THE INFLUENCE OF INITIAL CONDITIONS ON THE COURSE OF SOLIDIFICATION PROCESS

Romuald Szopa, Jarosław Siedlecki, Wioletta Wojciechowska

Institute of Mathematics and Computer Science, Czestochowa University of Technology

Abstract. The methods of sensitivity analysis are applied in order to determine the influence of pouring temperature (the initial condition) on the course of casting solidification. In the first part of the paper the macro model of the process is considered, while in the second part the micro/macro approach is taken into account. On the stage of numerical simulation the finite difference method is used. In the final part of the paper the examples of computations are shown.

1. Mathematical description (macro model)

The transient temperature field in the solidifying metal domain oriented in rectangular co-ordinate system (2D problem) is described by the following equation

$$X \in \Omega \ : \ c(T)\partial_t T = \partial_x\left[\lambda(T)\partial_x T\right] + \partial_y\left[\lambda(T)\partial_y T\right] \tag{1}$$

where $X = \{x,y\}$, $C(T)$ is the substitute thermal capacity per unit of volume [1, 2], $\lambda = \lambda(t)$ is the thermal conductivity, $T = T(X,t)$ is the temperature.
The energy equation for the mould domain is of the form

$$X \in \Omega_m \ : \ c_m \partial_t T_m = \lambda_m\left(\partial_{xx} T_m + \partial_{yy} T_m\right) \tag{2}$$

The boundary conditions on the outer surface of the mould (Γ_0) determine the continuity of heat flux between the mould and the environment (the Robin condition), but in the practice one can assume in this place the adiabatic condition $\lambda\partial_n T = 0$ ($\partial_n T$ denotes a normal derivative). On the contact surface between the casting and mould we have

$$X \in \Gamma_m \ : \ \begin{cases} -\lambda\partial_n T = -\lambda_m \partial_n T_m \\ T = T_m \end{cases} \tag{3}$$

The mathematical model is supplemented by the initial conditions

$$t = 0 \ : \ T(X,0) = T_0, \quad T_m(X,0) = T_{m0} \tag{4}$$

2. Mathematical description (micro/macro model)

In the case of micro/macro approach we consider the following equation describing the thermal processes in the casting domain

$$X \in \Omega \; : \; c(T)\partial_t T = \partial_x\left[\lambda(T)\partial_x T\right] + \partial_y\left[\lambda(T)\partial_y T\right] + L\partial_t f_s \tag{5}$$

where $c(T)$ is the volumetric specific heat, $f_s = f_s(X,t)$ is the volumetric solid state fraction at the point X, L is the volumetric latent heat. According to the Johnson-Mehl-Avrami-Kolmogoroff theory the temporary value of solid fraction f_S of the metal at the point considered is given by equation [3-5]

$$f_s(X,t) = 1 - \exp(-\omega) \tag{6}$$

where

$$\omega = \frac{4}{3}\pi \int_0^t \frac{\partial N}{\partial t}\left[\int_{t'}^{t} u(\tau)\mathrm{d}\tau\right]^3 \mathrm{d}t \tag{7}$$

In equation (7) N is a number of nuclei (more precisely: density [nuclei/m^3]), u is a rate of solid phase growth, t' is a moment of crystallization process beginning. If we assume the constant number of nuclei, then

$$\omega = \frac{4}{3}\pi \, N\left[\int_{t'}^{t} u(\tau)\mathrm{d}\tau\right]^3 \tag{8}$$

The solid phase growth (equiaxial grains) is determined by equation

$$u = \frac{\partial R}{\partial t} = \mu \Delta T^m \tag{9}$$

where R is a grain radius, μ is a growth coefficient $m \in [1,2]$, and

$$\Delta T = T_{cr} - T \tag{10}$$

is the undercooling below the solidification point T_{cr}.
The remaining equations and conditions are the same as in the case of the macro model.

3. Sensitivity analysis (macro model)

In order to determine the influence of the pouring temperature T_0 on the course of casting solidification the direct variant of sensitivity analysis has been used [6]. It should be pointed out that the substitute thermal capacity and also the thermal conductivity of the casting material are assumed to be the temperature-dependent and it causes that the sensitivity model differs in details from the typical ones.

So, we differentiate the governing equations with respect to parameter T_0

$$X \in \Omega \ : \ C_T U \partial_t T + C \partial_t U = \partial_x(\lambda \partial_x U) + \partial_y(\lambda \partial_y U) + \partial_x(\lambda_T U \partial_x T) + \partial_y(\lambda_T U \partial_y T) \tag{11}$$

where: $U = \partial T/\partial T_0$, $C_T = \mathrm{d}C/\mathrm{d}T$, $\lambda_T = \mathrm{d}\lambda/\mathrm{d}T$.

Now, we differentiate the equation (2) with respect to T_0

$$c_m \partial_t U_m = \lambda_m (\partial_{xx} U_m + \partial_{yy} U_m) \tag{12}$$

Where $U_m = \partial T_m/\partial T_0$.

If on the outer surface of the system we assume the no-flux condition then the adequate boundary condition takes a form: Denoting $X \in \Gamma_0$, $\partial_n U_m = 0$. On the contact surface we have

$$X \in \Gamma_m \ : \ \begin{cases} -\lambda \partial_n U = -\lambda_m \partial_n U_m \\ U = U_m \end{cases} \tag{13}$$

The problem is supplemented by the condition $U(X,0) = 1$, $U_m(X,0) = 0$. Summing up, if we assume that the thermal conductivity of casting material is a constant value then the sensitivity model is of the form

$$\begin{cases} X \in \Omega & : \ C\,\partial_t U = \lambda\left(\partial_{xx} U + \partial_{yy} U\right) - C_T\, U\, \partial_t T \\ X \in \Omega_m & : \ c_m\, \partial_t U_m = \lambda_m\, (\partial_{xx} U_m + \partial_{yy} U_m) \\ X \in \Gamma_0 & : \ \partial_n U_m = 0 \\ X \in \Gamma_m & : \ \begin{cases} -\lambda\, \partial_n U = -\lambda_m\, \partial_n U_m \\ U = U_m \end{cases} \\ t = 0 & : \ U = 1, \ U_m = 0 \end{cases} \tag{14}$$

4. Sensitivity analysis (micro/macro model)

Let us assume that the specific heat and the thermal conductivity of the casting material are the constant values (taking into account the small temperature interval in which the solidification process takes place this assumption is acceptable). The differentiation of the source term in equation (5), namely

$$Q_U = \frac{\partial}{\partial T_0}\left\{4\pi N L \mu\, \Delta T \left(\int_0^t \mu\, \Delta T d\tau\right)^2 \exp\left[-\frac{4}{3}\pi N \left(\int_0^t \mu\, \Delta T d\tau\right)^3\right]\right\} \tag{15}$$

gives

$$Q_U = 4\pi\, N\, L \exp\left(-\frac{4}{3}\pi N r_S^3\right)\times \left[4\pi\, N\, \mu\, \Delta T\, \rho_S\, r_S^4 - 2\mu\, \Delta T\, \rho_S\, r_S - \mu\, U_1\, r_S^2\right] \tag{16}$$

where

$$r_S = \int_0^t \mu\, \Delta T \mathrm{d}\tau, \quad \rho_S = \int_0^t \mu\, U_1 \mathrm{d}\tau \tag{17}$$

and finally

$$\begin{cases} X \in \Omega & : \quad c\,\partial_t U = \lambda\left(\partial_{xx} U + \partial_{yy} U\right) + Q_U \\ X \in \Omega_m & : \quad c_m\, \partial_t U_m = \lambda_m\, (\partial_{xx} U_m + \partial_{yy} U_m) \\ X \in \Gamma_0 & : \quad \partial_n U_m = 0 \\ X \in \Gamma_m & : \quad \begin{cases} -\lambda\, \partial_n U = -\lambda_m\, \partial_n U_m \\ U = U_m \end{cases} \\ t = 0 & : \quad U = 1,\ U_m = 0 \end{cases} \tag{18}$$

Above the value $m = 1$ in the formula (9) has been assumed. Both in the case of the macro model and the micro/macro one, the finite difference method has been used. The algorithms concerning the solution of the basic problem and the sensitivity one are very similar because the mathematical model of both tasks are similar, too.

5. Example of computations (macro model)

The bar of rectangular section (10×14 cm) made from Cu-Sn alloy (10%) is considered. The casting is produced in the sand mix which parameters are equal $\lambda_m = 2.28$ W/mK, $C_m = 2.320 \cdot 10^6$ J/m^{3}K. The thermal conductivity of the casting material equals $\lambda = 50$ W/mK. According to literature [7] the thermal capacity can be approximated by the piece-wise constant function: $C = 3.678 \cdot 10^6$ J/m^{3}K for $T > 990$°C and for T < 825°C, while $C = 14.558 \cdot 10^6$ J/m^{3}K for $T \in [825,990$°C]. In order to assure the differentiation are equal to $T = (X,0) = 1000$°C, $T_m(X,0) =$ = 30°C.

The quarter of domain is taken into account and its shape is marked in Figures 1 and 2. In Figure 1 the temperature field for time $t = 2$ and $t = 6$ minutes is shown.

Figure 2 illustrates the isolines of function U for the same times. The sensitivity analysis shows that the influence of pouring temperature on the temperature field is the most essential in the casting sub-domain and sand mix layer close to contact surface. In other words, the change of $T_0 = 1000^{\circ}$C to the value from interval

$[T_0\text{-}\Delta T_0,\ T_0+\Delta T_0]$ determines the essential fluctuations of temporary temperature field in these sub-domains.

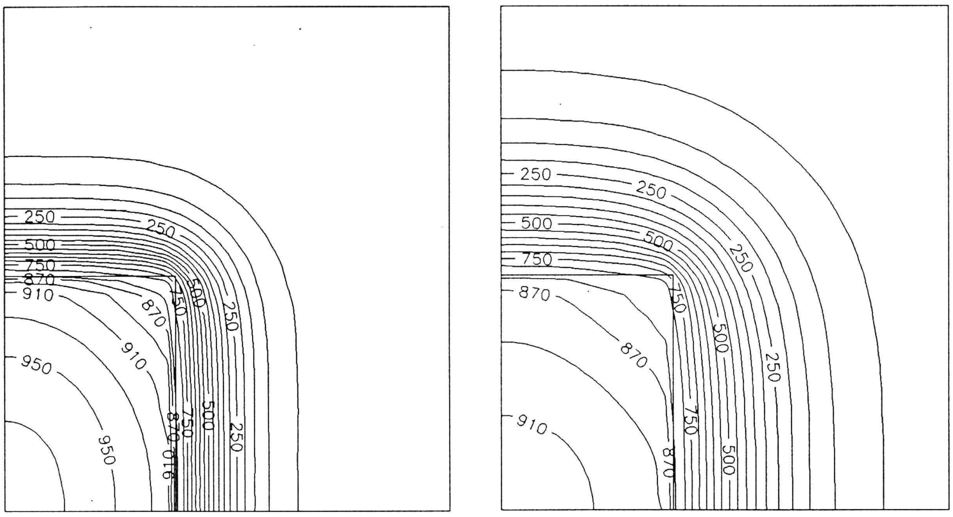

Fig. 1. Temperature field for 2 and 6 minutes

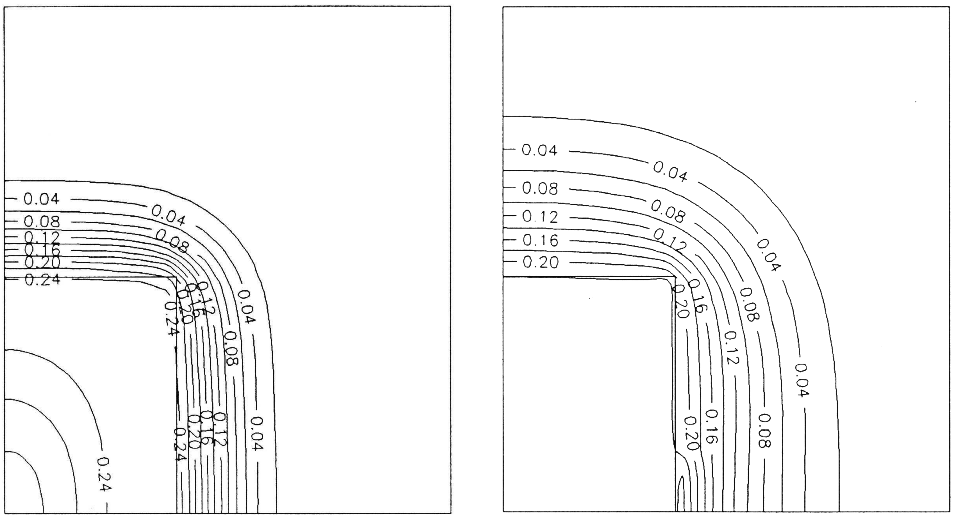

Fig. 2. Sensitivity field for 2 and 6 minutes

6. Example of computations (micro/macro model)

The aluminium casting in the form of plate ($2G$ = 5 cm) has been considered. The casting is produced in a typical sand mould. The parameters of metal equal

λ = 150 W/mK, c = 3 · 10^6 J/m^3K, L = 9.75 · 10^6 J/m^3, T_{cr} = 660°C, while λ_m = = 1.25 W/mK, c_m = 1.6 · 10^6 J/m^3K number of nuclei N = 5 · 10^{10} 1/m^3, growth coefficient μ = 3 · 10^{-6} m/sK, initial temperatures T_0 = 690°C, T_{m0} = 30°C. The geometry of the domain and the boundary conditions assumed allows to find the solution of the 1D problem in spite of this that the 2D computer program has been used.

In Figure 3 the sensitivity curves at the points 0.00125 (node 1), 0.01125 (node 5), 0.02125 (node 9) and 0.02875 m (node 12). The nodes 1, 5, 9 belong to the casting domain, the node 12 belongs to the mould domain.

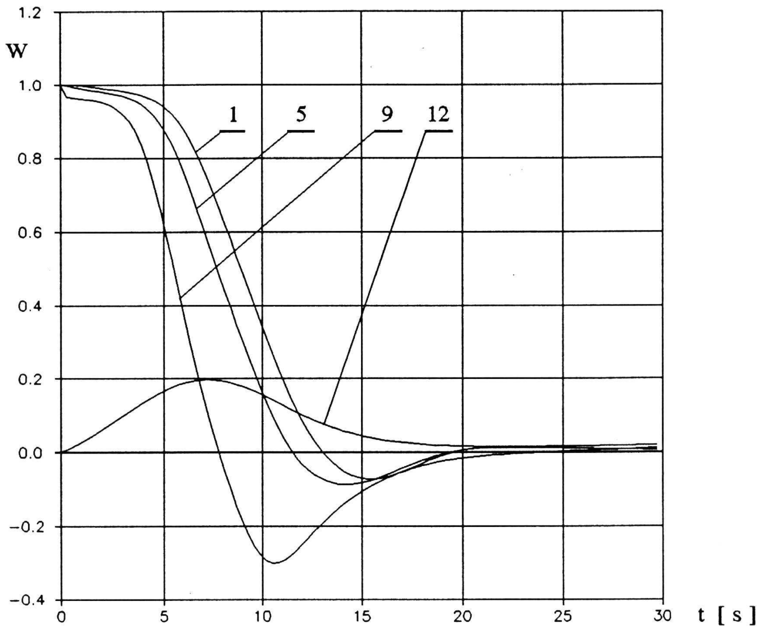

Fig. 3. Sensitivity curves

In Figure 4 the changes of temperature at the node 9 are shown. Using the sensitivity values the basic solution has been rebuilt on the solutions corresponding to changes of pouting temperature $\Delta T_0 = \pm 10$ K.

In Figure 5 the changes of temperature at the node 12 (mould) are shown. One can see that the influence of pouring temperature perturbations on the temperature field in the mould sub-domain is rather small.

Summing up, the methods of sensitivity analysis can be very effective tool for the investigations concerning the influence of the technological parameters on the course of casting solidification.

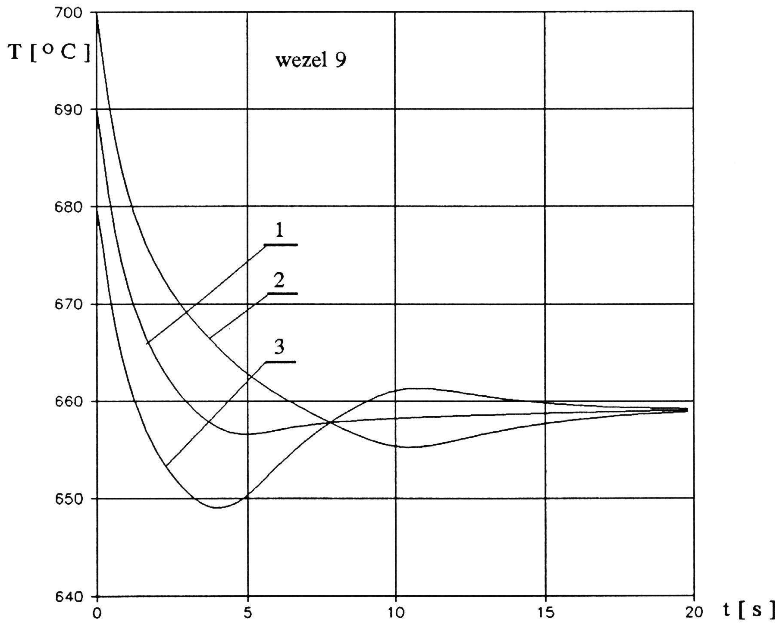

Fig. 4. The changes of temperature at node 9

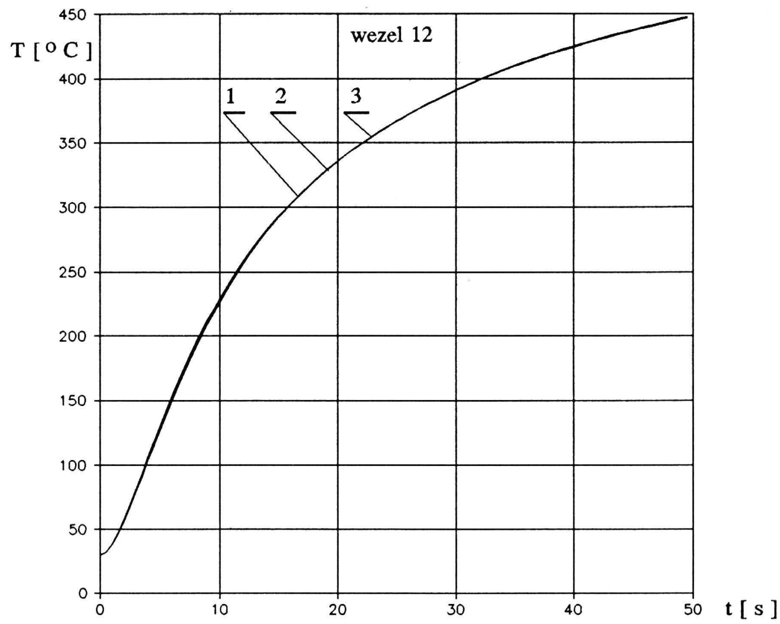

Fig. 5. The changes of temperature at node 12

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