Mathematical investigation of the process of substance crystallization in domains with complex geometry and its optimal control

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The optimal control problem of the metal solidification in casting is considered. The process is modeled by a three dimensional two phase initial-boundary value problem of the Stefan type.

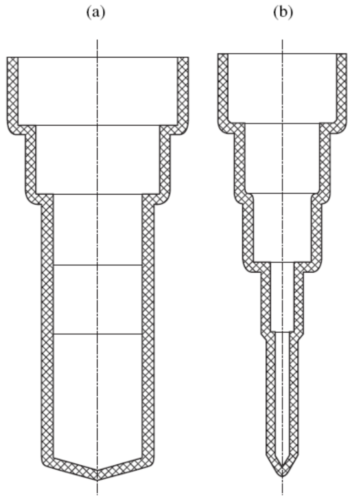

Fig. 1

An important stage in metal casting is the cooling and solidification of melted metal in the mold. The importance of this stage is explained by the fact that the quality of the resulting product depends on how the process of cooling and solidification proceeds. Stage of cooling and solidification can be described as follows. A mold with specified outer and inner boundaries (Fig. 1) is filled with liquid metal (the hatched area in Fig. 1 depicts the mold wall and the internal unhatched area shows the inside space filled with liquid metal). The mold and the metal inside it are heated up to prescribed temperatures T_{form} and T_{met} respectively. Next, the mold filled with metal (which is hereafter referred to as the object) begins to cool gradually under varying surrounding conditions. The different parts of its outer boundary are under different thermal conditions (i.e., the laws of heat exchange with the surroundings are different in these parts). Moreover, the thermal conditions vary with time.

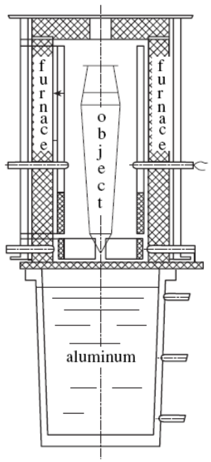

Fig. 2

The experimental setup for metal casting is shown on Fig. 2. It consists of upper and lower parts. The upper part of this setup consists of a furnace and a mold moving inside it. The lower part is a cooling bath representing a large tank filled with liquid aluminum whose temperature is somewhat higher than the aluminum melting point. The cooling of the liquid metal in the furnace proceeds as follows. On the one hand, the object is slowly immersed in the low temperature liquid aluminum (the coolant), which causes the solidification of the metal. On the other hand, the object gains heat from the furnace walls, which prevents the solidification process from proceeding too fast. According to numerous experiments of solidification in such setups, for a product of high quality to be obtained, it is desired that the phase boundary be as close to a plane as possible (no liquid metal bubbles inside the domain) and that it moves sufficiently slowly.

The process of cooling down of the object is described by the heat-type equation:

$$\frac{\partial H}{\partial t}=\frac{\partial}{\partial x}\left(K\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(K\frac{\partial T}{\partial z}\right), \quad (1)$$

$$(x,y,z)\in Q.$$

Here x, y, and z are the Cartesian coordinates of a point; t is time; Q is the domain (object) with a piecewise smooth boundary Γ; $T(x,y,z,t)$ is the substance temperature at the point with coordinates (x,y,z) at time t; K is the thermal conductivity of the substance. The heat content function $H\left(T(x,y,z,t)\right)$ is defined as

$$H\left(T(x,y,z,t)\right)=\begin{cases} H_1(T), & (x,y,z)\in metal,\\ H_2(T), & (x,y,z)\in mold,\end{cases}$$

$$H_1(T)=\begin{cases} \rho_S c_S T, & T<T_1,\\ \rho_S c_S T+\dfrac{\rho_S\gamma(T-T_1)}{T_2-T_1}, & T_1\le T<T_2,\\ \rho_L c_L(T-T_2)+R_S, & T\ge T_2,\end{cases}$$

$$H_2(T)=\rho_\Phi c_\Phi T, \qquad R_S=\rho_S c_S T_2+\rho_S\gamma,$$

γ is the specific heat of melting.

The thermal conductivity K is different for the metal and the mold:

$$K(T)=\begin{cases} K_1(T), & (x,y,z)\in metal,\\ k_\Phi, & (x,y,z)\in mold,\end{cases}$$

$$K_1(T)=\begin{cases} k_S, & T<T_1,\\ \dfrac{(k_L-k_S)T+k_ST_2-k_LT_1}{T_2-T_1}, & T_1\le T<T_2,\\ k_L, & T\ge T_2.\end{cases}$$

The constants c_S, c_L, c_Φ, ρ_S, ρ_L, ρ_Φ, k_S, k_L, k_Φ, T_1, and T_2 in these formulas are assumed to be known. Note that the metal can be present in two phases: solid and liquid. The domain separating the phases is determined by a narrow range of temperatures $[T_1,T_2]$, in which the thermodynamic coefficients change rapidly.

The mold and the metal are cooled via their interaction with the surroundings. The individual parts of the outer boundary of the object are in different thermal conditions. The basic types of thermal conditions at a point of the outer boundary of the object can be described as follows.

1) The point is in the liquid aluminum.
In this case, the following processes have to be taken into account:
(I) the heat lost by the object due to its own radiation;
(II) the heat gained from the surrounding liquid aluminum due to its radiation;
(III) the heat transfer due to thermal conduction between the liquid aluminum and the object.

2) The point is outside the liquid aluminum.
In this case, the following processes have to be taken into account:
(I) the heat lost by the object due to its own radiation;
(II) the heat gained from the emitting walls of the furnace;
(III) the heat gained from the emitting surface of the liquid aluminum.

The conditions of heat transfer with the surrounding medium are set on the boundary Γ of Q. These conditions depend on the given surface point and time and can be written in the general form:

$$\tilde{\alpha}T+\tilde{\beta}T_{\mathbf{n}}=\tilde{\gamma}. \quad (2)$$

Here $\tilde{\alpha}$, $\tilde{\beta}$, and $\tilde{\gamma}$ are given functions of the coordinates (x,y,z) of a point on Γ and the temperature $T(x,y,z,t)$, and $\frac{\partial T}{\partial \mathbf{n}}=T_{\mathbf{n}}$ is the derivative of T in the $\mathbf{n}$-direction (external normal to the surface Γ).

It should be noted that the thermodynamic coefficients have a jump at the metal-mold interface. Two conditions are set at this surface, namely, the temperature and the heat flux must be continuous.

Thus, to solve the direct problem is to determine a function $T(x, y, z, t)$ that satisfies Eq. (1) in Q, conditions (2) on the outer boundary Γ of Q, and the continuity conditions for the temperature and the heat flux at the metal-mold interface.

The optimal control problem is to choose a regime of metal cooling and solidification at which the solidification front has a preset shape or is close to it (namely, a plane orthogonal to the vertical axis of the object) and moves sufficiently slowly (at a speed close to the preset one). The evolution of the solidification front is affected by numerous parameters (the furnace temperature, the liquid aluminum temperature, the depth to which the object is immersed in the liquid aluminum, the speed at which the mold moves relative to the furnace, etc.). Dependence of the behaviour of the solidification front on the velocity of the object is of special interest in practice.

The speed $U(t)$ of the displacement of foundry mold in the melting furnace was chosen as the control. The cost function is:

$$I(U) = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} \iint_{S} [Z_{pl}(x, y, t) - z_*(t)]^2 dx dy dt. \quad (3)$$

Here t_1 is the time, when the crystallization front arises; t_2 is the time, when the crystallization of metal completes; $(x, y, Z_{pl}(x, y, t))$ are the real coordinates of the interface at the time t; $(x, y, z_*(t))$ are the desired coordinates of the interface at the time t; S is the largest cross section of the mold which is filled by metal. The control function may be restricted by some prescribed functions $U_1(t)$ and $U_2(t)$: $U_1(t) \le U(t) \le U_2(t)$.

The posed optimal control problem was studied in [1]-[3] for a mold in the form of a parallelepiped. In contrast to previous studies, the object under analysis has a complex geometric shape.

Due to the complex geometry of the object, we had to further elaborate the algorithm developed for computing an object of the simplest shape. First, at the interface of different parts of the object, there arose new elementary cells of complex geometry that were not encountered earlier. As a result, we had to modernize the algorithm for computing the heat balance in the system. Second, due to the new geometry of the object, the algorithm for computing the level of liquid aluminum in the cooling bath had to be improved. Finally, for the same reason, the algorithm for computing the heat flux to the object caused by the thermal radiation of the furnace and the surface of the liquid aluminum was modified. This is associated with the fact that some parts of the object surface are now shaded by others.

The object being investigated is approximated by the body, which consists of a finite number of rectangular parallelepipeds. The approximated body is placed mentally wholly into a certain large parallelepiped. In this large parallelepiped a basic rectangular grid is introduced in such a way that all external surfaces of the approximated body and the surfaces, which divide metal and form, coincide with the grid surfaces. Besides the basic grid, the auxiliary grid is built, whose surfaces are parallel to the surfaces of the basic grid and are displaced relative to it with a half-step in all directions. As a result this entire object being investigated is broken by the surfaces of auxiliary grid to the elementary volumes.

A numerical algorithm was developed for solving the initial-boundary value problem. Formulated direct problem is approximated on the constructed grid. For each elementary volume the equation of heat balance is written in the terms of heat content (see [1]). The finite-difference approximation of the heat balance equation is based on the Peaceman-Rachford scheme. In the computation of the direct problem primary attention was given to the evolution of the solidification front and to how it is affected by the parameters of the problem.

The control function is approximated by a piecewise constant function. As a result of such approximation the cost function is a function of finite number of variables. The minimum value of a cost function was found numerically using gradient methods. The approximate finite-difference evaluation of the cost functional gradient in the given optimal control problem is associated with huge difficulties (see [3]). In the work an effective method is proposed for evaluating the cost functional gradient in the optimal control problem. The method is based on the Fast Automatic Differentiation (FAD) technique (see [4]) and produces the exact value of the gradient.

When the gradient components are evaluated using the FAD-technique, despite the large number of gradient components, the required CPU time is not more than half of the CPU time required for solving the direct problem. This fact is supported by numerous computations and agrees with the conclusions drawn in [4]. That is why the exact evaluation of the cost functional gradient based on the Fast Automatic Differentiation technique seems a necessary unavoidable element of the solution to complicated optimal control problems, although this technique is rather cumbersome and the discrete adjoint problem and the gradient evaluation formulas are difficult to derive.

During the analysis of non-stationary problems, particularly when solving the optimal control problem of a complex dynamical system, it's often convenient and useful to have an opportunity to watch the dynamical progress of the whole process in study. For this reason a software that allows to draw a motion picture of any flat scalar field and to depict any stationary or moving object was developed (see [5]). This software is successfully used when solving the optimal problem in question for visualization of the whole crystallization process with a lot of details in a casting form with a complex geometry. Along with the temperature field there were depicted the borders of the casting form, the casting form, the interface and the areas of solidified metal. The use of the developed software also had influence on the new foundation of the optimal control problem in study.

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