Numerical analysis of thermal processes in domain of cast composite with spherical particles

M. Ciesielski a, B. Mochnacki b*

a Institute of Computer and Information Science, Częstochowa University of Technology
b Institute of Mathematics, Częstochowa University of Technology
Dąbrowskiego 73, 42-200 Częstochowa, Poland
*Corresponding author. E-mail address: bohdan.mochnacki@im.pcz.pl

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Abstract

Heat transfer proceeding in domain of cast composite with particles is considered. In particular the thermal processes in a sub-domain being the composition of single spherical particle (Pb) and adjoining metal matrix (Al) are analyzed. Initial temperatures of components correspond to solid state (particle) and liquid one (matrix). Numerical algorithm corresponding to a mathematical model of the boundary-initial problem discussed is constructed on the basis of control volume method. In the final part of the paper the examples of computations are shown.

Keywords: Cast composite, Solidification, Numerical modelling

1. Introduction

The macrostructure of material considered is shown in Figure 1 [1]. The governing equations concern the cubic sub-domain in which the single spherical particle is located at the central part of cube (the dimension of cube results from assumed particles density) – Figure 2. On the walls limiting the cubic sub-domain the no-flux boundary conditions are taken into account, in other words, the small temperature gradients in the interior of casting domain are considered (volumetric solidification). Initial temperature of metal matrix corresponds to the liquid state, while the initial temperature of particles corresponds to the solid one. Between particles and metal matrix the ideal thermal contact is assumed.

Fig. 1. a) The microstructure of AK9-Pb composite, b) One Pb particle with primary α phase crystals
Fig. 2. The cast composite domain

Summing up, the following boundary-initial problem is considered

\[ c_m(T) \frac{\partial T_m(x,t)}{\partial t} = \text{div}(\lambda_m(T) \nabla T_m(x,t)) + L_m \frac{\partial f_{SM}(x,t)}{\partial t}, \]  

where \( m = 1, 2 \) identifies the matrix and particle sub-domains, \( c_m \) is the volumetric specific heat, \( \lambda_m \) is the thermal conductivity, \( L_m \) is the volumetric latent heat, \( f_{SM} \) is the solid state fraction at the neighbourhood of point considered, \( T, x = \{ x_1, x_2, x_3 \} \), \( t \) denote temperature, spatial co-ordinates and time.

On the contact surface between matrix and particle the IV type of boundary condition is assumed

\[ \frac{\partial T_1(x,t)}{\partial n} = -\lambda_1 \frac{\partial T_2(x,t)}{\partial n}, \]

where \( \partial / \partial n \) denotes a normal derivative, while on the outer surface of the system

\[ \frac{\partial T_i(x,t)}{\partial n} = 0 \]  

The initial conditions are also given

\[ t = 0: \quad T_1(x,t) = T_{01}, \quad T_2(x,t) = T_{02} \]

The solidification (metal matrix) and melting (particle) proceed in a constant temperature \( T_{m*} \) (pure metals are considered). In this case the enthalpy related to an unit of volume is defined as follows

\[ H_m(T) = \int_0^T [c_m(\mu)]d\mu + L_m \eta_m(T) \]

where \( \eta_m(T) = 0 \) for \( T < T_{m*} \), \( \eta_m(T) = 1 \) for \( T > T_{m*} \) - see Figure 3. The definition (5) will be used on a stage of CVM equations construction (next chapter).

![Enthalpy-temperature diagram](image)

Fig. 3. Enthalpy-temperature diagram (solidification at constant temperature)

The practical and theoretical problems connected with cast composite solidification can be found, among others, in [1-5].

2. Control Volume Method (CVM)

The domain considered and its discretization is shown in Figure 4. One can see that the cubic CV are applied. The energy balances corresponding to heat exchange between the analyzed control volume \( \Delta V_i \) and adjoining control volumes (see Figure 5) results from the integration of energy equation with respect to time and volume \( \Delta V \). Let us consider the interval of time \( \Delta t \) while \( \Delta t = t^i + 1 - t^i \).

![Discretization of the domain considered](image)

Fig. 4. Discretization of the domain considered
Then
\[ \int_{t^i}^{t^f} \int_{CV} c_m(T) \frac{\partial T_m(x,t)}{\partial t} \, dV \, dt = \int_{t^i}^{t^f} \int_{CV} \text{div}(\lambda_m(T) \text{grad} T_m(x,t)) \, dV \, dt + \int_{t^i}^{t^f} \int_{CV} L_m \frac{\partial f_{Sm}(x,t)}{\partial t} \, dV \, dt \]

Using the Gauss-Ostrogradsky’s theorem one obtains
\[ \int_{t^i}^{t^f} \int_{CV} c_m(T) \frac{\partial T_m(x,t)}{\partial t} \, dV \, dt = \int_{t^i}^{t^f} \int_{CV} n \cdot (\lambda_m(T) \text{grad} T_m(x,t)) \, dA \, dr + \int_{t^i}^{t^f} \int_{CV} L_m \frac{\partial f_{Sm}(x,t)}{\partial t} \, dV \, dt \]

The approximation of the left-hand side of the energy equation (7) can be taken in the form
\[ \int_{t^i}^{t^f} \int_{CV} c_m(T) \frac{\partial T_m(x,t)}{\partial t} \, dV \, dt \equiv c_f \left( T^{f+1} - T^f \right) \Delta V_i \quad (8) \]

where \( c_f \) is an integral mean of thermal capacity and this value is approximated by the volumetric specific heat corresponding to the temperature \( T^f \). In a similar way one can approximate the last component in equation (7), namely
\[ \int_{t^i}^{t^f} \int_{CV} L_m \frac{\partial f_{Sm}(x,t)}{\partial t} \, dV \, dt \equiv L_f \left( f^{f+1} - f^f \right) \Delta V_i \quad (9) \]

The term determining heat conduction between \( \Delta V_i \) and its neighborhoods can be written in the form
\[ \int_{t^i}^{t^f} \left( \sum_{j=1}^{6} \lambda_{ij} \frac{T^{f+1}_{(j)} - T^f_{(j)}}{h_{(j)}} A_{(j)} \right) \, dA_{(j)} \]

where \( \lambda_{ij} \) is a mean thermal conductivity between nodes \( i \) and \( (j) \)
\[ \lambda_{ij} = \frac{2 \lambda_i \lambda_{(j)}}{\lambda_i + \lambda_{(j)}} \quad (11) \]

The energy balance written in the convention of “explicit” scheme takes the form
\[ c_f \left( T^{f+1} - T^f \right) \Delta V_i = \sum_{j=1}^{6} \lambda_{ij} \frac{T^{f+1}_{(j)} - T^f_{(j)}}{h_{(j)}} A_{(j)} \Delta t + L_f \left( f^{f+1} - f^f \right) \Delta V_i \quad (12) \]

from which
\[ T^{f+1} = T^f + \frac{\Delta t}{c_f \Delta V_i} \sum_{j=1}^{6} \lambda_{ij} \frac{T^{f+1}_{(j)} - T^f_{(j)}}{h_{(j)}} A_{(j)} + L_f \frac{c_f}{c_i} \left( f^{f+1} - f^f \right) \quad (13) \]

or
\[ T^{f+1} = T^f + \sum_{j=1}^{6} W_j \left( T^{f+1}_{(j)} - T^f_{(j)} \right) + L_f \frac{c_f}{c_i} \left( f^{f+1} - f^f \right) \quad (14) \]

where
\[ W_j = \frac{\lambda_{ij} A_{(j)} \Delta t}{c_f h_{(j)} \Delta V_i} \quad (15) \]

The stability condition
\[ 1 - \sum_{j=1}^{6} W_j > 0 \quad (16) \]
allows to determine the critical time step

\[ \Delta t < \left\{ \frac{\mu_i}{\sum_{j=1}^{n} \lambda_i \rho_i \Delta V_i} \right\}^{-1} \tag{17} \]

The similar equation can be used in the case of external CV (non-flux condition) but in formula (14) a part of coefficient \( W_j \) is equal to 0.

During the heating (cooling) processes proceeding in domain of \( \Delta V_i \) the following situation must be taken into account:

**Case 1:** If \( T_i^f \neq T_i^s \) then it is assumed that \( f_{S_i}^{f+1} = f_{S_i}^f \) and simultaneously \( T_i^{f+1} \) is calculated from eq. (14) – the last term in eq. (14) is equal to 0. In the case, where the calculated temperature \( T_i^{f+1} \) is \( T_i^{f+1} < T_i^s \) (for \( T_i^f > T_i^s \)) or \( T_i^{f+1} > T_i^s \) (for \( T_i^f < T_i^s \)) then it is assumed that \( T_i^{f+1} = T_i^s \), whereas new value of \( f_{S_i}^{f+1} \) is calculated on the basis of eq. (14), as

\[ f_{S_i}^{f+1} = f_{S_i}^f + \frac{c_i}{L_i} \left( T_i^s - T_i^f - \sum_{j=1}^{n} W_j \left( T_{i(j)}^f - T_i^f \right) \right) \tag{18} \]

The above relationship allows to start the solidification (melting) process at a constant temperature.

**Case 2:** If \( T_i^f = T_i^s \) then it is assumed that \( T_i^{f+1} = T_i^s \) and \( f_{S_i}^{f+1} \) is determined on the basis of eq. (14) (assuming \( T_i^{f+1} = T_i^s \)) as

\[ f_{S_i}^{f+1} = f_{S_i}^f - \frac{c_i}{L_i} \sum_{j=1}^{n} W_j \left( T_{i(j)}^s - T_i^s \right) \tag{19} \]

If the calculated value of \( f_{S_i}^{f+1} \) from eq. (19) is \( f_{S_i}^{f+1} > 1 \) then it is set \( f_{S_i}^{f+1} = 1 \) or if \( f_{S_i}^{f+1} < 0 \) then it is set \( f_{S_i}^{f+1} = 0 \). Next, the new value of \( T_i^{f+1} \) is calculated using eq. (14). In this way, the solidification (melting) process ends and at the same time starts cooling (heating) of metal.

The other variants of CVM application for numerical modeling of solidification one can find in [6-9].

3. Example of computation

The system of metal matrix (Al) and lead particle (Pb) is considered. The side of the cube is \( l = 173.65 \mu \mathrm{m} \), particle diameter is \( d = 100 \mu \mathrm{m} \) (the value of \( l \) has been determined such that the volume fraction of lead particle in the cube was 10%). Thermophysical parameters of sub-domains are equal – for Al: \( c_S = 2.916 \times 10^6 \), \( c_L = 3.07 \times 10^6 \) J/(m\(^3\) K), \( \lambda_S = 261 \), \( \lambda_L = 104 \) W/(m K), \( \gamma = 1.053 \times 10^3 \) J/m\(^3\), \( T^* = 660 \) °C, and for Pb: \( c_S = 1.966 \times 10^6 \), \( c_L = 1.579 \times 10^6 \) J/(m\(^3\) K), \( \lambda_S = 30.7 \), \( \lambda_L = 24.4 \) W/(m K), \( \gamma = 2.5316 \times 10^6 \) J/m\(^3\), \( T^* = 372 \) °C. The initial temperature of metal matrix is \( T_{0i} = 700 \) °C, the initial temperature of lead particle is \( T_{0f} = 20 \) °C.

In Figure 6 the course of isotherms corresponding to section A (see Figure 4) for times \( t = 0.01, 0.05, 0.1 \) ms are shown. In Figure 7 the temperature histories at the selected points are presented. The last Figure 8 shows the changes of \( f_S \) at the same set of points.

4. Conclusions

From the qualitative point of view the results of numerical simulations correspond to the real course of heat transfer process in the system particle-matrix. During the first stage of thermal
interactions the particle acts in a similar way as an internal chill. Close to the external surface of particle a thin film of solidified matrix is generated. Next the temperature of particle increases and the transition from solid to liquid state takes place. The thickness of solid aluminium film decreases, but during the time for which the simulation has been done the very thin solid film can be observed. The temperature of system declines - it results from the heterogeneous initial condition in the system considered. The further stages of cooling are determined by the boundary conditions given on the outer surface of casting but this process is not considered here.

The version of the CVM algorithm presented in this paper seems to be a quite effective tool for numerical modeling of thermal processes in domains being the composition of materials for which the solidification and melting proceeds at the constant temperature.

It should be pointed out that the similar problem (1D task has been considered) was numerically solved by R. Szopa [10, 11] and the solution basing on the combined variant of boundary element method has been applied.

The further investigation in the scope of paper subject should be connected with the change of mathematical model of heat conduction in the system particle-matrix, in particular the Cattaneo-Vernotte equation of dual phase lag model can be considered.

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References

