THE PARAMETRIC SENSITIVITY ANALYSIS OF SOLIDIFICATION PROCESS

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SUMMARY

In the paper the new results concerning the application of sensitivity analysis in the numerical modelling of solidification process is presented. This approach allows to investigate the influence of external conditions (thermophysical parameters of the mould, pouring temperature, initial mould temperature etc.) on the course of casting solidification. The model of thermal processes proceeding in the casting domain can be constructed both in the macro scale (the I generation model) and in the macro/micro scale (the II generation model). As an example of the macro approach the continuous casting technology is considered and the sensitivity with respect to the substitute heat transfer coefficient in the continuous casting mould region is analyzed. In the second part of the paper the macro/micro model is introduced and the similar problem is solved again.

Key words: casting solidification, sensitivity analysis, control volume method

1. FORMULATION OF THE MACRO PROBLEM

The continuous casting process is below considered. The basic energy equation describing the thermal processes in the domain of vertical, rectangular cast slab can be written in the form

\[ C(T) \left( \frac{\partial T}{\partial t} + w \frac{\partial T}{\partial z} \right) = \frac{\partial}{\partial x} \left[ \lambda(T) \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \lambda(T) \frac{\partial T}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \lambda(T) \frac{\partial T}{\partial z} \right] \]  (1)

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where $T = T(x, y, z, t)$, $C(T)$ is the substitute thermal capacity per unit of volume [1, 2], $\lambda(T)$ is the thermal conductivity, $w$ is the pulling rate - the cast slab shifts in $z$ direction (see: Figure 1). Formulating the equation (1) we assumed only the conductional heat transfer.

The substitute thermal capacity in equation (1) is defined in the following way [1, 2]

$$C(T) = c(T) - L \frac{df_s(T)}{dT}$$

(2)

where $c(T)$ is the volumetric specific heat, $L$ is the latent heat, $f_s$ is the volumetric solid state fraction at the point considered. If we denote by $T_L$ and $T_S$ the temperatures corresponding to the beginning and the end of solidification process then for $T < T_S$: $f_s = 1$, and for $T > T_L$: $f_s = 0$.

So, for the liquid and solid sub-domains $df_s/dT = 0$ and $C(T) = c(T)$, where $c(T)$ is the volumetric specific heat $c_L$ or $c_S$, correspondingly. In the mushy zone sub-domain the function describing the substitute thermal capacity depends on the course of $f_s(T)$ [1, 2, 3]. Because the equation (1) concerns the conventionally homogeneous domain therefore this approach to the alloys solidification modelling is called the one domain method.

The boundary conditions on the lateral surface of cast slab (the continuous casting mould region) are assumed in the form.
\[-\lambda(T)\frac{\partial T}{\partial n} = \alpha(T - T_w)\]  

(3)

where \( \frac{\partial T}{\partial n} \) is the normal derivative, \( \alpha \) is the substitute heat transfer coefficient [4], \( T_w \) is the cooling water temperature. On the upper surface of the casting (free surface of molten metal) the boundary condition of the 1st type (pouring temperature) can be taken into account. On the conventionally assumed bottom surface limiting the domain considered we can put \( \frac{\partial T}{\partial n} = 0 \), this means the adiabatic condition.

The initial condition resolves itself into the assumption, that a certain layer of molten metal directly over the starter bar has a pouring temperature \( T_p \). The starter bar allows to shut the continuous casting mould during the plant starting.

The numerous experiments show that conductional component of heat transfer corresponding to the direction of cast strand displacement is very small (in the case of steel castings this component constitutes about 5% of the heat conducted from the axis to the lateral surfaces). So, the equation (1) can be simplified to the 2D one. Let we rewrite the equation (4) in coordinate system ‘tied’ to a certain section of shifting casting, namely \( x' = x, \quad y' = y, \quad z' = z - ut \). It is easy to check up that we ‘lose’ in energy equation the component \( T_z \) and we obtain

\[
C(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x'} \left[ \lambda(T) \frac{\partial T}{\partial x'} \right] + \frac{\partial}{\partial y'} \left[ \lambda(T) \frac{\partial T}{\partial y'} \right]
\]

(4)

This approach is called ‘a wandering cross section method’ [5]. We consider the lateral section of the cast strand which position at the moment \( t = 0 \) corresponds to \( z = 0 \) (the initial condition has a form \( T(0) = T_p \)), while the boundary conditions on the periphery of this section are functions of time. If \( \Delta t_i \) corresponds to the ‘hold time’ of the section in the continuous casting mould region, then for \( 0 \leq t \leq \Delta t_i \) on the casting periphery the boundary condition for the primary cooling zone (e.g., heat flux) is assumed. For the next interval \( \Delta t_{i+1} \) we consider the boundary condition characterizing the heat transfer in the 1st sector of the secondary cooling zone etc.

2. SENSITIVITY ANALYSIS

In order to construct the sensitivity model respect to \( \alpha \) we differentiate the governing equations over this parameter (a direct approach is applied [6])

\[
\frac{dC(T)}{dT} U \frac{\partial T}{\partial t} + C(T) \frac{\partial U}{\partial t} = \frac{\partial}{\partial x} \left[ \frac{d\lambda(T)}{dT} U \frac{\partial T}{\partial x} + \lambda(T) \frac{\partial U}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{d\lambda(T)}{dT} U \frac{\partial T}{\partial y} + \lambda(T) \frac{\partial U}{\partial y} \right]
\]

(5)
In equation (5) we substitute again \( x' = x \), \( y' = y \), symbol \( \partial T / \partial \alpha = U \) denotes the sensitivity function.

Differentiating the condition (3) one has

\[
-\lambda \frac{\partial U}{\partial n} = T - T_0 + \alpha U
\]  

(6)

The initial condition takes a form: \( U(0) = 0 \).

The solution of the sensitivity problem allows, among others, to 'rebuild' the basic solution on the new solution corresponding to the optional new value of coefficient \( \alpha \). It results from the Taylor formula, namely

\[
T(x, y, t, \alpha \pm \Delta \alpha) = T(x, y, t, \alpha) \pm U(x, y, t, \alpha) \Delta \alpha
\]  

(7)

The distance \( \Delta \alpha \) should be not very big, of course.

As an example the following task is presented. The rectangular steel slab (0.44% C) with dimensions 0.6 \( \times \) 0.2[m] is considered. The pouring temperature equals 1550[°C], pulling rate: \( w = 0.017[\text{m/s}] \). The basic heat transfer coefficient in the primary cooling zone equals \( \alpha = 1500[\text{W/m}^2 \text{K}] \). The temperature field at the distance 0.6[m] from upper surface of the slab has been observed. The precise results will be shown below. For the nodes located near the corner of cast slab the nodal temperatures for \( \alpha = 1500 \) are collected on the left side of the page. The temperatures found directly for \( \alpha = 1700 \) are written in the middle of this page, while on the right side one can find the temperatures for \( \alpha = 1700 \) obtained on the basis of the sensitivity analysis:

<table>
<thead>
<tr>
<th>Nodes</th>
<th>Temperatures</th>
</tr>
</thead>
<tbody>
<tr>
<td>925</td>
<td>883 812 812 858 815 741 741 855 814 740 740</td>
</tr>
<tr>
<td>1259</td>
<td>1201 1046 812 1216 1155 986 741 1214 1155 987 740</td>
</tr>
<tr>
<td>1496</td>
<td>1478 1201 883 1492 1468 1155 816 1493 1471 1155 814</td>
</tr>
<tr>
<td>1512</td>
<td>1496 1259 925 1510 1492 1216 858 1510 1493 1215 855</td>
</tr>
</tbody>
</table>

The results presented show that the sensitivity analysis constitutes a very effective tool for estimation of the cooling conditions influence on the course of solidification.

3. THE SECOND GENERATION MODEL

We consider the following energy equation in the moving co-ordinate system (c.f. equation (4))
where $c(T)$ is the volumetric specific heat.

If we introduce the second generation model then the capacity of source function $Q$ results from the considerations called the micro/macro approach (e.g. [7, 8]). So, the problem of source function construction will be discussed. A temporary value of solid fraction $f_S$ of the metal at point considered is given by the Johnson-Mehl-Arrami-Kolmogorov type equation [7, 8]

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

where

$$\omega = \frac{4}{3} \pi \nu \int_0^\tau \frac{\partial N}{\partial t} \left[ \int_0^u \frac{d \tau}{\gamma} \right] d \tau$$

In equation (10) $N$ is a number of nuclei (more precisely: density [nuclei/m$^3$]), $\nu$ is the coefficient equal to 1 for the spherical grains and $\nu < 1$ for dendritic growth, $u$ is a rate of solid phase growth, $\tau$ is a moment of crystallization process beginning. The solid phase growth (equiaxial grains) is determined by equation

$$\frac{dR}{dt} = \mu \Delta T^p$$

where $R$ is a grain radius, $\mu$ is a growth coefficient, $p$ is the exponent from the interval $p \in [1, 2]$, and

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

is the undercooling below the solidification point $T_{cr}$. Additionally we assume the constant number of nuclei (the nucleation law is neglected) and the constant values of $c$ and $\lambda$. Then

$$\frac{\partial T}{\partial t} = \lambda \nabla^2 T + L \exp(-\omega) \frac{\partial \omega}{\partial t} = \lambda \nabla^2 T + Q$$

where
\[ Q = 4 \pi v N L \mu \Delta T^p \left[ \int_0^T \mu \Delta T^p \, dt \right]^2 \exp \left[ -\frac{4}{3} \pi v N \left( \int_0^T \mu \Delta T^p \, dt \right) \right] \] (14)

Equation (13) supplemented by the boundary condition (3) and the initial one constitutes a base for numerical computations of temperature field in the continuous casting domain.

4. SENSITIVITY OF THE MACRO/MICRO MODEL

In this chapter the sensitivity analysis of solidification process with respect to the heat transfer coefficient on the lateral surface of the casting is presented. Differentiation of the equations forming the mathematical model discussed with respect to \( \alpha \) leads to the additional boundary initial problem

\[
\begin{align*}
P \in \Omega: & \quad \frac{\partial U}{\partial t} = \lambda \left( \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} \right) + Q_v \\
P \in \Gamma: & \quad -\lambda \frac{\partial U}{\partial n} = \alpha (U - U_o) \\
t = 0: & \quad U = 0
\end{align*}
\] (15)

where \( P \in \Omega \) is the point from the interior of casting domain, \( P \in \Gamma \) is the boundary one, \( U = \partial T / \partial \alpha \). Denoting

\[ r_s = \int_0^T \mu \Delta T^p \, dt, \quad \rho_p = \int_0^T \mu \Delta T^p U \, dt \] (16)

we obtain

\[
Q_s = \frac{\partial Q}{\partial \alpha} = 4 p \pi v N L_v \exp \left( -\frac{4}{3} \pi v r_s \right) \\
\left[ 4 \pi v N \mu \Delta T^p \rho_p r_s^4 - 2 \mu \Delta T^p \rho_p r_s - \mu p U r_s^2 \Delta T^p \right] \] (17)

On the stage of numerical computations the value \( p = 1 \) has been assumed, integrals (16) have been found using the numerical methods. As the example the aluminium cast slab of dimensions 0.15\times0.15 [m] has been considered. The pulling rate is assumed to be \( w = 0.02 \) [m/s], while the pouring temperature \( T_0 = 700 \) [°C]. The following parameters of the metal have been introduced: \( \lambda = 150 \) [W/mK], \( c = 3 \times 10^6 \) [J/m^3K], \( L = 9.75 \times 10^8 \) [J/m^3], \( T_{cr} = 660 \) [°C], \( N = 10^{11} \) [nuclei/m^3], \( \mu = 3 \times 10^{-6} \) [m^3/sK], \( v = 1 \), \( p = 1 \). The heat transfer coefficient \( \alpha = 1200 \) [W/m^2K], cooling water temperature \( T_v = 30 \) [°C].
The Figures 2, 3, 4, 5 contain the results corresponding to distance $z = 0.6$ [m]. The possibility of the basic numerical solution transformation on the solution for the others cooling conditions is clearly visible. The possibilities of sensitivity analysis do not reduce only to the problems above presented. It is possible to consider the influence of casting and mould thermophysical parameters on the course of solidification, the influence of pouring temperature or parameters appearing in the Kolmogoroff model. Summing up, the sensitivity analysis constitutes a very effective tool for the solution of different problems from the scope of thermal theory of foundry processes.

REFERENCES


PARAMETRYCZNA ANALIZA WRAŻLIWOŚCI PROCESU KRZEPNIĘCIA

STRESZCZENIE

W pracy przedstawiono wyniki badań dotyczących wykorzystania metod analizy wrażliwości w numerycznym modelowaniu procesu krzepnięcia. Takie podejście pozwala badać wpływ zaburzeń parametrów procesu (parametrów termo fizycznych, temperatury zalewania, temperatury początkowej masy formierskiej itd.) na przebieg analizowanego procesu. Model procesów cieplnych zachodzących w krzepnącym odlewie może być formułowany zarówno w skali makro (modele I generacji), jak i makro/mikro (modele II generacji). Jako przykład zastosowań wykorzystano analizę wrażliwości procesu ciągłego odlewania stali na zmiany zastępczego współczynnika wymiany ciepła (model opisany w konwencji makro) oraz podobny problem dla wlewka aluminiowego (model II generacji). Na etapie obliczeń wykorzystano metodę bilansów elementarnych.

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