

## SENSITIVITY ANALYSIS OF CRYSTALLIZATION WITH RESPECT INTERNAL PARAMETERS

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**Abstract.** The solidification model basing on the Johnson-Mehl-Avrami-Kolmogoroff theory is discussed. Such model is called in literature 'the second generation' one. In particular the sensitivity analysis of the process with respect to the parameters appearing in the source term controlling the solidification is presented. The method allows, among other things, to analyze the influence of the 'internal' parameters on the temperature field in the system considered. On the stage of numerical computations the FDM is used. In the final part of the paper the example of computations is shown.

### 1. Mathematical model of solidification

The temperature field in the casting domain is described by the following equation

$$c_1 \frac{\partial T_1(x,t)}{\partial t} = \lambda_1 \nabla^2 T_1(x,t) + L \frac{\partial f_s(x,t)}{\partial t} \quad (1)$$

where  $T_1(x,t)$  is the casting temperature,  $f_s(x,t)$  is the solid state fraction at the point  $x$ ,  $c_1$  is the volumetric specific heat,  $\lambda_1$  is the thermal conductivity,  $L$  is the volumetric latent heat,  $x$  and  $t$  denote the spatial co-ordinates and time, correspondingly. The equation

$$c_2 \frac{\partial T_2(x,t)}{\partial t} = \lambda_2 \nabla^2 T_2(x,t) \quad (2)$$

describes the temperature field in the mould sub-domain. On the contact surface between casting and mould the continuity condition is given, this means

$$\begin{cases} -\lambda_1 \frac{\partial T_1(x,t)}{\partial n} = -\lambda_2 \frac{\partial T_2(x,t)}{\partial n} \\ T_1(x,t) = T_2(x,t) \end{cases} \quad (3)$$

On the outer surface of the system the Robin condition is taken into account

$$\Gamma_0 : -\lambda_2 \frac{\partial T_2(x,t)}{\partial n} = \alpha [T_2(x,t) - T_a] \quad (4)$$

where  $\alpha$  is the heat transfer coefficient,  $T_a$  is the ambient temperature. In equations (3) and (4)  $\partial T/\partial n$  denotes the normal derivative.

For  $t = 0$  the initial temperature field is known:

$$t = 0 : T_1(x,0) = T_{10}, \quad T_2(x,0) = T_{20} \quad (5)$$

where  $T_{10}$  is the pouring temperature and  $T_{20}$  is the initial temperature of the mould. A value of solid fraction  $f_s$  of metal at the point considered results from the Kolmogoroff type equation [1-3]

$$f_s = 1 - \exp(-\omega) \quad (6)$$

where

$$\omega = \omega(x,t) = \frac{4}{3} \pi v \int_0^t \frac{\partial N}{\partial t} \left[ \int_{t'}^t u d\tau \right]^3 dt \quad (7)$$

In equation (7)  $N$  is the nuclei density [nuclei/m<sup>3</sup>],  $u = u(x,t)$  is a rate of solid phase growth,  $v$  is the coefficient determining the type of crystallization (for  $v = 1$  we have the spherical growth),  $t'$  is a moment of crystallization process beginning. If we assume the constant number of nuclei, then

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

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

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

where  $R = R(x,t)$  is a grain radius,  $m \in [1, 2]$ ,  $\mu$  is a growth coefficient and

$$\Delta T = T^* - T \quad (10)$$

is the undercooling below the solidification point  $T^*$ . Additionally we assume that for  $T > T_{cr}$ :  $\Delta T = 0$ , in other words  $u = 0$  and then the lower limit in integrals (7) and (8) equals  $t' = 0$ . So

$$\omega = \frac{4}{3} \pi N \left[ \int_{t'}^t u(\tau) d\tau \right]^3 \quad (11)$$

Introducing (7) to equation (1) one obtains

$$c_1 \frac{\partial T_1}{\partial t} = \lambda_1 \nabla^2 T_1 + L \exp(-\omega) \frac{\partial \omega}{\partial t} \quad (12)$$

or

$$c_1 \frac{\partial T_1}{\partial t} = \lambda_1 \nabla^2 T_1 + 4\pi N L \nu \mu \Delta T^m \left( \int_0^t \mu \Delta T^m d\tau \right)^2 \exp \left[ -\frac{4}{3} \pi \nu N \left( \int_0^t \mu \Delta T^m d\tau \right)^3 \right] \quad (13)$$

## 2. Sensitivity with respect to internal parameters

The sensitivity analysis of the process with respect to the internal parameters (number of nuclei, growth coefficient, coefficient  $\nu$ ) will be presented, at the same time the direct method is applied [4, 5]. The direct approach reduces to the differentiation of the governing equations and the boundary-initial conditions over to parameters discussed.

The first step of sensitivity model construction consists in the differentiation of the boundary-initial problem with respect to the parameters considered.

Differentiation of the mathematical model with respect to  $p_i$  leads to the additional boundary initial problem in the form

$$\left\{ \begin{array}{l} x \in \Omega_1 : c_1 \frac{\partial}{\partial t} \left( \frac{\partial T_1}{\partial p_i} \right) = \lambda_1 \nabla^2 \left( \frac{\partial T_1}{\partial p_i} \right) + L \frac{\partial}{\partial t} \left( \frac{\partial f_s}{\partial p_i} \right) \\ x \in \Omega_2 : c_2 \frac{\partial}{\partial t} \left( \frac{\partial T_2}{\partial p_i} \right) = \lambda_2 \nabla^2 \left( \frac{\partial T_2}{\partial p_i} \right) \\ x \in \Gamma_{12} : \left\{ \begin{array}{l} \frac{\partial T_1}{\partial p_i} = \frac{\partial T_2}{\partial p_i} \\ -\lambda_1 \frac{\partial}{\partial n} \left( \frac{\partial T_1}{\partial p_i} \right) = -\lambda_2 \frac{\partial}{\partial n} \left( \frac{\partial T_2}{\partial p_i} \right) \end{array} \right. \\ x \in \Gamma_0 : -\lambda_2 \frac{\partial}{\partial n} \left( \frac{\partial T_2}{\partial p_i} \right) = \alpha \frac{\partial T_2}{\partial p_i} \\ t = 0 : \frac{\partial T_1}{\partial p_i} = 0, \quad \frac{\partial T_2}{\partial p_i} = 0 \end{array} \right. \quad (14)$$

where  $p_i = N, \nu, \mu$ . Denoting  $U_1 = \partial T_1 / \partial p_i$ ,  $U_2 = \partial T_2 / \partial p_i$  we have

$$\left\{ \begin{array}{l} x \in \Omega_1 : c_1 \frac{\partial U_1}{\partial t} = \lambda_1 \nabla^2 U_1 + Q_U \\ x \in \Omega_2 : c_2 \frac{\partial U_2}{\partial t} = \lambda_2 \nabla^2 U_2 \\ x \in \Gamma_{12} : \begin{cases} U_1 = U_2 \\ -\lambda_1 \frac{\partial U_1}{\partial n} = -\lambda_2 \frac{\partial U_2}{\partial n} \end{cases} \\ x \in \Gamma_0 : -\lambda_2 \frac{\partial U_2}{\partial n} = \alpha U_2 \\ t = 0 : U_1 = 0, \quad U_2 = 0 \end{array} \right. \quad (15)$$

The source term  $Q_U$  for different parameters  $p_i$  must be found separately. It is the product of the following components:

$$F_1 = 4\pi N L \nu \mu \Delta T^m \quad (16)$$

$$F_2 = \left( \int_0^t \mu \Delta T^m d\tau \right)^2 \quad (17)$$

$$F_3 = \exp \left[ -\frac{4}{3} \pi \nu N \left( \int_0^t \mu \Delta T^m d\tau \right)^3 \right] \quad (18)$$

Above functions will be differentiated with respect to parameter  $\nu$ . So:

$$\frac{\partial F_1}{\partial \nu} = 4\pi N L \mu (\Delta T^m - \nu m \Delta T^{m-1} U_1) \quad (19)$$

$$\frac{\partial F_2}{\partial \nu} = -2 \int_0^t \mu \Delta T^m d\tau \int_0^t \mu m \Delta T^{m-1} U_1 d\tau \quad (20)$$

and

$$\begin{aligned} \frac{\partial F_3}{\partial \nu} = & \exp \left[ -\frac{4}{3} \pi \nu N \left( \int_0^t \mu \Delta T^m d\tau \right)^3 \right] \times \\ & \left[ -\frac{4}{3} \pi N \left( \int_0^t \mu \Delta T^m d\tau \right)^3 + 4\pi N \nu \left( \int_0^t \mu \Delta T^m d\tau \right)^2 \cdot \int_0^t \mu m \Delta T^{m-1} U_1 d\tau \right] \end{aligned} \quad (21)$$

Denoting

$$r_S = \int_0^t \mu \Delta T d\tau, \quad \rho_S = \int_0^t \mu m \Delta T^{m-1} U_1 d\tau \quad (22)$$

we finally obtain

$$Q_U = 4\pi L N \mu r_S \exp\left(-\frac{4}{3}\pi N \nu r_S^3\right) \times \left[ \Delta T^m \left( r_S - 2\nu \rho_S - \frac{4}{3}\pi N \nu r_S^4 + 4\pi N \nu^2 r_S^3 \rho_S \right) - \nu m \Delta T^{m-1} r_S U_1 \right] \quad (23)$$

The very similar formula can be found for  $p_i = N$ . In the last case, this means  $p_i = \mu$  we have:

$$\frac{\partial F_1}{\partial \mu} = 4\pi L N \nu \left( \Delta T^m - \mu m \Delta T^{m-1} U_1 \right) \quad (24)$$

$$\frac{\partial F_2}{\partial \mu} = 2 \int_0^t \mu \Delta T^m d\tau \int_0^t \left( \Delta T^m - \mu m \Delta T^{m-1} U_1 \right) d\tau \quad (25)$$

and

$$\frac{\partial F_3}{\partial \mu} = \exp\left[-\frac{4}{3}\pi \nu N \left( \int_0^t \mu \Delta T^m d\tau \right)^3\right] \times \left[ -4\pi N \nu \left( \int_0^t \mu \Delta T^m d\tau \right)^2 \cdot \int_0^t \left( \Delta T^m - \mu m \Delta T^{m-1} U_1 \right) d\tau \right] \quad (26)$$

Denoting

$$r_S = \int_0^t \mu \Delta T^m d\tau, \quad \rho_S = \int_0^t \left( \Delta T^m - \mu m \Delta T^{m-1} U_1 \right) d\tau \quad (27)$$

we obtain

$$Q_U(x, t) = 4\pi L N \nu r_S \exp\left(-\frac{4}{3}\pi N \nu r_S^3\right) \times \left[ \Delta T^m \left( r_S + 2\mu \rho_S - 4\pi N \nu \mu r_S^3 \rho_S \right) - \mu m \Delta T^{m-1} r_S U_1 \right] \quad (28)$$

On the stage of numerical computations both the basic problem and the additional ones have been solved using the finite difference method.

### 3. Example of computations

The 1D problem (the plate solidification) is considered and the sensitivity with respect to growth coefficient is discussed. In particular the aluminium casting ( $2G = 5$  cm) produced in a typical sand mould is taken into account. The parameters  $\lambda_1 = 150$  W/mK,  $c_1 = 3 \cdot 10^6$  J/m<sup>3</sup>K,  $L = 9.75 \cdot 10^8$  J/m<sup>3</sup>,  $T^* = 660^\circ\text{C}$ ,  $N = 5 \cdot 10^{10}$  1/m<sup>3</sup>,  $\mu = 3 \cdot 10^{-6}$  m/sK<sup>2</sup>,  $m = 2$ ,  $\nu = 0.6$ ,  $\lambda_2 = 1.25$  W/mK,  $c_2 = 3 \cdot 10^6$  J/m<sup>3</sup>K. Initial temperatures  $T_{10} = 690^\circ\text{C}$  and  $T_{20} = 30^\circ\text{C}$ . In Figure 1 the sensitivity curves at the points  $x = 1.1, 1.6, 2.1$  and  $2.9$  cm (the nodes 5, 7, 9 belong to the casting domain, the node 12 belongs to the mould domain).

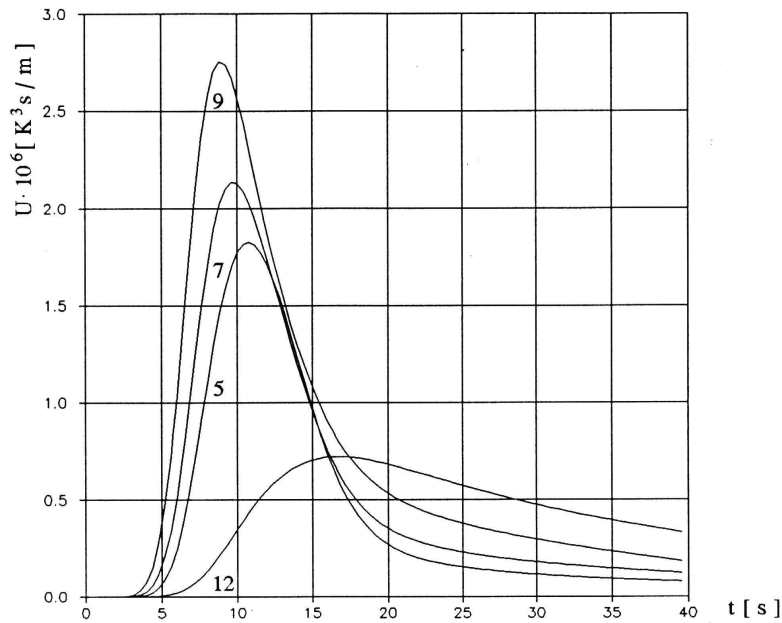
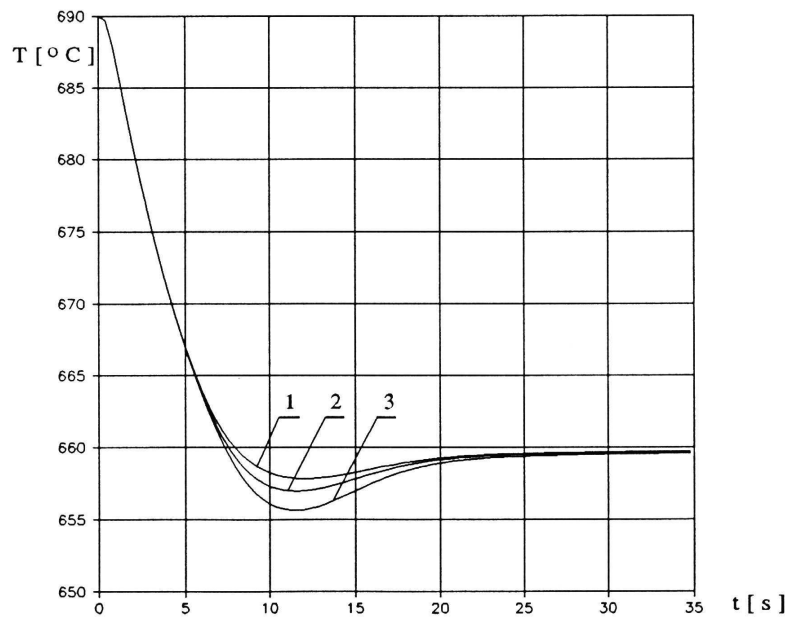
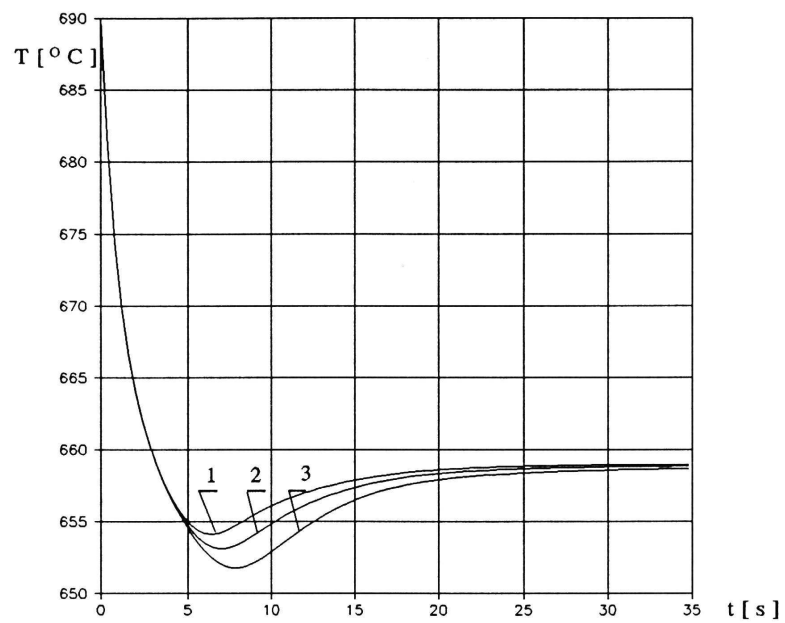


Fig. 1. Sensitivity curves

One can see that the sensitivity function in the casting sub-domain is essentially bigger than the same function in the mould sub-domain. So, the influence of parameter  $\mu$  perturbation can be visible as the changes of temperature field in  $\Omega_1$ . Figures 2 and 3 illustrate the cooling curves at the points  $x = 1.1$  and  $2.1$  cm. The symbol 2 corresponds to the basic value of growth coefficient, while the symbols 1 and 3 to the values of  $\mu$  equal  $\mu \pm 0.2\Delta\mu$ .

Fig. 2. Cooling curves at point  $x = 1.1$  cmFig. 3. Cooling curves at point  $x = 2.1$  cm

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