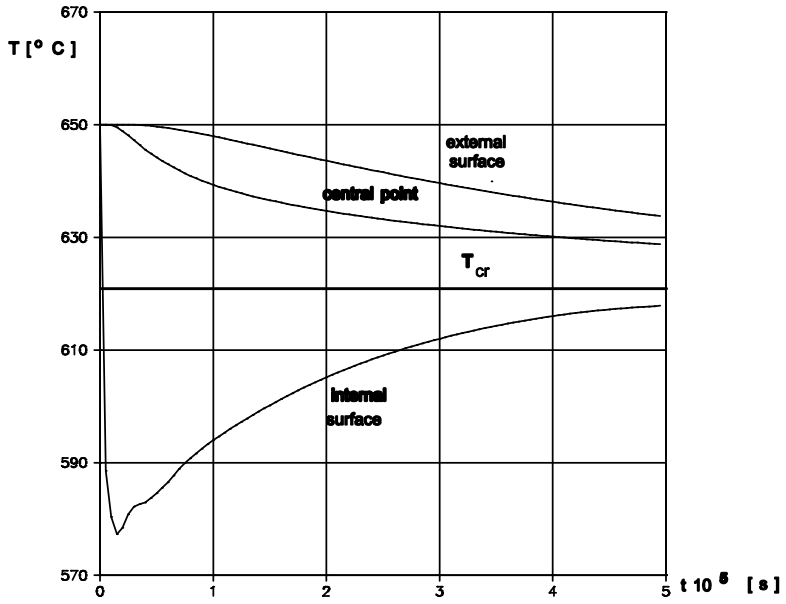

Fig. 5. Temperature history (metal matrix)

The following thermophysical parameters have been assumed [7]: thermal conductivity of lead $\lambda_1 = 30$ W/mK, thermal conductivity of Al-Si alloy $\lambda_2 = 90$ W/mK, latent heat of lead $L_1 = 2.92 \cdot 10^8$ J/m^3, latent heat of Al-Si alloy $L_2 = 9.5 \cdot 10^8$ J/m^3. The initial temperature of particle $T_{10} = 20°\text{C}$, initial temperature of Al-Si alloy $T_{20} = 650°\text{C}$. In Figures 4 and 5, as an example, the heating (cooling) curves in the particle with diameter 0.1 mm and metal matrix sub-domains are shown. One can see that for this particle dimension, the process proceeds very quickly and after a time $t = 3 \cdot 10^{-5}$ s, the whole domain of the particle is in a liquid state. Nevertheless, the particle acts to a certain degree as an internal chill because the temperature of the contact surface drops below the solidification point of the Al-Si alloy.

Summing up, the numerical model presented in this paper can be effectively applied for the analysis of thermal processes proceeding in the particle and metal matrix sub-domains.

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