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THE NUMERICAL ALGORITHM OF SOLIDIFICATION MODELLING USING THE MICRO-MACRO APPROACH

Mariusz Ciesielski

Institute of Mathematics and Computer Science, Czestochowa University of Technology, Poland
email: mariusz@imi.pcz.pl

Abstract. In this paper the numerical algorithm simulating the solidification process on the micro/macro level is presented. In order to solve the problem the control volume method is applied. The casting domain is covered by the mesh of regular macro-cells and next in every macro-cell the mesh of control volumes is generated. The control volumes correspond to the final shape of grains and they are approximated by the Thiessen polygons (2D task), while their central points correspond to the initial positions of nuclei (generated in a random way). The changes of temporary volumetric fraction of solid at the considered point from casting domain result from the laws determining the nucleation and nuclei growth. In the final part of the paper the example of computation is shown.

Introduction

For numerical modelling solidification process of pure metal or alloys, the macro models (the 1st generation models) and micro models (the 2nd generation models) are generally used [1]. The macro models base on phase diagrams without a direct relation with the microstructures of solidified metal, whereas in the micro models the microstructure evolution (nucleation and growth of the grains) during the solidification process is considered. Nucleation begins as the temperature of liquid metal decreases below the solidification point T^* and proceeds until the temperature begins to increase (recalescence point). Then the number of nuclei achieves a maximum value. After the nucleation, the grains radii increase continuously until volume of solid state fills the whole volume of casting domain. In this paper the model of crystallization process based on the Johnson-Mehl--Avrami-Kolmogorov (JMAK) theory [1, 2] is taken into account. The kinetics of nucleation and nuclei growth is proportional to the undercooling below T^*. The numerical solution of such micro-macro model gives information concerning solidification time, cooling curves, data concerning the undercooling and also the number and size of grains, etc.

On the stage of computations the control volume method (CVM) has been used. The control volumes correspond to the final shapes of grains (in other words, to the primary structure of the casting). In order to assure the correctness and exact-

ness of the algorithm proposed the control volumes in the shape of the Thiessen polygons are generated (the sectors joining the neighboring nodes are perpendicular to the surfaces limiting the control volumes) [3, 4]. The details concerning the generation of the mesh created by the Thiessen polygons can be found in [3, 5].

1. Mathematical modelling using control volume method

CVM constitutes the effective tool for numerical computations of the heat transfer processes. The domain analyzed is divided into n volumes. The CVM algorithm allows to find the transient temperature field at the set of nodes corresponding to the central points of control volumes. The nodal temperatures can be found on the basis of energy balances for successive volumes.

Let us consider the control volume ΔV_0 with central node x_0 - see Figure 1. It is assumed here that the thermal capacities and capacities of internal heat sources are concentrated in the nodes representing elements, while thermal resistances are concentrated in the sectors joining the nodes.

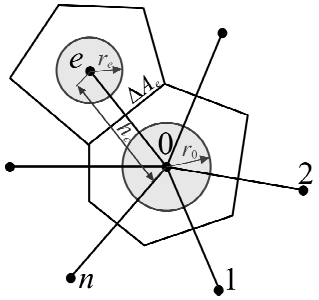

Fig 1. Control volume ΔV_0 and one of its neighboring control volumes ΔV_e

The change of enthalpy of control volume ΔV_0 equals [2, 6]

$$\Delta H_0 = c_0^f \left(T_0^{f+1} - T_0^f\right)\Delta V_0 \tag{1}$$

where c_0^f is the volumetric specific heat, f, f+1 denotes two successive time levels. We assume that the heat fluxes flowing to the ΔV_0 are proportional to the temperature differences at the moment $t = t^f$, then we shall obtain a solving system of the type 'explicit scheme'. So

$$Q_e = \left(T_e^f - T_0^f\right)\Delta A_e / R_{0e}^f \Delta t \tag{2}$$

where R_{0e}^f is the thermal resistance between points x_0 and x_e, ΔA_e surface limiting the domain ΔV_0 in direction e. If we denote as r_0^f and r_e^f the temporary grain radiuses at moment t^f and by h_e the distance between the nodes x_0, x_e then

$$R_{0e}^{f} = \frac{r_0^{f} + r_e^{f}}{\lambda_S} + \frac{h_e - \left(r_0^{f} + r_e^{f}\right)}{\lambda_L} \tag{3}$$

where λ_L and λ_S are the thermal conductivities of liquid and solid phases. The other definition of thermal resistance should be introduced for the boundary volumes [2].

Let us write the balance equation in explicit scheme

$$c_0^{f}\left(T_0^{f+1} - T_0^{f}\right)\Delta V_0 = \sum_e \frac{T_e^{f} - T_0^{f}}{R_{0e}^{f}} \Delta A_e \Delta t + \Delta V_0 q_V \Delta t \tag{4}$$

or

$$T_0^{f+1} = \sum_{e=0}^{n} W_e T_e^{f} + \frac{q_V \Delta t}{c_0^{f}} \tag{5}$$

where

$$W_e = \frac{\Delta t\, \Delta A_e}{c_0^{f} R_{0e}^{f}\, \Delta V_0} \quad \text{for } e > 0, \quad W_0 = 1 - \sum_{e=1}^{n} W_e \tag{6}$$

In order to assure the stability of above explicit scheme the coefficient W_0 must be positive.

The capacity of internal heat sources results from the formula

$$q_V = L \frac{\partial f_S}{\partial t} \tag{7}$$

where L is the volumetric latent heat, f_S is the solid state fraction at the neighborhood of considered point from casting domain. So, the capacity of internal heat sources equals

$$q_V = L \frac{f_S^{f+1} - f_S^{f}}{\Delta t} \tag{8}$$

The value of f_S for the control volume ΔV_0 we define as follows

$$f_S^{f} = \left[\frac{\pi (r_0^{f})^2}{|\Delta V_0|} \right]^{3/2} \tag{9}$$

Let us denote as ΔT_0 the undercooling below the solidification point at the node x_0:

$$\Delta T_0^{f} = T^{*} - T_0^{f} \tag{10}$$

According to [1], the solid phase growth (equiaxial grains) is determined by following formula

$$u = \frac{\mathrm{d}r(t)}{\mathrm{d}t} = \mu\, \Delta T^2(t) \tag{11}$$

where μ is the growth coefficient. The formula (11) allows to determine the temporary values of the r_0 changes and next to determine the local capacity of source function. The next formula

$$N(t) = \Psi\, \Delta T^2(t) \tag{12}$$

where Ψ is the nucleation coefficient, allows to calculate a number of nuclei in fixed casting volume.

2. Computational algorithm

At the beginning of computational algorithm, the casting domain is divided into the regular (e.g. in the shape of squares) macro-cells. In every macro-cell randomly set of central points is generated and next the mesh of control volumes (the Thiessen polygons) is created. The number of control volumes (or number of nuclei) in macro-cell depends on the maximum undercooling $\Delta T_{\max}$ below the solidification point T^*. This number is estimated on the basis of preliminary simulation with redundancy number of control volumes in order to determine average $\Delta T_{\max}$ in every macro-cell. Next, the value of $\Delta T_{\max}$ is substituted into formula (12) and the result is multiplied by the volume of macro-cell.

Heat transfer between two neighbouring macro-cells is transmitted through internal boundaries. For every internal boundary at every computational time step the heat flux flowing through these boundaries is calculated. The heat flux is determined on the basis of temperature difference at the control volumes that are adjacent to boundary. In this way specified heat fluxes (internal and external) constitute the boundary conditions for macro-cells at the next computational time step.

For every micro control volume filling macro-cell the changes of temperature are determined by eqn. (5). At every computational time step the average temperature T_{avg} in macro-cell is calculated. If $T_{\mathrm{avg}} < T^*$ then the number of nuclei is calculated from formula (12). In the case of difference between present and previous number of nuclei, the control volumes (only from undercooled and non-grained) are chosen in a random way and grains growth in these control volumes is begun. The growth of grain causes the increase of f_S and change of q_V in the control volume. The process of nucleation will go on until the all control volumes in macro-cell will be grained.

3. Example of numerical simulation

As the example testing the correctness of proposed algorithm, the aluminium bar (2D task) with dimensions 0.01m × 0.01m (see Figure 2) has been considered. The domain has been divided into 16 macro-cells. The substitute heat transfer coefficient $\alpha = 100$ W/(m^{2}K) (the Robin's boundary condition) at the bottom boundary has been assumed, at the same time the non-flux boundary conditions at the other boundaries have been applied. Initial casting temperature equals $T_0 =$ = 700°C, ambient temperature T_{amb} = 20°C, the thermophysical parameters of casting are the following: $c_S = 2.916 \cdot 10^6$, $c_L = 3.07 \cdot 10^6$ J/(m^3 K), $\lambda_S = 261$, $\lambda_L =$ = 104 W/(m K), $L = 1.053 \cdot 10^9$ J/m^3, $T^* = 660$°C, $\mu = 3 \cdot 10^{-6}$ m/(s K^2), $\Psi =$ = $4.6 \cdot 10^8$ grains/(m^3 K^2) or $\Psi = 6 \cdot 10^5$ grains/(m^2 K^2) (for 2D section).

After preliminary simulation the averages $\Delta T_{\max}$ in the macro-cells have been determined. The average $\Delta T_{\max}$ in each rows (looking from the bottom of Figure 2) is equal to: 3.63, 2.94, 2.66 and 2.61°C. Hence, the number of control volumes in macro-cell has been estimated to be 50, 33, 27 and 26 respectively. Total number of the control volumes is 544. In Figure 2 the size of grains after the time 30 s are shown. In Figure 3*a* the cooling curves (the average temperature) in the selected macro-cells *A*, *B*, *C* and *D* (see Figure 2) in casting domain are presented. In Figure 3*b* zoom of nucleation phase from Figure 3*a* and number of created nuclei (sum over all macro-cells) are shown.

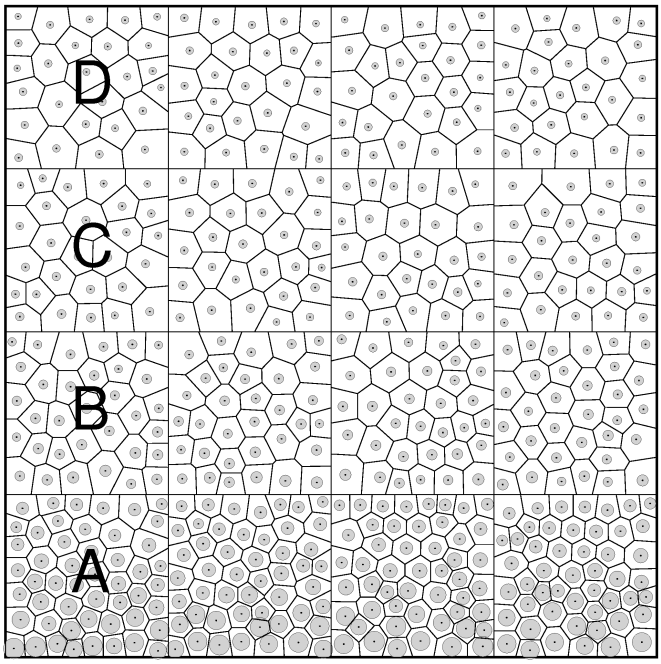

Fig. 2. Example of local primary structure after 30 s

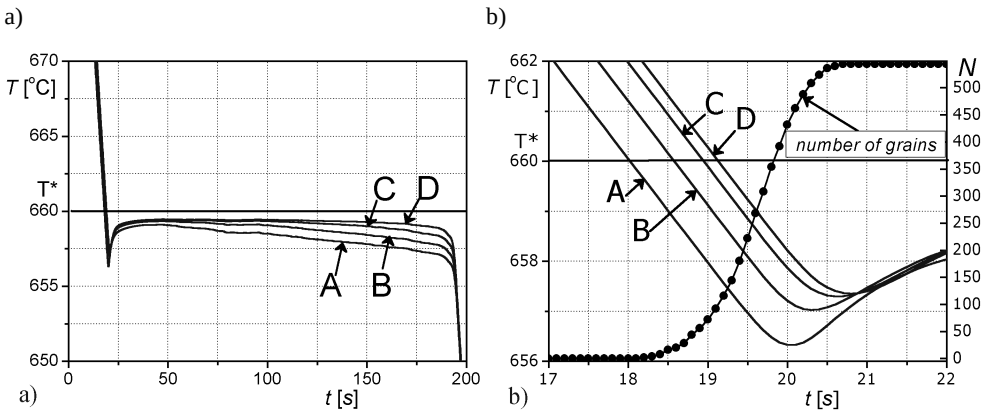

Fig. 3. The cooling curves in macro-cells *A*, *B*, *C* and *D* (a) and zoom of nucleation phase and number of created grains (b)

Conclusions

The micro-macro approach for modelling of solidification problem is very attractive and creating the new possibilities of scientific researches. The control volumes in the shape of Thiessen polygons correspond to the final shapes of grains. For every macro-cell we can calculate average maximum of undercooling and on the basis of undercooling we can estimate total number of created grains. These data give the information about concentration of grains in whole casting domain. The program worked out by the author of this paper creates adequate meshes in every macro-cell on the basis of the set of central nodes whose positions can be generated in a random way.

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