SENSITIVITY OF LINEAR CRYSTALLIZATION MODEL WITH RESPECT TO EXTERNAL PARAMETERS

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Abstract. In the paper the micro/macro model proposed by Stefanescu is analyzed. In particular the sensitivity of temperature field with respect to external parameters is discussed. The external parameters correspond to the mould volumetric specific heat and thermal conductivity. The others parameters, for instance, heat transfer coefficient between mould and environment can be also taken into account. On the stage of numerical realization the generalized variant of the finite differences method is applied.

Introduction

The sensitivity analysis allows to estimate the mutual connections between the solidification and cooling processes proceedings in the casting domain and the external parameters resulting from the technology conditions. Here the geometrical and thermophysical parameters of the mould subdomain can be taken into account. In the paper we limit to the analysis of the influence of mould volumetric specific heat and its thermal conductivity on the course of thermal phenomena in the casting-mould domain. The problem is essential from the practical point of view because the mould parameters can be treated as the interval variables $c_2 \pm \Delta c_2$, $\lambda_2 \pm \Delta \lambda_2$ and we know only the mean values c_2, λ_2. If $T(x, t, c_2, \lambda_2)$ denotes a temperature field dependent on geometrical co-ordinates x, time t, and parameters c_2, λ_2, then using the Taylor formula we have

$$T\left(x, t, c_2 \pm \Delta c_2, \lambda_2\right) = T\left(x, t, c_2, \lambda_2\right) \pm \frac{\partial T\left(x, t, c_2, \lambda_2\right)}{\partial c_2} \Delta c_2 \tag{1}$$

$$T\left(x, t, c_2, \lambda_2 \pm \Delta \lambda_2\right) = T\left(x, t, c_2, \lambda_2\right) \pm \frac{\partial T\left(x, t, c_2, \lambda_2\right)}{\partial \lambda_2} \Delta \lambda_2 \tag{2}$$

Above, it was assumed that the perturbation concerns only the parameter c_2 or λ_2, but we can consider (using the similar formula) the simultaneous perturbations of the both parameters simultaneously.

Introducing the sensitivity functions $V = \partial T / \partial c_2$ and $U = \partial T / \partial \lambda_2$ we obtain

$$T\left(x, t, c_2 \pm \Delta c_2, \lambda_2\right) = T\left(x, t, c_2, \lambda_2\right) \pm V\left(x, t, c_2, \lambda_2\right) \Delta c_2 \tag{3}$$

$$T\left(x, t, c_2, \lambda_2 \pm \Delta \lambda_2\right) = T\left(x, t, c_2, \lambda_2\right) \pm U\left(x, t, c_2, \lambda_2\right) \Delta \lambda_2 \tag{4}$$

The knowledge of sensitivity fields V and U allows to determine the influence of parameters c_2, λ_2 perturbations on the course of function T, and to obtain the solution concerning the transient temperature field in the casting - mould domain in the form of interval one.

1. Governing equations

The energy equation determining the casting solidification can be written in the form [1, 2]

$$x \in \Omega_1: \quad c_1(T) \frac{\partial T_1(x, t)}{\partial t} = \operatorname{div}\left[\lambda_1(T) \operatorname{grad} T_1(x, t)\right] + L \frac{\partial f_S(x, t)}{\partial t} \tag{5}$$

where Ω_1 is a casting domain, c_1 is a volumetric specific heat, λ_1 is a thermal conductivity, L is a volumetric latent heat, f_S is a volumetric solid state fraction at the considered point from casting domain. The local value of f_S is given as follows [3]

$$f_S(x, t) = N(x, t) \; V(x, t) \tag{6}$$

where N is a local grains density [grains/m^3], V is a temporary single grain volume. The solidification goes to the end when $f_S = 1$. The equation (6) corresponds to the so-called linear model [3]. In literature the exponential model presented by Mehl-Johnson-Avrami-Kolmogoroff is also discussed [4-6].
If we consider the spherical grains then

$$\frac{\partial f_S(x, t)}{\partial t} = 4\pi \left[\frac{R(x, t)^3}{3} \frac{\partial N(x, t)}{\partial t} + R(x, t)^2 \frac{\partial R(x, t)}{\partial t} N(x, t) \right] \tag{7}$$

where R is a grain radius. The last equation can be also modified in order more exactly to take into account the final stages of crystallization (the mutual connections between the grains) and then the following formula is proposed [3]

$$\frac{\partial f_S(x, t)}{\partial t} = 4\pi \left[\frac{R(x, t)^3}{3} \frac{\partial N(x, t)}{\partial t} + R(x, t)^2 \frac{\partial R(x, t)}{\partial t} N(x, t) \right] \left[1 - f_S(x, t)\right] \tag{8}$$

Additionally it is assumed that:

- A number of nuclei N is proportional to the second power of undercooling below the solidification point T^*

$$N(x,\,t) = \Psi \,\Delta T^2(x,\,t) \tag{9}$$

where Ψ is the nucleation coefficient, $\Delta T = T^* - T_1(x,\,t)$ is the undercooling. It should be pointed out that the nucleation stops when $\Delta T(x,\,t+\Delta t) < \Delta T(x,\,t)$.

- The temporary and local solidification rate is proportional to the undercooling below the solidification point T^*

$$u(x,\,t) = \frac{\partial R(x,\,t)}{\partial t} = \mu\left[T^* - T_1(x,\,t)\right]^m \tag{10}$$

where μ is a growth coefficient, $m \in [1,\,2]$ (see [1]).

The equation determining the temperature field $T_2(x,\,t)$ in the mould subdomain is similar to (5) (without the source term), namely

$$x \in \Omega_2 : \quad c_2(T)\frac{\partial T_2(x,\,t)}{\partial t} = \operatorname{div}\left[\lambda_2(T)\,\operatorname{grad} T_2(x,\,t)\right] \tag{11}$$

where Ω_2 is a mould domain, c_2 is a mould volumetric specific heat, λ_2 is a mould thermal conductivity.

On the contact surface the continuity condition should be assumed, in particular in the case of an ideal contact it takes a form

$$x \in \Gamma_{1,2} : \quad \begin{cases} -\lambda_1 \dfrac{\partial T_1(x,\,t)}{\partial n} = -\lambda_2 \dfrac{\partial T_2(x,\,t)}{\partial n} \\ T_1(x,\,t) = T_2(x,\,t) \end{cases} \tag{12}$$

where $\partial/\partial n$ denotes a normal derivative.

On the outer surface of the mould the Robin condition with heat transfer coefficient α is given

$$x \in \Gamma_{2,a} : \quad -\lambda_2 \frac{\partial T_2(x,\,t)}{\partial n} = \alpha\left[T_2(x,\,t) - T_a\right] \tag{13}$$

at the same time T_a is an ambient temperature. The initial conditions (pouring temperature and initial mould temperature) are also known.

2. The sensitivity models

Below, the direct variant of parametric sensitivity analysis is applied [7, 8]. Then the sensitivity models result from the differentiation of energy equations and boundary-initial conditions with respect to c_2 and λ_2 (mould parameters). Denoting $V_1 = \partial T_1 / \partial c_2$, $V_2 = \partial T_2 / \partial c_2$ we have (the constant values of c_1, λ_1, c_2, λ_2 and the constant nuclei density N are assumed)

$$
\begin{cases}
x \in \Omega_1 : & c_1 \dfrac{\partial V_1}{\partial t} = \lambda_1 \nabla^2 V_1 + Q_1 \\
x \in \Omega_2 : & c_2 \dfrac{\partial V_2}{\partial t} = \lambda_2 \nabla^2 V_2 - \dfrac{\partial T_2}{\partial t} \\
x \in \Gamma_{1,2} : & \begin{cases} V_1 = V_2 \\ -\lambda_1 \dfrac{\partial V_1}{\partial n} = -\lambda_2 \dfrac{\partial V_2}{\partial n} \end{cases} \\
x \in \Gamma_{2,a} : & -\lambda_2 \dfrac{\partial V_2}{\partial n} = \alpha V_2 \\
t = 0 : & V_1 = 0, \quad V_2 = 0
\end{cases}
\tag{14}
$$

where Q_1 is the source function resulting from the last term of equation (5).
Because

$$
\frac{\partial f_S}{\partial t} = 4\pi N \mu \Delta T^m \left[\int_0^t \mu \Delta T^m \, \mathrm{d}\tau \right]^2 = F_1 \cdot F_2
\tag{15}
$$

and

$$
\frac{\partial F_1}{\partial c_2} = -4\pi N \mu m \Delta T^{m-1} \frac{\partial T_1}{\partial c_2}
\tag{16}
$$

$$
\frac{\partial F_2}{\partial c_2} = -2 \int_0^t \mu \Delta T^m \, \mathrm{d}\tau \int_0^t \mu m \Delta T^{m-1} \frac{\partial T_1}{\partial c_2} \, \mathrm{d}\tau = -2 r_S \rho_S
\tag{17}
$$

therefore

$$
Q_1 = -4\pi N L \mu \Delta T^{m-1} r_S \left(m V_1 r_S + 2 \Delta T \rho_S \right)
\tag{18}
$$

The same form of source function Q_1 appears in the case of sensitivity model with respect to λ_2. This one is of the form

$$
\begin{cases}
x \in \Omega_1: & c_1 \dfrac{\partial U_1}{\partial t} = \lambda_1 \nabla^2 U_1 + Q_1 \\
x \in \Omega_2: & c_2 \dfrac{\partial U_2}{\partial t} = \lambda_2 \nabla^2 U_2 - \dfrac{c_2}{\lambda_2} \dfrac{\partial T_2}{\partial t} \\
x \in \Gamma_{1,2}: & \begin{cases} U_1 = U_2 \\ -\lambda_1 \dfrac{\partial U_1}{\partial n} = -\lambda_2 \dfrac{\partial U_2}{\partial n} - \dfrac{\partial T_2}{\partial n} \end{cases} \\
x \in \Gamma_{2,a}: & -\lambda_2 \dfrac{\partial U_2}{\partial n} = \alpha U_2 + \dfrac{\partial T_2}{\partial n} \\
t = 0: & U_1 = 0, \quad U_2 = 0
\end{cases}
\tag{19}
$$

where $U_1 = \partial T_1 / \partial \lambda_2$, $U_2 = \partial T_2 / \partial \lambda_2$. Generally speaking the model of sensitivity V is a little simpler than model of sensitivity U. Both models are coupled with the basic one concerning the transient temperature field in the system casting-mould.

3. Numerical solution of sensitivity problem

The first example concerns the 1D task (the computer program has been prepared for 2D problems, but introducing the adequate boundary conditions we have obtained 1D solution).

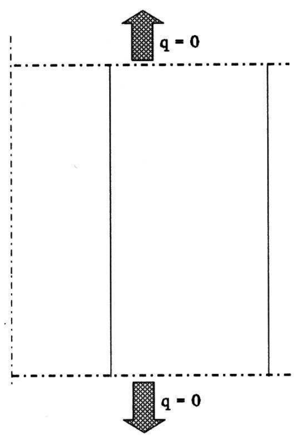

Fig. 1. Casting - mould domain

The thickness of the casting equals 5 cm, thickness of the mould 20 cm. Parameters of casting material (aluminium): λ_1 = 150 W/mK, $c_1 = 3 \cdot 10^6$ J/m^{3}K, $L = 9.75 \cdot 10^8$ J/m^3, $T^* = 660$°C, mould parameters: $\lambda_2 = 1.25$ W/mK, $c_2 = 1.6 \cdot 10^6$ J/m^{3}K.

The constant number of nuclei $N = 5 \cdot 10^{10}$ 1/m^3 was assumed, growth coefficient $\mu = 3 \cdot 10^{-6}$ m/sK^2, initial temperatures $T_{10} = 690^{\circ}$C and $T_{20} = 30^{\circ}$C, correspondingly. The basic value of λ_2 has been disturbed and $\Delta\lambda_2 = \pm 0.25$ W/mK. In Figure 2 the curves of sensitivity U for points x_i = 0.01125 ('1' - casting) and 0.02875 '2', 0.04375 '3', 0.05875 '4' - mould are shown.

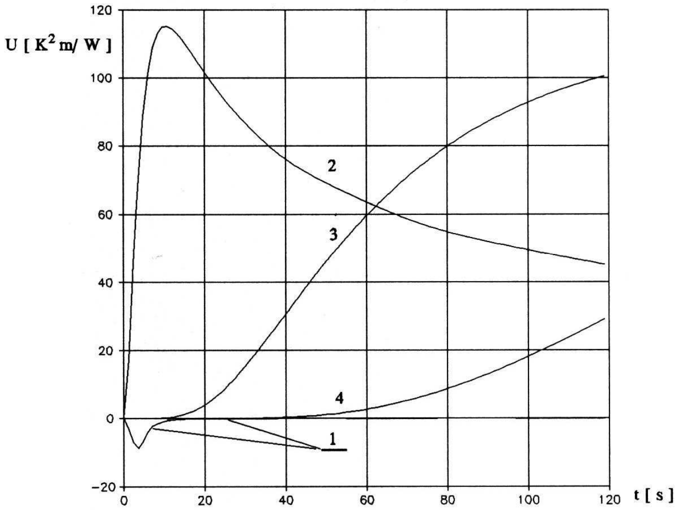

Fig. 2. Sensitivity curves

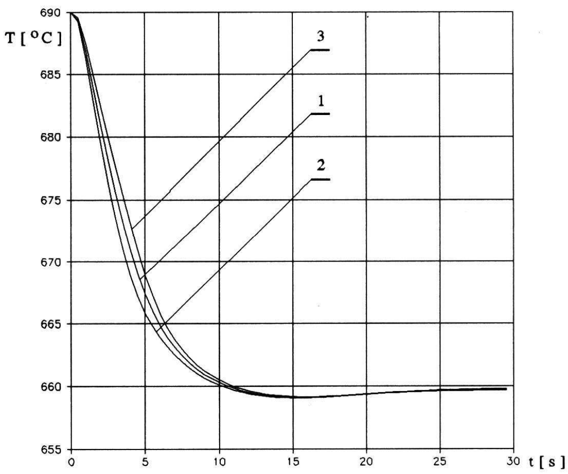

Fig. 3. Cooling curves for different λ_2

One can see that the temperature field in the casting domain is rather not 'sensitive' to thermal conductivity of mould. Only at the initial stages of the process the influence of λ_2 is visible. From the view-point of numerical simulation it is quite good situation because we can introduce to the program approximate values of λ_2 and obtain the correct results concerning the kinetics of casting solidification. The sensitivity U_2 changes in the bigger scope. The maximum of this function is located close to the contact surface and next shifts to the center of mould sub-domain. In Figure 3 the cooling curves at the point $x = 0.02125$ m and $\lambda_2 = 1.25$ (curve 1) and for disturbed values ($\Delta\lambda_2 = 0.25$) found using the Taylor Formula are shown. The differences are visible, but not essential from the practical point of view.

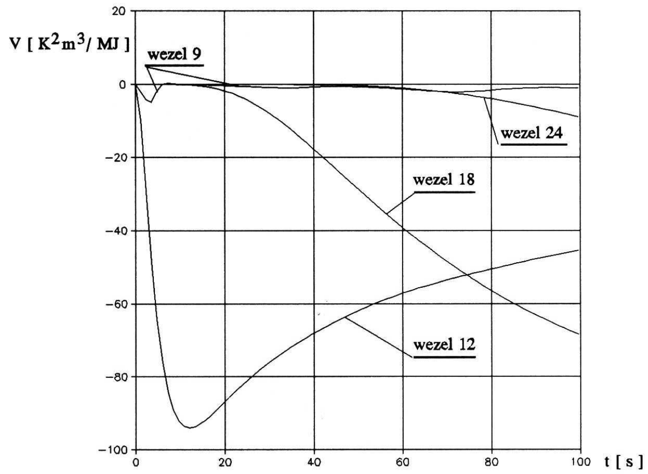

Fig. 4. Sensitivity V at selected points

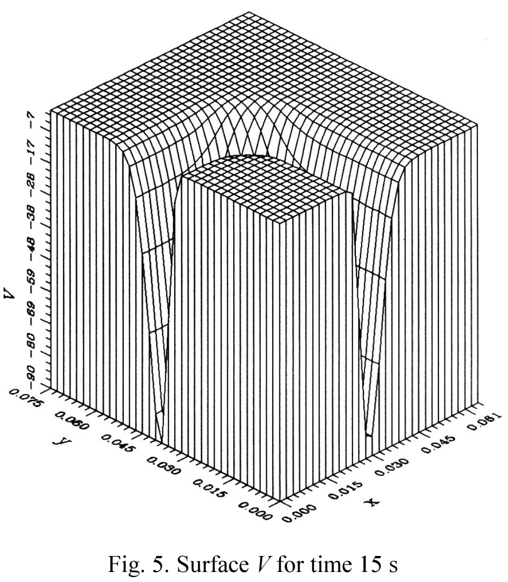

Fig. 5. Surface V for time 15 s

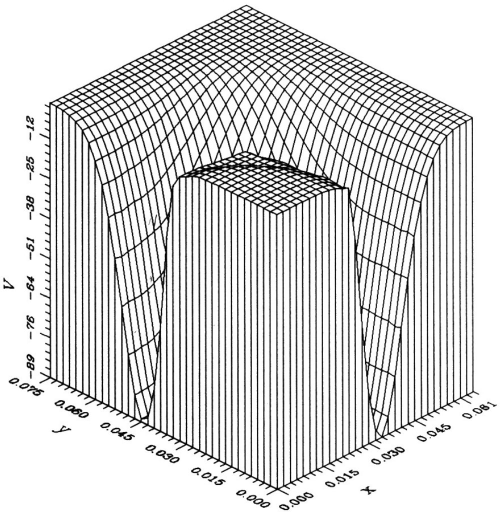

Fig. 6. Surface V for time 60 s

Now the results concerning the sensitivity V will be discussed. The basic value of c_2 equals $c_2 = 1.6 \cdot 10^6$ J/m^{3}K. In Figure 4 the courses of sensitivity function at the points $x_9 = 0.01125$ (casting), $x_{12} = 0.02875$, $x_{18} = 0.04375$, $x_{24} = 0.05875$ m (mould).

The sensitivity V in the mould sub-domain is negative, it can be explained in physical way.

The same computer program has been used for the analysis of 2D tasks. The rectangular aluminium bar (0.05×0.07 m) made in the typical sand mould has been considered. The input data have been the same as previously. As an example the distribution of sensitivity V in the casting-mould system for times 15 i 60 s are shown.

4. Final remarks

The sensitivity methods constitute the very effective tool for analysis of the heat transfer processes proceeding in the system casting-mould. The direct application of such methods allows to generalize the basic solution on the infinite number of others solutions concerning the disturbed values of technological and physical parameters. Additionally the methods of sensitivity analysis can be used for numerical solution of inverse problems from the scope of thermal theory of foundry processes [1]. The details concerning the generalized variant of FDM which was here used on the stage of numerical simulation can be found in [9, 10].

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