SECOND GENERATION SOLIDIFICATION MODEL. SENSITIVITY WITH RESPECT TO MOULD PARAMETERS

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Abstract. In the paper the solidification model basing on the Mehl-Johnson-Avrami--Kolmogorov theory is discussed. In particular the sensitivity analysis of solidification process with respect to the mould parameters is presented. The method allows, among other things, to analyze the influence of the mould parameters on the temperature field in the system considered. The casting-mould domain is treated as a 2D one. On the stage of numerical computations the boundary element method is used. In the final part of the paper the example of computations is shown.

1. Mathematical background

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

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

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, λ_1 is the thermal conductivity, L is the volumetric latent heat, $x = \{x_1,\ x_2\}$ and t denote the spatial co-ordinates and time, correspondingly.
The equation

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

describes the temperature field in the mould sub-domain. Along the contact surface between casting and mould the continuity condition is given:

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

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

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

where α is the heat transfer coefficient, T_a is the ambient temperature. In equations (3) and (4) $\partial(\cdot)/\partial n$ denotes the normal derivative.
For $t = 0$ the initial temperature field is known:

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

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 the metal at point considered results from the Kolmogorov type equation [1-3]

$$f_S = 1 - \exp(-\omega) \tag{6}$$

where

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

In equation (7) N is the nuclei density, nucl./m^3, $u = u(x, t)$ is a rate of solid phase growth, t' is a moment of crystallization process beginning. If we assume the constant number of nuclei, then

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

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

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

where $R = R(x, t)$ is a grain radius, μ is a growth coefficient and

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

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

$$\omega = \frac{4}{3}\pi N \left[\int_0^t \mu \Delta T \,\mathrm{d}\tau \right]^3 \tag{11}$$

Introducing (7) to equation (1) one obtains

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

or

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

2. Sensitivity analysis

Now we will present the sensitivity analysis of solidification process with respect to the mould parameters (thermal conductivity and volumetric specific heat) at the same time the direct method is applied. The direct approach requires the considerations corresponding the sensitivity of distinguished parameters separately, but from the theoretical and practical points of view such approach is essentially simpler than the adjoining one [4].
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 λ_2 leads to the additional boundary initial problem in the form

$$\begin{cases} x \in \Omega_1 : & c_1 \dfrac{\partial}{\partial t}\left(\dfrac{\partial T_1}{\partial \lambda_2}\right) = \lambda_1 \nabla^2 \left(\dfrac{\partial T_1}{\partial \lambda_2}\right) + L_V \dfrac{\partial}{\partial t}\left(\dfrac{\partial f_S}{\partial \lambda_2}\right) \\ x \in \Omega_2 : & c_2 \dfrac{\partial}{\partial t}\left(\dfrac{\partial T_2}{\partial \lambda_2}\right) = \lambda_2 \nabla^2 \left(\dfrac{\partial T_2}{\partial \lambda_2}\right) + \dfrac{c_2}{\lambda_2}\dfrac{\partial T_2}{\partial t} \\ x \in \Gamma_{12} : & \begin{cases} \dfrac{\partial T_1}{\partial \lambda_2} = \dfrac{\partial T_2}{\partial \lambda_2} \\ -\lambda_1 \dfrac{\partial}{\partial n}\left(\dfrac{\partial T_1}{\partial \lambda_2}\right) = -\dfrac{\partial T_2}{\partial n} - \lambda_1 \dfrac{\partial}{\partial n}\left(\dfrac{\partial T_2}{\partial \lambda_2}\right) \end{cases} \\ x \in \Gamma_0 : & -\lambda_2 \dfrac{\partial}{\partial n}\left(\dfrac{\partial T_2}{\partial \lambda_2}\right) = \alpha \dfrac{\partial T_2}{\partial \lambda_2} + \dfrac{\partial T_2}{\partial n} \\ t = 0 : & \partial T_1 / \partial \lambda_2 = 0, \quad \partial T_2 / \partial \lambda_2 = 0 \end{cases} \quad (14)$$

We denote $U_1 = \partial T_1 / \partial \lambda_2$, $U_2 = \partial T_2 / \partial \lambda_2$ and

$$r_S = \int_0^t \mu \Delta T \, d\tau, \quad \rho_U = \int_0^t \mu U_1 \, d\tau \quad (15)$$

Then

$$q_1 = L_V \frac{\partial}{\partial t}\left(\frac{\partial f_S}{\partial \lambda_2}\right) = 4\,\pi\, N\, L_V \,\exp\left(-\frac{4}{3}\pi\, N\, r_S^3\right)\times \\ \times\left[4\,\pi\, N\,\mu\,\Delta T\,\rho_U\, r_S^4 - 2\,\mu\,\Delta T\,\rho_U\, r_S - \mu\, U_1\, r_S^2\right] \tag{16}$$

In this place the Schwarz theorem and the rules of the complex function differentiation can be used. Finally, the boundary initial problem (14) can be written in the form

$$\begin{cases} x\in\Omega_1: & c_1 \dfrac{\partial U_1}{\partial t} = \lambda_1\,\nabla^2\, U_1 + q_1 \\ x\in\Omega_2: & c_2 \dfrac{\partial U_2}{\partial t} = \lambda_2\,\nabla^2\, U_2 + \dfrac{c_2}{\lambda_2}\dfrac{\partial T_2}{\partial t} \\ x\in\Gamma_{12}: & \begin{cases} U_1 = U_2 \\ -\lambda_1 \dfrac{\partial U_1}{\partial n} = -\dfrac{\partial T_2}{\partial n} - \lambda_1 \dfrac{\partial U_2}{\partial n} \end{cases} \\ x\in\Gamma_0: & -\lambda_2 \dfrac{\partial U_2}{\partial n} = \alpha\, U_2 + \dfrac{\partial T_2}{\partial n} \\ t=0: & U_1 = 0,\quad U_2 = 0 \end{cases} \tag{17}$$

Now, we differentiate the basic model with respect to c_2:

$$\begin{cases} x\in\Omega_1: & c_1 \dfrac{\partial}{\partial t}\left(\dfrac{\partial T_1}{\partial c_2}\right) = \lambda_1\,\nabla^2\left(\dfrac{\partial T_1}{\partial c_2}\right) + L_V \dfrac{\partial}{\partial t}\left(\dfrac{\partial f_S}{\partial c_2}\right) \\ x\in\Omega_2: & c_2 \dfrac{\partial}{\partial t}\left(\dfrac{\partial T_2}{\partial c_2}\right) = \lambda_2\,\nabla^2\left(\dfrac{\partial T_2}{\partial c_2}\right) - \dfrac{\partial T_2}{\partial c_2} \\ x\in\Gamma_{12}: & \begin{cases} \dfrac{\partial T_1}{\partial c_2} = \dfrac{\partial T_2}{\partial c_2} \\ -\lambda_1 \dfrac{\partial}{\partial n}\left(\dfrac{\partial T_1}{\partial c_2}\right) = -\lambda_2 \dfrac{\partial}{\partial n}\left(\dfrac{\partial T_2}{\partial c_2}\right) \end{cases} \\ x\in\Gamma_0: & -\lambda_2 \dfrac{\partial}{\partial n}\left(\dfrac{\partial T_2}{\partial c_2}\right) = \alpha \dfrac{\partial T_2}{\partial c_2} \\ t=0: & \partial T_1/\partial c_2 = 0,\quad \partial T_2/\partial c_2 = 0 \end{cases} \tag{18}$$

Denoting $V_1 = \partial T_1 / \partial c_2$, $V_2 = \partial T_2 / \partial c_2$ and

$$\rho_V = \int_0^t \mu V_1 \, \mathrm{d}\tau \tag{19}$$

we obtain the formula determining the source function

$$\begin{gathered} q_2 = L_V \frac{\partial}{\partial t}\left(\frac{\partial f_S}{\partial c_2}\right) = -4\pi N L_V \exp\left(-\frac{4}{3}\pi N r_S^3\right) \times \\ \times \left[2\mu \Delta T \rho_V r_S + \mu V_1 r_S^2 + 4\pi N \mu \Delta T \rho_V r_S^4\right] \end{gathered} \tag{20}$$

So, the problem (18) can be written as follows:

$$\begin{cases} x \in \Omega_1: & c_1 \dfrac{\partial V_1}{\partial t} = \lambda_1 \nabla^2 V_1 + q_2 \\ x \in \Omega_2: & c_2 \dfrac{\partial V_2}{\partial t} = \lambda_2 \nabla^2 V_2 - \dfrac{\partial T_2}{\partial t} \\ x \in \Gamma_{12}: & \begin{cases} V_1 = V_2 \\ -\lambda_1 \dfrac{\partial V_1}{\partial n} = -\lambda_1 \dfrac{\partial V_2}{\partial n} \end{cases} \\ x \in \Gamma_0: & -\lambda_2 \dfrac{\partial V_2}{\partial n} = \alpha V \\ t = 0: & V_1 = 0, \quad V_2 = 0 \end{cases} \tag{21}$$

In order to determine the sensitivity of the process analyzed one should solve simultaneously the basic problem and two additional boundary-initial problems described by equations (17) and (21). The mutual connections between the basic model and systems (17) and (21) require the knowledge of temporary temperature field in the casting-mould domain. So, in order to solve the additional boundary-initial problems the solution of the basic one must be known.

3. Method of numerical solution

On the stage of numerical computation the control volume method (CVM) has been applied. The domain considered has been divided into N 2D control volumes, additionally the time grid with the step Δt has been introduced. The energy balance for the control volume considered ΔV_0 and the transition from t to $t + \Delta t$ can be written in the form

$$\Delta H_0 = \Delta t \sum_{e=1}^{m} Q_{0\,e}^{s} + \Delta t \int_{\Delta V_0} q \, \mathrm{d}V \tag{22}$$

where: ΔH_0 is the change of control volume entalphy during the time Δt, the index s is equal to f or $f + 1$ (in the problem considered the explicit scheme has been used and $s = f$), q is the capacity of internal heat sources. The quantity of heat exchanged between the control volume ΔV_0 and adjoining ones equals

$$Q_{0\,e}^{s} \, \Delta t = \frac{T_e^s - T_0^s}{R_e^f} \Delta A_e \, \Delta t \tag{23}$$

where: ΔA_e is the surface limiting ΔV_0 in direction e, R_e^f is the thermal resistance

$$R_e^f = \frac{0.5\, h_e}{\lambda_0^f} + \frac{0.5\, h_e}{\lambda_e^f} \tag{24}$$

while h_e is the distance between central points of ΔV_0 and ΔV_e.
The component corresponding to internal heat sources is transformed to the form

$$\int_{\Delta V_0} q \, \mathrm{d}V = q_0 \mid \Delta V_0 \mid \tag{25}$$

where q_0 is the mean capacity of source function.
The change of enthalpy ΔH_0 results from the formula

$$\Delta H_0 = c_0^f \left(T_0^{f+1} - T_0^f \right) \mid \Delta V_0 \mid \tag{26}$$

where c_0^f is the volumetric specific heat of control volume considered.
Taking into account the last formulas we have

$$c_0^f \left(T_0^{f+1} - T_0^f \right) \mid \Delta V_0 \mid = \sum_{e=1}^{m} \frac{T_e^s - T_0^s}{R_e^f} \Delta A_e \, \Delta t + q_{V0} \mid \Delta V_0 \mid \Delta t \tag{27}$$

or

$$T_0^{f+1} = T_0^f + \frac{\Delta t}{c_0^f} \left(\sum_{e=1}^{m} \frac{T_e^s - T_0^s}{R_e^f} F_e + q_{V0} \right) \tag{28}$$

where $F_e = \Delta A_e / \Delta V_0$. We denote

$$A_\mathrm{e} = \frac{F_e \, \Delta t}{c_0^f \, R_e^f}, \quad B = \frac{q_0 \, \Delta t}{c_0^f} \tag{29}$$

and then

$$T_0^{f+1}=T_0^f+\sum_{e=1}^{m}\left(T_e^s-T_0^s\right)A_e+B \tag{30}$$

or

$$T_0^{f+1}=T_0^f+\sum_{e=1}^{m}T_e^s\,A_e-T_0^s\sum_{e=1}^{m}A_e+B \tag{31}$$

For the explicit scheme we have $s=f$. So

$$T_0^{f+1}=\left(1-\sum_{e=1}^{m}A_e\right)T_0^f+\sum_{e=1}^{m}T_e^f\,A_e+B \tag{32}$$

or

$$T_0^{f+1}=\sum_{e=0}^{m}T_e^f\,A_e+B \tag{33}$$

where

$$A_0=1-\sum_{e=1}^{m}A_e \tag{34}$$

The problem of the boundary conditions modelling is a very simple. For the control volumes being in the thermal contact with the environment (the Robin condition), the thermal resistance is defined as follows

$$R_e^f=\frac{0.5\,h_e}{\lambda_0^f}+\frac{1}{\alpha} \tag{35}$$

where α is the heat transfer coefficient, additionally in a place of adequate T_e^f the ambient temperature appears. The condition between casting and mould is modelled in a natural way (see: definition of thermal resistance). The stability of the above scheme is assured if the coefficient $A_0>0$ for every control volume.

As an example we consider the quarter of the rectangular aluminium bar (0.05×0.07 m) produced in the sand mix mould. The parameters of casting material are equal to $\lambda_1=150$ W/mK, $c_1=3\cdot 10^6$ J/m$^3\cdot$K, $L=9.75\cdot 10^8$ J/m^3, solidification point $T_{cr}=660^{\circ}$C. The parameters of the mould: $\lambda_2=2.25$ W/mK, $c_1=2.261\cdot 10^6$ J/m$^3\cdot$K. The constant number of nuclei $N=10^{10}$ l/m^3 has been assumed, growth coefficient: $\mu=3\cdot 10^{-6}$ ms/K [7]. Initial temperatures: $T_{10}=700^{\circ}$C, $T_{20}=30^{\circ}$C. The solution of the problem give the big number of information concerning the course of the process.

For instance, in Figure 1 the effect of varying values of thermal conductivity λ_2 on the temperature is shown (cooling curves correspond to the point from casting domain located close to the boundary). The basic solution has been found for λ_2 = 2.25 W/mK, while the others results from the sensitivity analysis under the assumption that $\Delta\lambda_2$ = 0.25. In this place the Taylor formula has been used

$$T\left(\lambda_0 \pm \Delta\lambda\right) = T\left(\lambda_0\right) \pm U\,\Delta\,\lambda \tag{36}$$

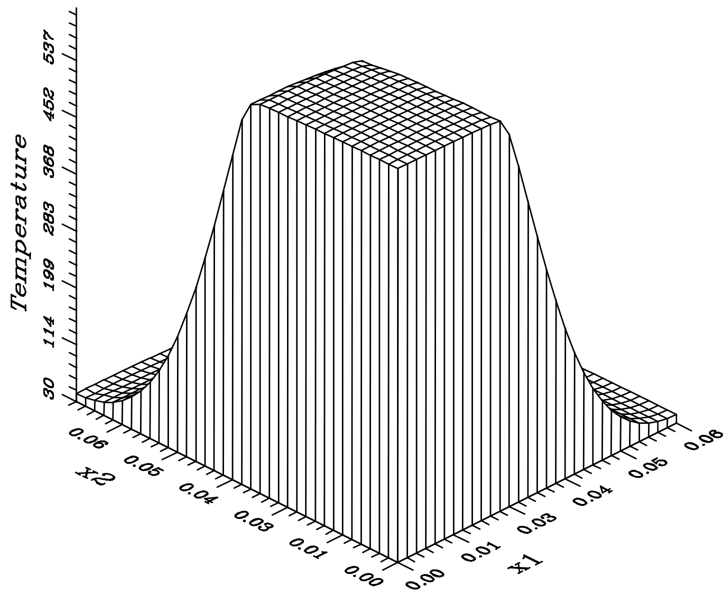

Fig. 1. Temperature distribution (t = 120 s)

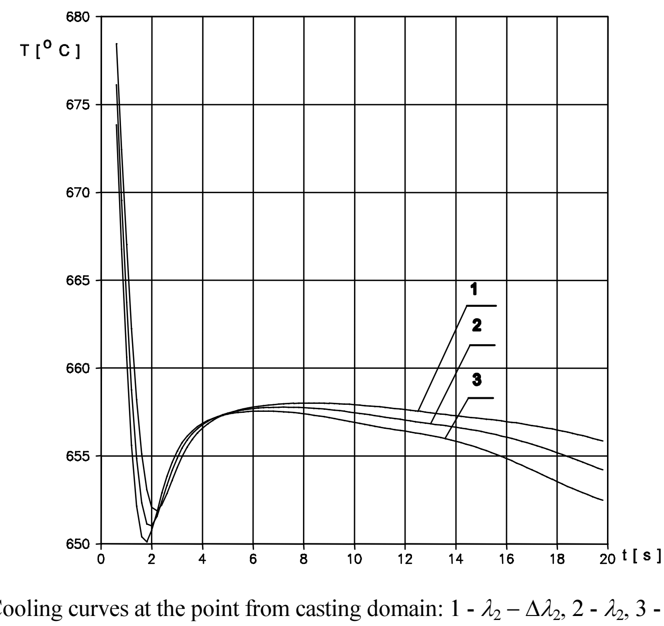

Fig. 2. Cooling curves at the point from casting domain: 1 - $\lambda_2 - \Delta\lambda_2$, 2 - λ_2, 3 - $\lambda_2 + \Delta\lambda_2$

In order to test the exactness and effectiveness of the method proposed the computations have been vealized in two variants. At first the border values of λ_2 ($\lambda_2 = 2$ and $\lambda_2 = 2.5$) have been assumed and for these input data the direct solution has been found. Next the same solution has been constructed on the basis of $\lambda = 2.25$ and the formula (36) has been applied. It turned out that the both solutions are practically the same. This fact confirms the correctness of the algorithm both on the stage of mathematical model and also the numerical computation. In Figure 2 the temperature field for time $t = 120$ s is shown.

Summing up, the presented algorithm using the control volume method for the numerical computations of temperature sensitivity is quite exact and effective and can be applied for analysis of the heat transfer processes in the system casting-mould-environment.

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