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Optimal control for one complex dynamic system, II

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Abstract. 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. A numerical algorithm for solving the direct problem was presented in the first part of this article, published in [1]. The optimal control problem was solved numerically using the gradient method. The gradient of the cost function was found with the help of conjugate problem. The discreet conjugate problem was posed with the help of Fast Automatic Differentiation technique.

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6 Calculation of the gradient in the optimal control problem

6.1 The canonical form of the discrete version of the direct problem

The variational problem formulated in Section 2 (part I) was solved numerically by gradient methods. To calculate the gradient of the function the Fast Automatic Differentiation (FAD) methodology [2] was used.

In accordance with the FAD-methodology, all equations, that approximate the direct problem, have to be presented in a special, so-called, canonical form that we will give below.

For this canonical form to be more compact, let us introduce the following designations.

For all $i = \overline{0, I}$, $l = \overline{0, L}$ let us designate as (X_m) and (X_f) these $(N+2)$-dimentional vectors:

$$(X_m)^j_{0il} = -\left(r_1(\beta^j_{0il})\beta^j_{0il} + q^j_1\right)\Big|_{S^{1x-}_{0il}}, \quad (X_f)^j_{0il} = -\left(r_2(\beta^j_{0il})\beta^j_{0il} + q^j_2\right)\Big|_{S^{2x-}_{0il}},$$

$$(X_m)^j_{nil} = R^j_{n-1}\frac{\beta^j_{nil} - \beta^j_{n-1,il}}{h^x_{n-1}}, \quad (X_f)^j_{nil} = B^j_{n-1}\frac{\beta^j_{nil} - \beta^j_{n-1,il}}{h^x_{n-1}}, \quad (n = \overline{1, N}),$$

$$(X_m)^j_{N+1,il} = \left(r_1(\beta^j_{Nil})\beta^j_{Nil} + q^j_1\right)\Big|_{S^{1x+}_{Nil}}, \; (X_f)^j_{N+1,il} = \left(r_2(\beta^j_{Nil})\beta^j_{Nil} + q^j_2\right)\Big|_{S^{2x+}_{Nil}}.$$

For all $n = \overline{0, N}$, $l = \overline{0, L}$ let us designate as (Y_m) and (Y_f) these $(I+2)$-dimentional vectors:

$$(Y_m)^j_{n0l} = -\left(r_1(\beta^j_{n0l})\beta^j_{n0l} + q^j_1\right)\Big|_{S^{1y-}_{n0l}}, \quad (Y_f)^j_{n0l} = -\left(r_2(\beta^j_{n0l})\beta^j_{n0l} + q^j_2\right)\Big|_{S^{2y-}_{n0l}},$$

$$(Y_m)^j_{nil} = \widehat{R}^j_{i-1}\frac{\beta^j_{nil}-\beta^j_{n,i-1,l}}{h^y_{i-1}}, \qquad (Y_f)^j_{nil} = \widehat{B}^j_{i-1}\frac{\beta^j_{nil}-\beta^j_{n,i-1,l}}{h^y_{i-1}}, \quad i=\overline{1,I},$$

$$(Y_m)^j_{n,I+1,l} = \Big(r_1(\beta^j_{nIl})\beta^j_{nIl}+q^j_1\Big)\Big|_{S^{1y+}_{nIl}}, \; (Y_f)^j_{n,I+1,l} = \Big(r_2(\beta^j_{nIl})\beta^j_{nIl}+q^j_2\Big)\Big|_{S^{2y+}_{nIl}}.$$

For all $n=\overline{0,N}$, $i=\overline{0,I}$ let us designate as (Z_m) and (Z_f) these $(L+2)$-dimentional vectors:

$$(Z_m)^j_{ni0} = -\Big(r_1(\beta^j_{ni0})\beta^j_{ni0}+q^j_1\Big)\Big|_{S^{1z-}_{ni0}}, \quad (Z_f)^j_{ni0} = -\Big(r_2(\beta^j_{ni0})\beta^j_{ni0}+q^j_2\Big)\Big|_{S^{2z-}_{ni0}},$$

$$(Z_m)^j_{nil} = \widetilde{R}^j_{l-1}\frac{\beta^j_{nil}-\beta^j_{ni,l-1}}{h^z_{l-1}}, \qquad (Z_f)^j_{nil} = \widetilde{B}^j_{l-1}\frac{\beta^j_{nil}-\beta^j_{ni,l-1}}{h^z_{l-1}}, \quad l=\overline{1,L},$$

$$(Z_m)^j_{ni,L+1} = \Big(r_1(\beta^j_{niL})\beta^j_{niL}+q^j_1\Big)\Big|_{S^{1z+}_{niL}}, \; (Z_f)^j_{ni,L+1} = \Big(r_2(\beta^j_{niL})\beta^j_{niL}+q^j_2\Big)\Big|_{S^{2z+}_{niL}}.$$

Here and further the subscripts m and f indicate the belonging of the variable to the metal or to the form respectively.

Taking into account the introduced designations the three subproblems that approximate the direct problem can be written for all $j=\overline{0,J-1}$ in the following form:

x – direction

$$E^{j+\frac{1}{3}}_{nil} = E^j_{nil} + \omega^{j+1}_{nil}\Big[S^{1x+}_{nil}(X_m)^{j+\frac{1}{3}}_{n+1,il} - S^{1x-}_{nil}(X_m)^{j+\frac{1}{3}}_{nil} + S^{2x+}_{nil}(X_f)^{j+\frac{1}{3}}_{n+1,il} -$$
$$-S^{2x-}_{nil}(X_f)^{j+\frac{1}{3}}_{nil} + S^{1y+}_{nil}(Y_m)^j_{n,i+1,l} - S^{1y-}_{nil}(Y_m)^j_{nil} + S^{2y+}_{nil}(Y_f)^j_{n,i+1,l} - S^{2y-}_{nil}(Y_f)^j_{nil} +$$
$$+S^{1z+}_{nil}(Z_m)^j_{ni,l+1} - S^{1z-}_{nil}(Z_m)^j_{nil} + S^{2z+}_{nil}(Z_f)^j_{ni,l+1} - S^{2z-}_{nil}(Z_f)^j_{nil}\Big],$$

y – direction

$$E^{j+\frac{2}{3}}_{nil} = E^{j+\frac{1}{3}}_{nil} + \omega^{j+1}_{nil}\Big[S^{1y+}_{nil}(Y_m)^{j+\frac{2}{3}}_{n,i+1,l} - S^{1y-}_{nil}(Y_m)^{j+\frac{2}{3}}_{nil} + S^{2y+}_{nil}(Y_f)^{j+\frac{2}{3}}_{n,i+1,l} -$$
$$-S^{2y-}_{nil}(Y_f)^{j+\frac{2}{3}}_{nil} + S^{1x+}_{nil}(X_m)^{j+\frac{1}{3}}_{n+1,il} - S^{1x-}_{nil}(X_m)^{j+\frac{1}{3}}_{nil} + S^{2x+}_{nil}(X_f)^{j+\frac{1}{3}}_{n+1,il} - S^{2x-}_{nil}(X_f)^{j+\frac{1}{3}}_{nil} +$$
$$+S^{1z+}_{nil}(Z_m)^{j+\frac{1}{3}}_{ni,l+1} - S^{1z-}_{nil}(Z_m)^{j+\frac{1}{3}}_{nil} + S^{2z+}_{nil}(Z_f)^{j+\frac{1}{3}}_{ni,l+1} - S^{2z-}_{nil}(Z_f)^{j+\frac{1}{3}}_{nil}\Big],$$

z – direction

$$E^{j+1}_{nil} = E^{j+\frac{2}{3}}_{nil} + \omega^{j+1}_{nil}\Big[S^{1z+}_{nil}(Z_m)^{j+1}_{ni,l+1} - S^{1z-}_{nil}(Z_m)^{j+1}_{nil} + S^{2z+}_{nil}(Z_f)^{j+1}_{ni,l+1} -$$
$$-S^{2z-}_{nil}(Z_f)^{j+1}_{nil} + S^{1x+}_{nil}(X_m)^{j+\frac{2}{3}}_{n+1,il} - S^{1x-}_{nil}(X_m)^{j+\frac{2}{3}}_{nil} + S^{2x+}_{nil}(X_f)^{j+\frac{2}{3}}_{n+1,il} - S^{2x-}_{nil}(X_f)^{j+\frac{2}{3}}_{nil} +$$
$$+S^{1z+}_{nil}(Z_m)^{j+\frac{2}{3}}_{ni,l+1} - S^{1z-}_{nil}(Z_m)^{j+\frac{2}{3}}_{nil} + S^{2z+}_{nil}(Z_f)^{j+\frac{2}{3}}_{ni,l+1} - S^{2z-}_{nil}(Z_f)^{j+\frac{2}{3}}_{nil}\Big],$$

$$n=\overline{0,N}; \qquad i=\overline{0,I}; \qquad l=\overline{0,L}.$$

Let us introduce the following two-dimensional vectors:

$$S_{nil}^{x+} = \begin{bmatrix} S_{nil}^{1x+} \\ S_{nil}^{2x+} \end{bmatrix}, \qquad S_{nil}^{x-} = \begin{bmatrix} S_{nil}^{1x-} \\ S_{nil}^{2x-} \end{bmatrix}, \qquad S_{nil}^{y+} = \begin{bmatrix} S_{nil}^{1y+} \\ S_{nil}^{2y+} \end{bmatrix},$$

$$S_{nil}^{y-} = \begin{bmatrix} S_{nil}^{1y-} \\ S_{nil}^{2y-} \end{bmatrix}, \qquad S_{nil}^{z+} = \begin{bmatrix} S_{nil}^{1z+} \\ S_{nil}^{2z+} \end{bmatrix}, \qquad S_{nil}^{z-} = \begin{bmatrix} S_{nil}^{1z-} \\ S_{nil}^{2z-} \end{bmatrix},$$

$$n = \overline{0,N}; \qquad i = \overline{0,I}; \qquad l = \overline{0,L};$$

$$(X_{mf})_{nil}^j = \begin{bmatrix} (X_m)_{nil}^j \\ (X_f)_{nil}^j \end{bmatrix} \qquad n = \overline{0,N+1}; \qquad i = \overline{0,I}; \qquad l = \overline{0,L};$$

$$(Y_{mf})_{nil}^j = \begin{bmatrix} (Y_m)_{nil}^j \\ (Y_f)_{nil}^j \end{bmatrix} \qquad n = \overline{0,N}; \qquad i = \overline{0,I+1}; \qquad l = \overline{0,L};$$

$$(Z_{mf})_{nil}^j = \begin{bmatrix} (Z_m)_{nil}^j \\ (Z_f)_{nil}^j \end{bmatrix} \qquad n = \overline{0,N}; \qquad i = \overline{0,I}; \qquad l = \overline{0,L+1}.$$

Note that $S_{nil}^{x+} = S_{n+1,il}^{x-}$, $n = \overline{0,N-1}$;

$$S_{nil}^{y+} = S_{n,i+1,l}^{y-},\ i = \overline{0,I-1}; \quad S_{nil}^{z+} = S_{ni,l+1}^{z-},\ l = \overline{0,L-1}.$$

Let us introduce also designations for the following scalar products:

$$\widetilde{X}_{nil}^j = \left(S_{nil}^{x-}, (X_{mf})_{nil}^j\right), \qquad \widetilde{X}_{N+1,il}^j = \left(S_{Nil}^{x+}, (X_{mf})_{N+1,il}^j\right),$$

$$\widetilde{Y}_{nil}^j = \left(S_{nil}^{y-}, (Y_{mf})_{nil}^j\right), \qquad \widetilde{Y}_{n,I+1,l}^j = \left(S_{nIl}^{y+}, (Y_{mf})_{n,I+1,l}^j\right),$$

$$\widetilde{Z}_{nil}^j = \left(S_{nil}^{z-}, (Z_{mf})_{nil}^j\right), \qquad \widetilde{Z}_{ni,L+1}^j = \left(S_{niL}^{z+}, (Z_{mf})_{ni,L+1}^j\right),$$

$$n = \overline{0,N}; \qquad i = \overline{0,I}; \qquad l = \overline{0,L}.$$

Note that $\widetilde{X}_{nil}^j$ for all $n = \overline{1,N}$ is a function of two variables: E_{nil}^j and $E_{n-1,il}^j$; $\widetilde{X}_{0il}^j$ is a function of one variable E_{0il}^j, and $\widetilde{X}_{N+1,il}^j$ is also a function of one variable E_{Nil}^j. Similar statements are valid for $\widetilde{Y}_{nil}^j$ and $\widetilde{Z}_{nil}^j$.

With the aid of introduced designations the last three subproblems can be for $j = \overline{0,J-1}$ written in this compact form:

x − direction

$$E_{nil}^{j+\frac{1}{3}} = E_{nil}^j + \omega_{nil}^{j+1}\left(\widetilde{X}_{n+1,il}^{j+\frac{1}{3}} - \widetilde{X}_{nil}^{j+\frac{1}{3}} + \widetilde{Y}_{n,i+1,l}^j - \widetilde{Y}_{nil}^j + \widetilde{Z}_{ni,l+1}^j - \widetilde{Z}_{nil}^j\right), \quad (24)$$

y − direction

$$E_{nil}^{j+\frac{2}{3}} = E_{nil}^{j+\frac{1}{3}} + \omega_{nil}^{j+1}\left(\widetilde{Y}_{n,i+1,l}^{j+\frac{2}{3}} - \widetilde{Y}_{nil}^{j+\frac{2}{3}} + \widetilde{X}_{n+1,il}^{j+\frac{1}{3}} - \widetilde{X}_{nil}^{j+\frac{1}{3}} + \widetilde{Z}_{ni,l+1}^{j+\frac{1}{3}} - \widetilde{Z}_{nil}^{j+\frac{1}{3}}\right), \quad (25)$$

z − direction

$$E_{nil}^{j+1}=E_{nil}^{j+\frac{2}{3}}+\omega_{nil}^{j+1}\left(\widetilde{Z}_{ni,l+1}^{j+1}-\widetilde{Z}_{nil}^{j+1}+\widetilde{X}_{n+1,il}^{j+\frac{2}{3}}-\widetilde{X}_{nil}^{j+\frac{2}{3}}+\widetilde{Y}_{n,i+1,l}^{j+\frac{2}{3}}-\widetilde{Y}_{nil}^{j+\frac{2}{3}}\right), \qquad (26)$$

$$n=\overline{0,N} \qquad i=\overline{0,I} \qquad l=\overline{0,L}.$$

The cost functional $I(U)$ is approximated by the function $F(U)$ with the aid of the trapezoids method:

$$I(U)\cong F(U)=\frac{1}{2(t_2-t_1)}\left(\tau^{j_1+1}f^{j_1}+\sum_{j=j_1+1}^{j_2-1}(\tau^j+\tau^{j+1})f^j+\tau^{j_2}f^{j_2}\right).$$

Here j_1 is the ordinal number of the mesh point of the temporal grid which corresponds to the moment t_1, j_2 is the ordinal number of the mesh point of the temporal grid which corresponds to the moment t_2,

$$f^j=\sum_{n=n_1}^{n_2}\sum_{i=i_1}^{i_2}\left(Z_{ni}^j-z_*^j\right)^2 h_n^x h_i^y,$$

n_1, n_2 and i_1, i_2 are the ordinal numbers of the mesh points of the three-dimensional spacial grid along the Ox and Oy axes respectively which define the boundaries of the section S (i.e. $mesS=(x_{n_2}-x_{n_1})\times(y_{i_2}-y_{i_1})$), $Z_{ni}^j=Z_{pl}(x_n,y_i,t^j)$, $z_*^j=z_*(t^j)$.

Matrix elements Z_{ni}^j $\left(n=\overline{n_1,n_2},\quad i=\overline{i_1,i_2}\right)$ for each temporal layer j are defined by linear interpolation of the temperature field, obtained as a result of solving the direct problem. Let x_n, y_i, z_l be the coordinates of the mesh point of the spacial grid. For each mesh point $(x_n,y_i)\in S$, $(n=\overline{n_1,n_2},\ i=\overline{i_1,i_2})$ we find such index l_* for which one of the following conditions is valid: either $\beta\left(E_{ni,l_*+1}^j\right)\le T_{pl}\le\beta\left(E_{nil_*}^j\right)$, or $\beta\left(E_{ni,l_*}^j\right)\le T_{pl}\le\beta\left(E_{ni,l_*+1}^j\right)$.

Then

$$Z_{ni}^j=\frac{(z_{l_*+1}-z_{l_*})T_{pl}+(z_{l_*}\beta_{ni,l_*+1}^j-z_{l_*+1}\beta_{nil_*}^j)}{\beta_{ni,l_*+1}^j-\beta_{nil_*}^j}.$$

Each equation of the selected discrete version of the direct problem (24)–(26) is presented in the canonical form (27) in accordance with the FAD-methodology:

$$E_{nil}^j=\Psi\left((n,i,l,j),\Lambda_{(n,i,l,j)},U_{(n,i,l,j)}\right). \qquad (27)$$

Here $\Lambda_{(n,i,l,j)}$ is the set of all $E_{\alpha\beta\gamma}^{\nu}$ with such indices α, β, γ and ν that corresponding elements occur in the right side of the equality (27); $U_{(n,i,l,j)}$ is the set of all components of the control vector U^ν $\quad(U^\nu=U(t^\nu))$ that occur in the right side of the equality (27). In spite of the fact that the control depends only on temporal index j the set $U_{(n,i,l,j)}$ is marked also by the spacial indices n, i, and l in order to emphasize the fact that the influence of this control is different at different spacial points.

To calculate the components of the gradient of the function $F(U)$ along the components of the vector U^j we will use the following relation, which is the generalization of a similar relation in [**?**]:

$$\frac{dF}{dU^j}=\frac{\partial F}{\partial U^j}+\sum_{(\alpha,\beta,\gamma,\nu)\in\overline{K}_{(n,i,l,j)}}\Psi^T_{u^j}\left((\alpha,\beta,\gamma,\nu),\Lambda_{(\alpha,\beta,\gamma,\nu)},U_{(\alpha,\beta,\gamma,\nu)}\right)p^{\nu}_{\alpha\beta\gamma},\ j=\overline{1,J}, \quad (28)$$

where $p^{\nu}_{\alpha\beta\gamma}$ are the conjugate variables (impulses), determined from solving the following system of linear algebraic equations

$$p^j_{nil}=\frac{dF}{dE^j_{nil}}+\sum_{(\alpha,\beta,\gamma,\nu)\in\overline{Q}_{(n,i,l,j)}}\Psi^T_{E^j_{nil}}\left((\alpha,\beta,\gamma,\nu),\Lambda_{(\alpha,\beta,\gamma,\nu)},U_{(\alpha,\beta,\gamma,\nu)}\right)p^{\nu}_{\alpha\beta\gamma}, \quad (29)$$

$$n=\overline{0,N},\qquad i=\overline{0,I},\qquad l=\overline{0,L},\qquad j=\overline{1,J}.$$

Index sets $\overline{Q}_{(n,i,l,j)}$ and $\overline{K}_{(n,i,l,j)}$ are determined by the following relations:

$$\overline{Q}_{(n,i,l,j)}=\left\{(\alpha,\beta,\gamma,\nu):E^j_{nil}\in\Lambda_{(\alpha,\beta,\gamma,\nu)}\right\},\overline{K}_{(n,i,l,j)}=\left\{(\alpha,\beta,\gamma,\nu):u^j\in U_{(\alpha,\beta,\gamma,\nu)}\right\}.$$

The system of linear algebraic equations (29) for determining the impulses p^j_{nil} is usually called the conjugate problem.

Let us introduce the following designations for a number of derivatives that will be used to write our conjugate problem in a compact form:

$$\forall i=\overline{0,I}\quad\text{and}\quad\forall l=\overline{0,L}$$

$$(D_{x+})^j_{nil}=\frac{\partial\widetilde{X}^j_{nil}}{\partial E^j_{nil}},\quad(D_{x-})^j_{nil}=\frac{\partial\widetilde{X}^j_{nil}}{\partial E^j_{n-1,il}},\quad(n=\overline{1,N}),\quad(D_{x+})^j_{0il}=\frac{\partial\widetilde{X}^j_{0il}}{\partial E^j_{0il}},$$

$$(D_{x-})^j_{0il}=0,\quad(D_{x+})^j_{N+1,il}=0,\quad(D_{x-})^j_{N+1,il}=\frac{\partial\widetilde{X}^j_{N+1,il}}{\partial E^j_{Nil}};$$

$$\forall n=\overline{0,N}\quad\text{and}\quad\forall l=\overline{0,L}$$

$$(D_{y+})^j_{nil}=\frac{\partial\widetilde{Y}^j_{nil}}{\partial E^j_{nil}},\quad(D_{y-})^j_{nil}=\frac{\partial\widetilde{Y}^j_{nil}}{\partial E^j_{n,i-1,l}},\quad(i=\overline{1,I}),\quad(D_{y+})^j_{n0l}=\frac{\partial\widetilde{Y}^j_{n0l}}{\partial E^j_{n0l}},$$

$$(D_{y-})^j_{n0l}=0,\quad(D_{y+})^j_{n,I+1,l}=0,\quad(D_{y-})^j_{n,I+1,l}=\frac{\partial\widetilde{Y}^j_{n,I+1,l}}{\partial E^j_{nIl}};$$

$$\forall n=\overline{0,N}\quad\text{and}\quad\forall i=\overline{0,I}$$

$$(D_{z+})^j_{nil}=\frac{\partial\widetilde{Z}^j_{nil}}{\partial E^j_{nil}},\quad(D_{z-})^j_{nil}=\frac{\partial\widetilde{Z}^j_{nil}}{\partial E^j_{ni,l-1}},\quad(l=\overline{1,L}),\quad(D_{z+})^j_{ni0}=\frac{\partial\widetilde{Z}^j_{ni0}}{\partial E^j_{ni0}},$$

$$(D_{z-})^j_{ni0}=0,\quad(D_{z+})^j_{ni,L+1}=0,\qquad(D_{z-})^j_{ni,L+1}=\frac{\partial\widetilde{Z}^j_{ni,L+1}}{\partial E^j_{niL}}.$$

For the differentiation to be valid, the functions $\beta(E^j_{nil})$, $\Omega_1(E^j_{nil})$ and $\Omega_2(E^j_{nil})$ were smoothed out in the neighborhood of their salient points.

Usage of the FAD-methodology leads us to the following systems of equations for determining the impulses.

6.2 The conjugate problem

6.2.1 Initial conditions for the impulses

In order to obtain the adjoint variables on the last temporal layer $j = J$, it is necessary for all $n = \overline{0, N}$ and $i = \overline{0, I}$ to solve the following system of $(L+1)$ linear algebraic equations for the variables p^j_{nil} $(l = \overline{0, L})$:

$$p^J_{ni0} = \omega^J_{ni0}\left((D_{z-})^J_{ni1} - (D_{z+})^J_{ni0}\right)p^J_{ni0} - \omega^J_{ni1}(D_{z-})^J_{ni1}p^J_{ni1} + \frac{\partial F}{\partial E^J_{ni0}},$$

$$p^J_{nil} = \omega^J_{ni,l-1}(D_{z+})^J_{nil}p^J_{ni,l-1} + \omega^J_{nil}\left((D_{z-})^J_{ni,l+1} - (D_{z+})^J_{nil}\right)p^J_{nil} -$$
$$-\omega^J_{ni,l+1}(D_{z-})^J_{ni,l+1}p^J_{ni,l+1} + \frac{\partial F}{\partial E^J_{nil}}, \quad (l = \overline{1, L-1}),$$

$$p^J_{niL} = \omega^J_{ni,L-1}(D_{z+})^J_{niL}p^J_{ni,L-1} + \omega^J_{niL}\left((D_{z-})^J_{ni,L+1} - (D_{z+})^J_{niL}\right)p^J_{niL} + \frac{\partial F}{\partial E^J_{niL}}.$$

It is possible to give to this system a more compact form if for all $n = \overline{0, N}$ and $i = \overline{0, I}$ to assume that

$$\omega^J_{ni,-1} = \omega^J_{ni,L+1} = 0 \quad \text{and} \quad p^J_{ni,-1} = p^J_{ni,L+1} = 0.$$

As a result we will obtain:

$$p^J_{nil} = \omega^J_{ni,l-1}(D_{z+})^J_{nil}p^J_{ni,l-1} + \omega^J_{nil}\left((D_{z-})^J_{ni,l+1} - (D_{z+})^J_{nil}\right)p^J_{nil} -$$
$$-\omega^J_{ni,l+1}(D_{z-})^J_{ni,l+1}p^J_{ni,l+1} + \frac{\partial F}{\partial E^J_{nil}}, \quad l = \overline{0, L}. \tag{30}$$

6.2.2 First subproblem for the impulses (y-direction)

In order to calculate the impulses $p^{j+\frac{2}{3}}_{nil}$ on the temporal sublayer $(j + 2/3)$ $(j = \overline{J-1, 0})$ it is necessary to solve a linear algebraic system of $(I + 1)$ equations for all $n = \overline{0, N}$ and $l = \overline{0, L}$. This system can be written down more compactly if we make the following assumption:

$$\omega^{j+1}_{n,-1,l} = \omega^{j+1}_{n,I+1,l} = \omega^{j+1}_{-1,il} = \omega^{j+1}_{N+1,il} = 0,$$

$$p^{j+\frac{2}{3}}_{n,-1,l} = p^{j+\frac{2}{3}}_{n,I+1,l} = p^{j+1}_{n,-1,l} = p^{j+1}_{n,I+1,l} = p^{j+1}_{-1,il} = p^{j+1}_{N+1,il} = 0,$$
$$n = \overline{0, N}, \qquad i = \overline{0, I}, \qquad l = \overline{0, L}, \qquad j = \overline{J-1, 0}.$$

As a result we will have:

$$p_{nil}^{j+\frac{2}{3}} = \omega_{n,i-1,l}^{j+1}(D_{y+})_{nil}^{j+\frac{2}{3}} p_{n,i-1,l}^{j+\frac{2}{3}} + \omega_{nil}^{j+1}\left((D_{y-})_{n,i+1,l}^{j+\frac{2}{3}} - (D_{y+})_{nil}^{j+\frac{2}{3}}\right) p_{nil}^{j+\frac{2}{3}} -$$

$$-\omega_{n,i+1,l}^{j+1}(D_{y-})_{n,i+1,l}^{j+\frac{2}{3}} p_{n,i+1,l}^{j+\frac{2}{3}} + \xi_{nil}^{j+\frac{2}{3}}, \qquad (31)$$

where

$$\xi_{nil}^{j+\frac{2}{3}} = p_{nil}^{j+1} + \omega_{n-1,il}^{j+1}(D_{x+})_{nil}^{j+\frac{2}{3}} p_{n-1,il}^{j+1} + \omega_{nil}^{j+1}\left((D_{x-})_{n+1,il}^{j+\frac{2}{3}} - (D_{x+})_{nil}^{j+\frac{2}{3}}\right) p_{nil}^{j+1} -$$

$$-\omega_{n+1,il}^{j+1}(D_{x-})_{n+1,il}^{j+\frac{2}{3}} p_{n+1,il}^{j+1} + \omega_{n,i-1,l}^{j+1}(D_{y+})_{nil}^{j+\frac{2}{3}} p_{n,i-1,l}^{j+1} + \omega_{nil}^{j+1}\Big((D_{y-})_{n,i+1,l}^{j+\frac{2}{3}} -$$

$$-\left.(D_{y+})_{nil}^{j+\frac{2}{3}}\right) p_{nil}^{j+1} - \omega_{n,i+1,l}^{j+1}(D_{y-})_{n,i+1,l}^{j+\frac{2}{3}} p_{n,i+1,l}^{j+1} + \frac{\partial F}{\partial E_{nil}^{j+\frac{2}{3}}}, \quad i = \overline{0, I}.$$

The formulation of other two subproblems for calculating the impulses will be provided only in the final compact form. If we assume that

$$\omega_{n,-1,l}^{j} = \omega_{n,I+1,l}^{j} = \omega_{-1,il}^{j} = \omega_{N+1,il}^{j} = \omega_{ni,-1}^{j} = \omega_{ni,L+1}^{j} = 0,$$

$$p_{-1,il}^{j+\frac{1}{3}} = p_{N+1,il}^{j+\frac{1}{3}} = p_{-1,il}^{j+\frac{2}{3}} = p_{N+1,il}^{j+\frac{2}{3}} = p_{ni,-1}^{j+\frac{2}{3}} = p_{ni,L+1}^{j+\frac{2}{3}} = 0,$$

$$p_{ni,-1}^{j} = p_{ni,L+1}^{j} = p_{ni,-1}^{j+\frac{1}{3}} = p_{ni,L+1}^{j+\frac{1}{3}} = p_{n,-1,l}^{j+\frac{1}{3}} = p_{n,I+1,l}^{j+\frac{1}{3}} = 0,$$

$$n = \overline{0, N}, \qquad i = \overline{0, I}, \qquad l = \overline{0, L}, \qquad j = \overline{0, J},$$

it is similar to how this was done for the first subproblem.

6.2.3 Second subproblem for the impulses (x-direction)

In order to calculate the adjoint variables $p_{nil}^{j+\frac{1}{3}}$ on the temporal sublayer $j + 1/3 \quad (j = \overline{J-1, 0})$ it is necessary to solve the following linear algebraic system of $(N + 1)$ equations for all $i = \overline{0, I}$ and $l = \overline{0, L}$:

$$p_{nil}^{j+\frac{1}{3}} = \omega_{n-1,il}^{j+1}(D_{x+})_{nil}^{j+\frac{1}{3}} p_{n-1,il}^{j+\frac{1}{3}} + \omega_{nil}^{j+1}\left((D_{x-})_{n+1,il}^{j+\frac{1}{3}} - (D_{x+})_{nil}^{j+\frac{1}{3}}\right) p_{nil}^{j+\frac{1}{3}} -$$

$$-\omega_{n+1,il}^{j+1}(D_{x-})_{n+1,il}^{j+\frac{1}{3}} p_{n+1,il}^{j+\frac{1}{3}} + \xi_{nil}^{j+\frac{1}{3}}, \qquad (32)$$

where

$$\xi_{nil}^{j+\frac{1}{3}} = p_{nil}^{j+\frac{2}{3}} + \omega_{n-1,il}^{j+1}(D_{x+})_{nil}^{j+\frac{1}{3}} p_{n-1,il}^{j+\frac{2}{3}} + \omega_{nil}^{j+1}\left((D_{x-})_{n+1,il}^{j+\frac{1}{3}} - (D_{x+})_{nil}^{j+\frac{1}{3}}\right) p_{nil}^{j+\frac{2}{3}} -$$

$$-\omega_{n+1,il}^{j+1}(D_{x-})_{n+1,il}^{j+\frac{1}{3}} p_{n+1,il}^{j+\frac{2}{3}} + \omega_{ni,l-1}^{j+1}(D_{z+})_{nil}^{j+\frac{1}{3}} p_{ni,l-1}^{j+\frac{2}{3}} + \omega_{nil}^{j+1}\Big((D_{z-})_{ni,l+1}^{j+\frac{1}{3}} -$$

$$-\left.(D_{z+})_{nil}^{j+\frac{1}{3}}\right) p_{nil}^{j+\frac{2}{3}} - \omega_{ni,l+1}^{j+1}(D_{z-})_{ni,l+1}^{j+\frac{1}{3}} p_{ni,l+1}^{j+\frac{2}{3}} + \frac{\partial F}{\partial E_{nil}^{j+\frac{1}{3}}}, \quad n = \overline{0, N}.$$

6.2.4 Third subproblem for the impulses (z-direction)

In order to calculate the adjoint variables p^j_{nil} on temporal layer j ($j = \overline{J-1,1}$) it is necessary to solve the following linear algebraic system of $(L+1)$ equations for all $n = \overline{0,N}$ and $i = \overline{0,I}$:

$$p^j_{nil} = \omega^j_{ni,l-1}(D_{z+})^j_{nil}p^j_{ni,l-1} + \omega^j_{nil}\left((D_{z-})^j_{ni,l+1} - (D_{z+})^j_{nil}\right)p^j_{nil} - \\ -\omega^j_{ni,l+1}(D_{z-})^j_{ni,l+1}p^j_{ni,l+1} + \xi^j_{nil}, \quad (33)$$

where

$$\xi^j_{nil} = p^{j+\frac{1}{3}}_{nil} + \omega^{j+1}_{n,i-1,l}(D_{y+})^j_{nil}p^{j+\frac{1}{3}}_{n,i-1,l} + \omega^{j+1}_{nil}\left((D_{y-})^j_{n,i+1,l} - (D_{y+})^j_{nil}\right)p^{j+\frac{1}{3}}_{nil} - \\ -\omega^{j+1}_{n,i+1,l}(D_{y-})^j_{n,i+1,l}p^{j+\frac{1}{3}}_{n,i+1,l} + \omega^{j+1}_{ni,l-1}(D_{z+})^j_{nil}p^{j+\frac{1}{3}}_{ni,l-1} + \omega^{j+1}_{nil}\left((D_{z-})^j_{ni,l+1} - \right. \\ \left. - (D_{z+})^j_{nil}\right)p^{j+\frac{1}{3}}_{nil} - \omega^{j+1}_{ni,l+1}(D_{z-})^j_{ni,l+1}p^{j+\frac{1}{3}}_{ni,l+1} + \frac{\partial F}{\partial E^j_{nil}}, \quad l = \overline{0,L}.$$

Systems (30)–(33) approximate the initial-boundary value problem for the reverse thermal conductivity equation.

Each of systems (30)–(33) is solved with the aid of tridiagonal Gaussian elimination. Solving these three subproblems successively for all $j = \overline{J,0}$ allows us to obtain the values of the adjoint variables in the following order: p^J_{nil}, $p^{(J-1)+2/3}_{nil}$, $p^{(J-1)+1/3}_{nil}$, $p^{(J-1)}_{nil}$,...,$p^{1+1/3}_{nil}$, p^1_{nil}, $p^{0+2/3}_{nil}$, $p^{0+1/3}_{nil}$, ($n = \overline{0,N}, i = \overline{0,I}, l = \overline{0,L}$).

In the first two subproblems (i.e. in the systems of equations (31)–(32)) all derivatives $\frac{\partial F}{\partial E^{j+2/3}_{nil}}$ and $\frac{\partial F}{\partial E^{j+1/3}_{nil}}$ ($j = \overline{J-1,0}$, $n = \overline{0,N}$, $i = \overline{0,I}$, $l = \overline{0,L}$) are equal to zero. In the last subproblem (33) only derivatives $\frac{\partial F}{\partial E^j_{nil_*}}$ and $\frac{\partial F}{\partial E^j_{ni,l_*+1}}$ are not equal to zero. They are calculated using the following formulas:

$$\frac{\partial F}{\partial E^j_{nil_*}} = \frac{\mu^j}{t_2 - t_1}\left(Z^j_{ni} - z^j_*\right)\frac{\partial \beta(E^j_{nil_*})}{\partial E^j_{nil_*}} \cdot \frac{(z_{l_*+1} - z_{l_*})(T_{pl} - \beta(E^j_{ni,l_*+1}))}{\left(\beta(E^j_{ni,l_*+1}) - \beta(E^j_{nil_*})\right)^2}h^x_n h^y_i,$$

$$\frac{\partial F}{\partial E^j_{ni,l_*+1}} = \frac{\mu^j}{t_2 - t_1}\left(Z^j_{ni} - z^j_*\right)\frac{\partial \beta(E^j_{ni,l_*+1})}{\partial E^j_{ni,l_*+1}} \cdot \frac{(z_{l_*} - z_{l_*+1})(T_{pl} - \beta(E^j_{nil_*}))}{\left(\beta(E^j_{ni,l_*+1}) - \beta(E^j_{nil_*})\right)^2}h^x_n h^y_i,$$

where $\mu^{j_1} = \tau^{j_1+1}$, $\mu^j = \tau^j + \tau^{j+1}(j = \overline{j_1+1, j_2-1})$, $\mu^{j_2} = \tau^{j_2}$.

6.3 Gradient of the objective function of the discrete optimal control problem

Let us examine the first case, when the control function $U(t)$ is selected as the dependence on time of the displacement of the foundry mold in the melting furnace, namely, the z-coordinate of the lower bound of the wall of the furnace $Z_{Sou}(t)$. This parameter enters into the expressions that determine the functions $q_1(t)$ and $q_2(t)$ when the considered cell is located outside of the liquid aluminum. The control function $U(t)$ is approximated by a piecewise constant function that has constant values in each time interval $[t^j, t^{j+1}]$. Namely, we assume that on this time interval control equals to $U(t) = Z_{Sou}(t^{j+1}) = Z_{Sou}^{j+1}$. Consequently, $q_1^{j+1/3} = q_1^{j+2/3} = q_1^{j+1}$ and $q_2^{j+1/3} = q_2^{j+2/3} = q_2^{j+1}$.

According to the FAD-methodology, the components of the gradient of the objective function are calculated from the following formula:

$$
\begin{aligned}
\frac{dF}{dU^j} = \frac{\partial F}{\partial U^j} &+ \sum_{n=0}^{N}\sum_{i=0}^{I}\left(\omega_{niL}^j \frac{\partial \widetilde{Z}_{ni,L+1}^j}{\partial U^j} p_{niL}^j - \omega_{ni0}^j \frac{\partial \widetilde{Z}_{ni0}^j}{\partial U^j} p_{ni0}^j\right) + \\
&+ \sum_{n=0}^{N}\sum_{l=0}^{L}\left(\omega_{nIl}^j \frac{\partial \widetilde{Y}_{n,I+1,l}^{j-\frac{1}{3}}}{\partial U^j} p_{nIl}^j - \omega_{n0l}^j \frac{\partial \widetilde{Y}_{n0l}^{j-\frac{1}{3}}}{\partial U^j} p_{n0l}^j\right) + \\
&+ \sum_{i=0}^{I}\sum_{l=0}^{L}\left(\omega_{Nil}^j \frac{\partial \widetilde{X}_{N+1,il}^{j-\frac{1}{3}}}{\partial U^j} p_{Nil}^j - \omega_{0il}^j \frac{\partial \widetilde{X}_{0il}^{j-\frac{1}{3}}}{\partial U^j} p_{0il}^j\right) + \\
&+ \sum_{n=0}^{N}\sum_{l=0}^{L}\left(\omega_{nIl}^j \frac{\partial \widetilde{Y}_{n,I+1,l}^{j-\frac{1}{3}}}{\partial U^j} p_{nIl}^{j-\frac{1}{3}} - \omega_{n0l}^j \frac{\partial \widetilde{Y}_{n0l}^{j-\frac{1}{3}}}{\partial U^j} p_{n0l}^{j-\frac{1}{3}}\right) + \\
&+ \sum_{i=0}^{I}\sum_{l=0}^{L}\left(\omega_{Nil}^j \frac{\partial \widetilde{X}_{N+1,il}^{j-\frac{2}{3}}}{\partial U^j} p_{Nil}^{j-\frac{1}{3}} - \omega_{0il}^j \frac{\partial \widetilde{X}_{0il}^{j-\frac{2}{3}}}{\partial U^j} p_{0il}^{j-\frac{1}{3}}\right) + \qquad (34) \\
&+ \sum_{n=0}^{N}\sum_{i=0}^{I}\left(\omega_{niL}^j \frac{\partial \widetilde{Z}_{ni,L+1}^{j-\frac{2}{3}}}{\partial U^j} p_{niL}^{j-\frac{1}{3}} - \omega_{ni0}^j \frac{\partial \widetilde{Z}_{ni0}^{j-\frac{2}{3}}}{\partial U^j} p_{ni0}^{j-\frac{1}{3}}\right) + \\
&+ \sum_{i=0}^{I}\sum_{l=0}^{L}\left(\omega_{Nil}^j \frac{\partial \widetilde{X}_{N+1,il}^{j-\frac{2}{3}}}{\partial U^j} p_{Nil}^{j-\frac{2}{3}} - \omega_{0il}^j \frac{\partial \widetilde{X}_{0il}^{j-\frac{2}{3}}}{\partial U^j} p_{0il}^{j-\frac{2}{3}}\right) + \\
&+ \sum_{n=0}^{N}\sum_{l=0}^{L}\left(\omega_{nIl}^j \frac{\partial \widetilde{Y}_{n,I+1,l}^{j-1}}{\partial U^j} p_{nIl}^{j-\frac{2}{3}} - \omega_{n0l}^j \frac{\partial \widetilde{Y}_{n0l}^{j-1}}{\partial U^j} p_{n0l}^{j-\frac{2}{3}}\right) + \\
&+ \sum_{n=0}^{N}\sum_{i=0}^{I}\left(\omega_{niL}^j \frac{\partial \widetilde{Z}_{ni,L+1}^{j-1}}{\partial U^j} p_{niL}^{j-\frac{2}{3}} - \omega_{ni0}^j \frac{\partial \widetilde{Z}_{ni0}^{j-1}}{\partial U^j} p_{ni0}^{j-\frac{2}{3}}\right), \quad j = \overline{1, J}.
\end{aligned}
$$

Since the functional $F(U)$ does not depend explicitly on the control vector $\{U^j\}$, all components $\frac{\partial F}{\partial U^j} = 0$.

Let us give an example of calculation of one of the derivatives that occur in formula (34):

$$\frac{\partial \widetilde{X}^{j-\frac{2}{3}}_{N+1,il}}{\partial U^j} = S^{2x+}_{Nil}\frac{\partial\left((X_f)^{j-\frac{2}{3}}_{N+1,il}\right)}{\partial U^j} = S^{2x+}_{Nil}\frac{\partial\left(\left(q_2^j\right)\Big|_{S^{2x+}_{Nil}}\right)}{\partial U^j}.$$

It's taken into account here that cells with the indices (N,i,l), $(i=\overline{0,I},\ l=\overline{0,L})$ don't contain metal. Therefore $(X_m)^{j-\frac{2}{3}}_{N+1,il} = 0$. If at the moment $t=t^j$ cell with number (N,i,l) is located in the liquid aluminum, then $\frac{\partial\left(\left(q_2^j\right)|_{S^{2x+}_{Nil}}\right)}{\partial U^j} = \frac{\partial\left(\left(q_2^j\right)|_{S^{2x+}_{Nil}}\right)}{\partial Z^j_{Sou}} = 0$ and, therefore $\frac{\partial \widetilde{X}^{(j-1)+1/3}_{N+1,il}}{\partial U^j} = 0$. But if at the moment $t=t^j$ this cell is located outside of the liquid aluminum, then (according to (20) and (21))

$$\frac{\partial\left(\left(q_2^j\right)\Big|_{S^{2x+}_{Nil}}\right)}{\partial Z^j_{Sou}} = \frac{\partial\left(\varphi_s+\varphi_a\right)}{\partial Z^j_{Sou}} =$$

$$= \frac{\partial(q_s(X_s,Y_{Sou}-y_i+L_{Sou},Z_{Sou}-z_l+H_{Sou})-q_s(X_s,Y_{Sou}-y_i,Z_{Sou}-z_l+H_{Sou}))}{\partial Z^j_{Sou}}+$$

$$+\frac{\partial\left(q_s\left(X_s,Y_{Sou}-y_i,Z_{Sou}-z_l\right)-q_s\left(X_s,Y_{Sou}-y_i+L_{Sou},Z_{Sou}-z_l\right)\right)}{\partial Z^j_{Sou}}+$$

$$+\frac{\partial(q_a(Z_a,Y_{al}-y_i+L_{al},X_{al}-X_b+H_{al})-q_a(Z_a,Y_{al}-y_i,X_{al}-X_b+H_{al}))}{\partial Z^j_{Sou}}.$$

The third argument of the function q_s and the first argument of the function q_a depend on the value Z^j_{Sou}. According to formulas (22) and (23) (see part I) we have:

$$\widetilde{q}_s(\xi,l,h) \equiv \frac{\partial q_s(\xi,l,h)}{\partial h} = M_S\left[\frac{\xi^2}{\eta^3}\arctan\left(\frac{l}{h}\right)+\frac{l\xi^2}{\eta^2(\eta^2+l^2)}\right],$$

$$\widetilde{q}_a(\xi,l,h) \equiv \frac{\partial q_a(\xi,l,h)}{\partial \xi} = -M_a\cdot\frac{l}{\xi^2+l^2}-\frac{M_a}{\eta^2}\left[\left(\eta-\frac{\xi^2}{\eta}\right)\arctan\left(\frac{l}{\eta}\right)-\frac{l\xi^2}{\eta^2+l^2}\right],$$

where $\eta=\sqrt{\xi^2+h^2}$. Thus,

$$\frac{\partial\left(\left(q_2^j\right)\Big|_{S^{2x+}_{Nil}}\right)}{\partial Z^j_{Sou}} = \widetilde{q}_s\left(X_s,Y_{Sou}-y_i+L_{Sou},Z_{Sou}-z_l+H_{Sou}\right)-$$

$$-\widetilde{q}_s\left(X_s,Y_{Sou}-y_i,Z_{Sou}-z_l+H_{Sou}\right)+$$

$$+\widetilde{q}_s\left(X_s,Y_{Sou}-y_i,Z_{Sou}-z_l\right)-\widetilde{q}_s\left(X_s,Y_{Sou}-y_i+L_{Sou},Z_{Sou}-z_l\right)+$$

$$+\left[\widetilde{q}_a(Z_a, Y_{al}-y_i+L_{al}, X_{al}-X_b+H_{al})-\widetilde{q}_a(Z_a, Y_{al}-y_i, X_{al}-X_b+H_{al})\right]\cdot\frac{\partial Z_a}{\partial Z^j_{Sou}},$$

$$\frac{\partial Z_a}{\partial Z^j_{Sou}}=\begin{cases}-1, & \text{object did not reach the surface of aluminum,}\\ -1-\dfrac{X_b\cdot Y_b}{L_{al}\cdot H_{al}-X_b\cdot Y_b}, & \text{object reached the surface of aluminum.}\end{cases}$$

There is a special practical interest in the dependence of the solidification front on the speed $\widetilde{u}(t)$ of the displacement of the object. In this case the speed of the displacement of the foundry mold in the melting furnace is selected as the control function. Z-coordinate of the lower bound of the wall of the furnace $Z_{Sou}(t)$ is determined with the aid of the speed $\widetilde{u}(t)$ as follows:

$$Z_{Sou}(t^j)=Z_{Sou}(t^{j-1})-\tau^j\widetilde{u}(t^j),\quad \text{or}\quad Z_{Sou}(t^j)=\widetilde{z}-\sum_{k=1}^{j}\tau^k\widetilde{u}(t^k),$$

where $\widetilde{z}$ is the z-coordinate of the lower bound of the wall of the furnace at the initial time. In this case the component of the gradient of the function $F(\widetilde{u})$ along the components of vector $\{\widetilde{u}^j\}$, $\big(\widetilde{u}^j=\widetilde{u}(t^j)\big)$, are calculated using the following formula:

$$\frac{dF}{d\widetilde{u}^j}=\frac{\partial F}{\partial\widetilde{u}^j}-\tau^j\sum_{k=j}^{J}\left(\frac{dF}{dU^k}-\frac{\partial F}{\partial U^k}\right), j=\overline{1,J}, \tag{35}$$

where $\frac{dF}{dU^k}(k=\overline{1,J})$ are calculated using the formula (34). Due to the specific character of the functional in the considered problem, $\frac{\partial F}{\partial\widetilde{u}^j}=\frac{\partial F}{\partial U^j}=0$, $(j=\overline{1,J})$.

Let us give the formula for calculating the gradient of the functional in the case, when the speed function $\widetilde{u}(t)$ in the temporal section $[0,t^J]$ was approximated by piecewise constant function with an arbitrary number of segments.

The time interval $[0,t^J]$ is divided in Θ "large" subintervals. The function $\widetilde{u}(t)$ has a constant value on each subinterval. Each of these subintervals contains β elementary intervals $[t^{j-1},t^j]$. Thus, $\widetilde{u}^{(s-1)\beta+\alpha}=\widetilde{v}^s$, $(\alpha=\overline{1,\beta})$, where $\widetilde{v}^s$ $(s=\overline{1,\Theta})$ is given. Then the component of the gradient of the objective function $F(U)$ along the components of vector $\{\widetilde{v}^s\}$, $(s=\overline{1,\Theta})$, are calculated using the following formula:

$$\frac{dF}{d\widetilde{v}^s}=\sum_{\alpha=1}^{\beta}\frac{dF}{d\widetilde{u}^{(s-1)\beta+\alpha}},\quad s=\overline{1,\Theta}, \tag{36}$$

where derivatives $\frac{dF}{d\widetilde{u}^j}$ are determined with the aid of relation (35).

Let us point out also that the systems of equations (30)–(33) don't depend on the choice of the control function.

Let us especially note that the value of the gradient of the objective function, calculated according to formulas (34)–(36), is precise for the selected approximation of the optimal control problem.

The calculation of the approximate value of the gradient of the objective function with the aid of the finite-difference method in this optimal control problem is connected with enormous difficulties [3].

The machine time needed for calculation of the gradient components using the approach presented here (based on the FAD-methodology) is not more than half of machine time needed for solving the direct problem.

Therefore, in spite of the difficulties connected with obtaining the discrete version of the conjugate problem and the gradient, it seems unavoidable finding the precise value of the gradient of the objective function using the FAD-methodology while solving complex problems of optimal control.

7 Numerical results of solving the optimal control problem

The speed $\widetilde{u}(t)$ of the displacement of foundry mold in the melting furnace was chosen as the control $U(t)$. The formulated optimal control problem was solved numerically using the gradient method. During the solution of the optimal control problem the time interval $[0, t^J]$ was divided into N parts (subintervals). The control function $U(t)$ was approximated by piecewise constant function, so that for each of subintervals it was constant. The components of the gradient of the objective function are calculated using the formula (36).

The optimal control problem was studied for a rectangular parallelepiped. The previous parameters of the problem, indicated in the fifth section (part I), were used, with the exception of some given below:

$$T_{Sou} = 1900.15, \qquad T_{al} = 1033.15, \qquad L_{Sou} = 0.350, \qquad H_{Sou} = 0.380,$$

$$X_b = 0.040, \quad Y_b = 0.060, \quad Z_b = 0.180.$$

The parallelepiped was immersed into the liquid aluminum to 5/6 of its height. The number t^J, which determines the length of the time interval $[0, t^J]$, was equal to 3299 s. Z-coordinate $z_*(t)$ of the desired solidification front changed with a constant velocity $U_*(t) = 0.1mm/s$. Calculations were performed for different numbers N of subintervals, on which the control function $U(t)$ was constant.

In Fig. 16a the dependence of the optimal cost functional $J(U)$ upon the number N of subintervals is represented. It is obtained as the result of the solution of optimization problem. Here N has the following values: 1, 2, 4, 12, 24, 600. As shown in Fig. 16a, the optimal value of the functional decreases noticeably for the small values of N, and for the great values of $N (N > 30)$ it weakly diminishes and comes out to a certain constant asymptotical value. Fig. 16b is a fragment of Fig. 16a in which there is no point corresponding to the value $N = 600$. This makes it possible to examine more precisely the dependence of the optimal value of the cost functional upon the number of subintervals for low values of N.

In Figures 17 the optimal trajectories of the foundry mold are shown. These are those trajectories with which optimum values of functional examined above are obtained (see Fig. 16), namely, for $N = 1, 2, 4, 12, 24, 600$. Numbers near the curves indicate the number N of subintervals used. The convergence of the optimal trajectories to a certain limit function when the number N increase is visible in Figures 17. Let us note that the qualitatively correct structure of optimal trajectory is already obtained for $N = 12$. Further increase of the number N only smoothes the optimal trajectory.

Figure 18 shows the behavior of the standard deviation of the real solidification front from the desired one for several control functions. Standard deviation is determined by the formula

$$D(t) = \sqrt{\frac{1}{|S|} \iint\limits_{S} \left[Z_{pl}(x, y, t) - z_*(t)\right]^2 dxdy}, \tag{37}$$

where $|S|$ is the area of the cross section S. Curve 1 in Fig. 18 corresponds to the regime when the foundry mold is moved with a small constant velocity $\widetilde{u}(t) = 0.083mm/s$ relative to the furnace. Curve 2, just as curve 1, corresponds to the regime with a constant velocity of the displacement of the foundry mold, but $\widetilde{u}(t) = 0.150mm/s$. Curve 3 corresponds to such displacement of foundry mold when the functional (3) reaches the minimum value. All these calculations were performed for $N = 24$.

The advantages of the optimal process of metal crystallization are vividly shown by the figures given below. Figures 19-21 illustrate isotherms for different times in two cross sections through the object's vertical axis of symmetry parallel to the parallelepiped faces. Since the object is symmetric about the vertical axis, the figures present only halves of the cross sections. Figures 19a, 20a, 21a (first experiment) illustrate the process of metal solidification in a mold moving relative to the furnace with the constant speed $\widetilde{u}(t) = 0.417mm/min$. Figures 19b, 20b, 21b (second experiment) correspond to a mold moving with the optimal speed, corresponding $N = 4$.

Figures 19–21 show that the isotherms are concentrated within the mold. Moreover, the results of the second experiment are superior to those of the first one. First, the phase boundary in the second experiment is closer to a horizontal plane. Second, bubbles of liquid metal form and collapse inside the casting in the first experiment (Fig. 21a), which results in a casting of poor quality, whereas no bubbles are observed in the second experiment. Third, the process of solidification in the first experiment proceeds too quickly (for about 962 s.), which also degrades the casting. In the second experiment, the solidification process lasts roughly twice as long as in the first (1930 s.).

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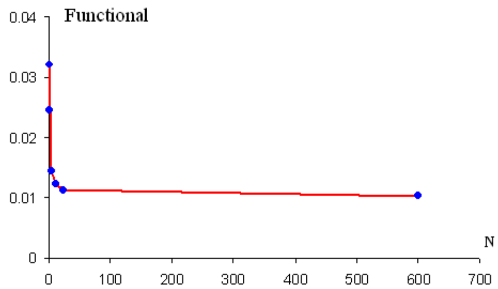

Fig. 16a

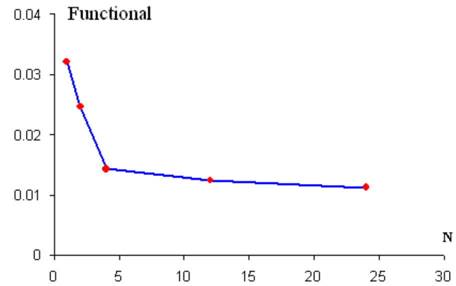

Fig. 16b

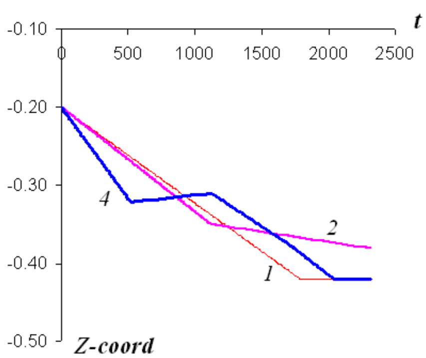

Fig. 17a

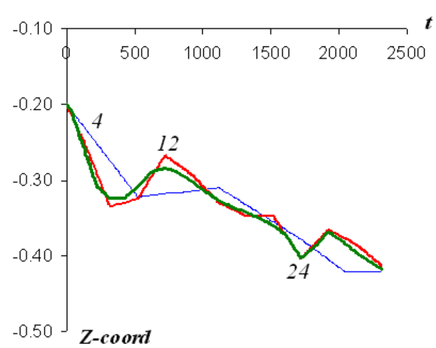

Fig. 17b

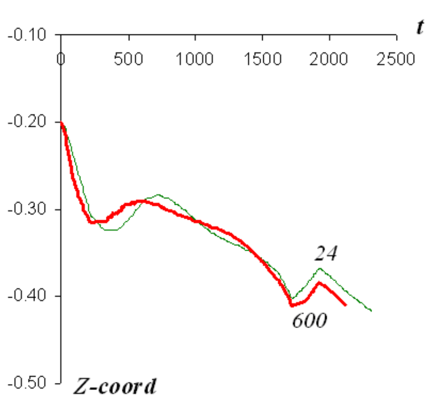

Fig. 17c

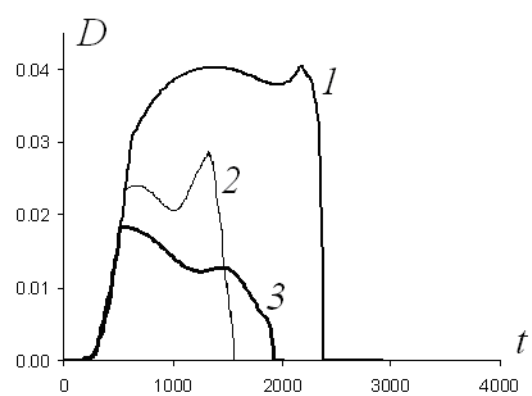

Fig. 18

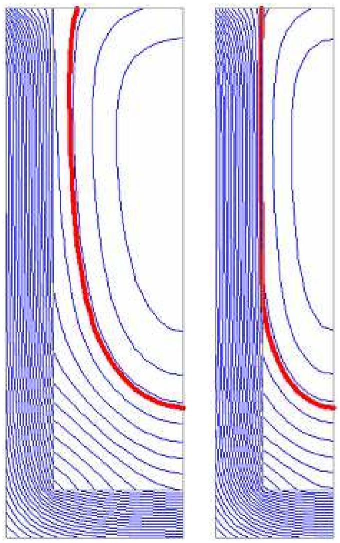

Fig. 19a

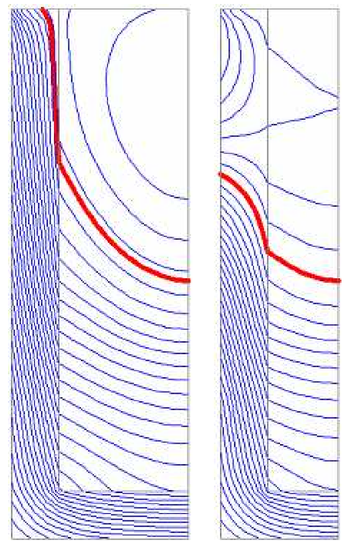

Fig. 19b

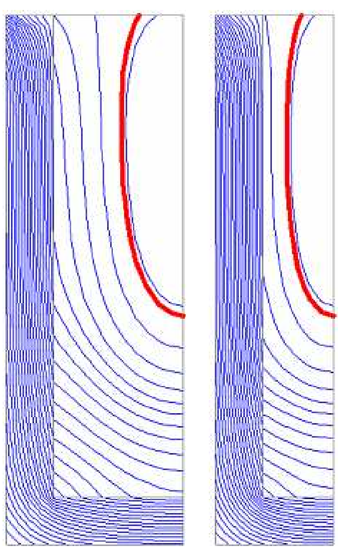

Fig. 20a

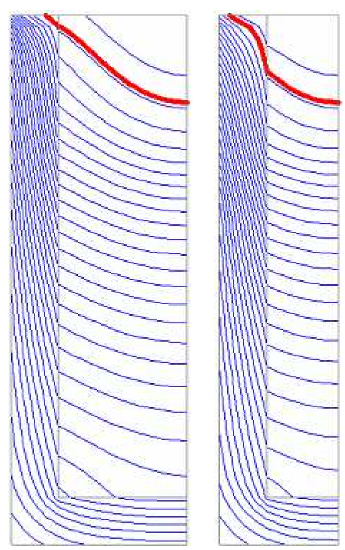

Fig. 20b

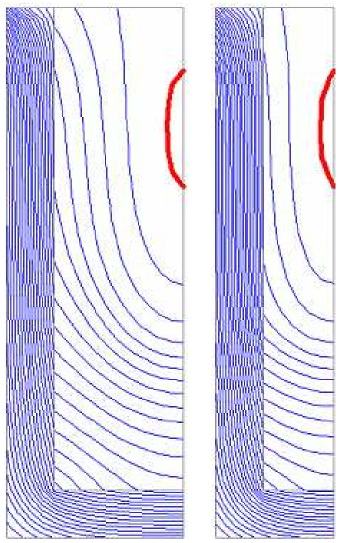

Fig. 21a

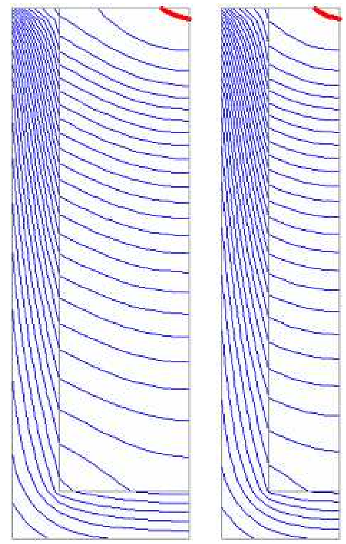

Fig. 21b

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