

## A method for treating two-dimensional thermophysical problems in regions with complex geometry

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In paper [1] a method was developed to treat the filling of a cavity with a viscous incompressible fluid. The substantial part of it was the construction of a metric mapping from the Euclidean space of the real process into a Riemannian space so as to geometrize the continuity equation. Along with this a boundary fitted coordinate system is obtained, which carries some information about the peculiarities of the flow.

In the present work the method of construction of coordinate systems, developed in [1], is applied to regions with complicated geometry. In it the thermophysical problem (this implies cooling and crystallisation) for a cast is treated and numerically solved. The joint treatment of hydrodynamic and thermophysical problems in one coordinate system is convenient for practical applications.

In order to do the presentation self-sufficient, in section 1 we describe the method of constructing the coordinate system and metric from [1]. The components of the metric tensor in the whole region are obtained as functions, defined on one of the boundary surfaces which further is called basic (the surface  $S^1$  on Fig. 1). In section 2 these components are obtained in an explicit form in two-dimensional region with a static geometry. In sections 3 and 4 the finite difference scheme and the form of the boundary conditions of II and III kind are obtained for equation of heat transfer. The presence of coordinate effects requires increased accuracy in the realization of the numerical scheme. That is why the coefficients of equation (II) are computed on an auxiliary grid with smaller step and afterward are averaged between the points of the principal grid. In section 5 the process of crystallization in an interval is described by the method of the equivalent heat capacity. In order to evaluate  $C_E(T)$  from (24) at the ends of the interval of crystallization (where it's influence on the process is stronger), a phenomenological model, developed in [5], is used. In the last section the results from the numerical computations are presented.

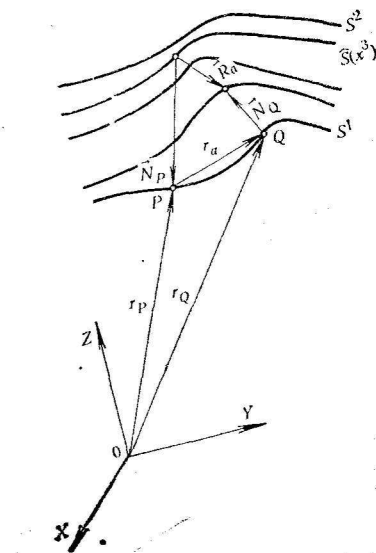


Fig. 1

## 1. Construction of the Riemannian space. Equation of heat transfer

Further the Greek indices  $\alpha, \beta; \dots$  take values  $\alpha, \beta, \dots = 1, 2$ ; the Latin indices  $i, j, k, \dots = 1, 2, 3$ .

Let us consider a medium, bounded by two surfaces  $S^1$  and  $S^2$  at a distance  $h(x^1, x^2)$ , measured on the normal of  $S^1$ , where  $x^1$  and  $x^2$  are the curvilinear coordinates on  $S^1$ . The metric space is constructed as a direct product of a one parameter family of surfaces  $\widehat{S}$  with metric, congruent with the geometry of  $S^1$  and  $S^2$ , and the field of the normal to  $S^1$  vectors. Let  $r_\alpha$  are vectors in  $S^1$ , tangent to the coordinate curves  $x^\alpha$ :  $r_\alpha = \frac{\partial R}{\partial x^\alpha}$ , where  $R$  is the vector from an external coordinate system  $K_0$  to the point  $Q$  on  $S^1$ . The metric on  $S^1$  will be  $g_{\alpha\beta} = (r_\alpha, r_\beta)$ , where the scalar product is defined by the external Euclidean metric in  $K_0$ . Then  $N|_Q = \frac{r_\alpha \times r_\beta}{g^2}|_Q$  is the unit vector

at the point  $Q$  on  $S^1$ . The components of the second quadratic form on the basic surface  $S^1$  are  $b_{\alpha\beta} = -(N, r_\alpha, r_\beta)$ , [4]. We parametrize the intermediate surfaces  $\widehat{S}$  by  $x, 0 \leq x \leq 1$ . Then for two points  $A$  and  $B$  on  $\widehat{S}$ , located over  $P$  and  $Q$  on  $S^1$ , is deduced:

$$R_A = R_P + xhN_P; \quad R_B = R_Q + xhN_Q.$$

Let  $P$  and  $Q$  are located on the coordinate curve  $x^\alpha$ . It follows that on  $\widehat{S}$ :

$$(1) \quad \widehat{r}_\alpha = r_\alpha + \lim_{P \rightarrow Q} \frac{x(h_Q N_Q - h_P N_P)}{\|P - Q\|} = r_\alpha - xhb_\alpha^c r_c + xN(\nabla h, r_\alpha).$$

The metric  $G_{\alpha\beta}$  on  $\widehat{S}$  is derived from (1):

$$(2) \quad G_{\alpha\beta} = (\widehat{r}_\alpha, \widehat{r}_\beta) = g_{\alpha\beta} - 2xhb_{\alpha\beta} + x^2 h^3 b_{\alpha\gamma} b_\beta^\gamma + x^2 (\nabla h, r_\alpha) (\nabla h, r_\beta).$$

We choose  $x$  as the third coordinate. The metric of the Riemannian space

$$(3) \quad \text{becomes: } G_{\alpha\beta} = (\widehat{r}_\alpha, \widehat{r}_\beta); \quad G_{\alpha\beta} = -xh(\nabla h, r_\alpha)/G_{\alpha\alpha}^{\frac{1}{2}}; \quad G_{33} = h^2.$$

The equation of heat transfer, written in the metric (2, 3) is:

$$(4) \quad c\rho \frac{\partial T}{\partial t} = \lambda(G^{22}T_{,\eta\eta} + G^{33}T_{,xx} + 2G^{23}T_{,x\eta}) + G^{22}T_{,\eta}\lambda_{,\eta} + G^{33}T_{,x}\lambda_{,x} + G^{23}(T_{,x}\lambda_{,\eta} + T_{,\eta}\lambda_{,x}) + \lambda \left[ (G^{\frac{1}{2}} G^{22})_{,\eta} T_{,\eta} + (G^{\frac{1}{2}} G^{33})_{,x} T_{,x} + (G^{\frac{1}{2}} G^{23})_{,\eta} T_{,x} + (G^{\frac{1}{2}} G^{23})_{,x} T_{,\eta} \right] / G^{\frac{1}{2}}.$$

## 2. Derivation of the metric

Let  $r = (x^2 + y^2)^{\frac{1}{2}} = \Theta(z)$  is the coordinate curve on  $S^1$ , with values in  $K_0$ . We compute the differentials of coordinate curves:

$$(5) \quad dr = B(z)dz; \quad d\eta^2 = dz^2(1 + B^2).$$

If  $dr^1$  and  $dr^2$  are two orthogonal vectors on  $S^1$ , their components in  $K_0$  are:

$$(6) \quad dr^1 = r(-\sin \varphi, \cos \varphi, 0)d\varphi$$

$$dr^2 = \frac{1}{(1+B^2)^{\frac{1}{2}}} (B \cos \varphi, B \sin \varphi, 1)d\eta.$$

The scalar products of  $dr^1$  and  $dr^2$  define the components of  $g_{\alpha\beta}$ :

$$g_{11}=r^2, \quad g_{22}=1, \quad g^{\frac{1}{2}}=r.$$

Also in  $K_0$  we obtain the components of the normal vector  $N$  and of its derivatives along the new coordinate lines:

$$(7) \quad \begin{aligned} N &= \frac{dr^1 \times dr^2}{\frac{1}{g^2}} = \frac{1}{(1+B^2)^{\frac{1}{2}}} (\cos \varphi, \sin \varphi, -B) \\ \partial_\varphi N &= \frac{1}{(1+B^2)^{\frac{1}{2}}} (-\sin \varphi, \cos \varphi, 0) \\ \partial_\eta N &= -\frac{\dot{B}}{(1+B^2)^{\frac{1}{2}}} (B \cos \varphi, B \sin \varphi, 1), \end{aligned}$$

where  $\dot{B} = \partial_\eta B$ ;  $\partial_\eta = \frac{1}{(1+B^2)^{\frac{1}{2}}} \partial z$ . The second quadratic form is derived from (7) with the formulae  $b_{\alpha\beta} = -(N, r^\beta)$ :

$$(8) \quad b_{11} = -\frac{r}{(1+B^2)^{\frac{1}{2}}}, \quad b_{12} = -\frac{1}{r(1+B^2)^{\frac{1}{2}}}; \quad b_{22} = \frac{\dot{B}}{1+B^2}, \quad b_2^2 = b_{22}.$$

From (5)÷(8) the components of the metric tensor (3) in the region are computed as functions, defined on  $S^1$ :

$$(9) \quad \begin{aligned} G_{11} &= \left( r + x \frac{h}{(1+B^2)^{\frac{1}{2}}} \right)^2; \quad G_{22} = \left( 1 - x \frac{\dot{B}h}{1+B^2} \right)^2 + (x\dot{h})^2. \\ G_{33} &= h^2; \quad G_{23} = xh\dot{h} \end{aligned}$$

### 3. Finite difference schemes for the equation of heat transfer

The equation (4) is written down in a coordinate system  $(x, \eta)$ , applying a three point discretization with a varying step, [3, 6, 8]. The points along  $\eta$  are marked by the indices  $J=1, \dots, NY$ , and along  $X$  — by indices  $K=1, \dots, NX$ .

$$(10) \quad \begin{aligned} \dot{B}(J) &= 2 \left( \frac{R(J+1)-R(J)}{Z(J+1)-Z(J)} - \frac{R(J)-R(J-1)}{Z(J)-Z(J-1)} \right) \frac{1}{(Z(J+1)-Z(J-1))(1+B^2)^{\frac{1}{2}}} \\ \dot{h}(J) &= (h(J+1)-h(J-1))/(\Delta\eta(J+1)-\Delta\eta(J)) \\ \Delta\eta(J) &= ((Z(J)-Z(J+1))^2 + (R(J)-R(J+1))^2)^{\frac{1}{2}}. \end{aligned}$$

From (10) the components of the metric (9) are determined. For the internal points of the region and at  $\lambda = \text{const}$ , we obtain from (4):

$$(11) \quad c_p \frac{\partial T}{\partial t}(J, K) = \frac{1}{G^2 \left( J + \frac{1}{2}, K + \frac{1}{2} \right)} \left\{ \left[ A(J+1, K)(T(J+1, K) - T(J, K)) - A(J, K)(T(J, K) - T(J-1, K)) \right] \frac{1}{\Delta\eta(J)} + [B(J, K+1)(T(J, K+1) - T(J, K)) - B(J, K)(T(J, K) - T(J-1, K))] \frac{1}{\Delta\eta(J)} \right\}$$

$$\begin{aligned}
& -T(J, K-1)) \Big] \frac{1}{\Delta x} + [C(J-1, K)(T(J-1, K-1) - T(J-1, K+1)) - C(J+1, K)(T(J+1, K-1) \\
& - T(J+1, K+1)) + C(J, K-1)(T(J-1, K-1) - T(J+1, K-1)) \\
& - C(J, K+1)(T(J, K+1) - T(J+1, K+1))] \frac{1}{\Delta \eta(J) + \eta(J-1)} \Big\}.
\end{aligned}$$

The components of the metric (9) are computed in an auxiliary and more dense coordinate grid, and then are used to obtain the coefficients  $A$ ,  $B$  and  $C$ :

$$A(J+1, K) = 2\lambda \left( G_{11} \left( J + \frac{1}{2}, K \right) G_{33} \left( J + \frac{1}{2}, K \right) \right)^{\frac{1}{2}} / (\Delta \eta(J) G_{22}^{\frac{1}{2}}(J, K) + \Delta \eta(J+1) G_{22}^{\frac{1}{2}}(J+1, K))$$

$$B(J, K+1) = 2\lambda \left( G_{11} \left( J, K + \frac{1}{2} \right) G_{22} \left( J, K + \frac{1}{2} \right) \right)^{\frac{1}{2}} / \Delta x \left( G_{33}^{\frac{1}{2}}(J, K+1) + G_{33}^{\frac{1}{2}}(J, K) \right)$$

$$C(J, K) = \lambda G^{23}(J, K) G^{\frac{1}{2}}(J, K) / 2\Delta x.$$

For the boundary points in the direction of  $x$  we deduce:

$$\begin{aligned}
(12) \quad C\rho \frac{\partial T}{\partial t}(J, K) &= \frac{1}{G^{\frac{1}{2}} \left( J + \frac{1}{2}, K + \frac{1}{2} \right)} \left\{ [A(J+1, K)(T(J+1, K) - T(J, K)) - A(J, K)(T(J, K) \right. \\
& - T(J-1, K))] / \Delta \eta(J) + [B(J, K+1)(T(J, K+1) - T(J, K)) - D(J, K)(T(J, K) - T^S(J))] \frac{1}{\Delta x} \\
& + [C(J-1, K)(T(J-1, K-1) - T(J-1, K)) - C(J+1, K)(T(J+1, K-1) - T(J+1, K)) \\
& + C(J, K-1)(T(J-1, K-1) - T(J+1, K-1)) - C(J, K)(T(J-1, K) \\
& \left. - T(J+1, K))] \frac{1}{\Delta \eta(J-1) - \Delta \eta(J)} \right\},
\end{aligned}$$

where  $D(J, K) = G_{11} \left( \left( J, K + \frac{1}{2} \right) G_{22} \left( J, K + \frac{1}{2} \right) \right)^{\frac{1}{2}}$ . The other boundaries are treated similarly. Let  $T^S(J)$  be the temperature of the surface, which is determined by the boundary conditions, which are in the general case:

$$(13) \quad \lambda \frac{\partial T}{\partial N} \Big|_{S^1} + \alpha_1 T \Big|_{S^1} = \alpha_0 T^L.$$

After a three-point approximation of  $\frac{\partial T}{\partial n} \Big|_{S^1}$  by Lagrange polynomial:

$$(14) \quad T^S(J) = \left( \alpha_0 T^L - \frac{\lambda}{h(J)} \frac{4T(J, 1) - T(J, 2)}{2\Delta x} \right) / \left( \alpha_1 T(J, 1) - \frac{3}{2} \frac{\lambda}{h(J)\Delta x} \right),$$

where  $T^L$  is the external temperature. On the surface  $S^2$  the expression for  $T^S(J)$  is more complex. It will be derived in the next section.

#### 4. Coordinate effects

It could be seen from (9) that the coordinate system is not orthogonal. This creates fictitious heat fluxes, which are compensated by adding to every element complementary sources, described in (11) and (12) by the terms, containing  $C(J, K)$ .

Another problem, resulting from the coordinate effects, is the derivation of the boundary conditions of II and III kind. The normal derivative  $(\nabla T, n)|_{S^2}$  does not coincide in direction and value with the derivative  $\frac{\partial T}{\partial N}$ . Let:

$$(15) \quad (\nabla T, N)|_{S^2} = \frac{1}{G_{33}^2} \frac{\partial T}{\partial x}|_{S^2}; \quad (\nabla T, \eta)|_{S^2} = \frac{1}{G_{22}^2} \frac{\partial T}{\partial \eta}|_{S^2}.$$

The derivative  $(\nabla T, n)|_{S^2}$  could be represented as a linear combination of the two derivatives (15):

$$(16) \quad \frac{\partial T}{\partial n}|_{S^2} = \frac{A_1(x, \eta)}{G_{33}^2(x, \eta)} \frac{\partial T}{\partial x}|_{S^2} + \frac{A_2(x, \eta)}{G_{22}^2(x, \eta)} \frac{\partial T}{\partial \eta}|_{S^2}.$$

In order to determine the coefficients  $A_1(x, \eta)$  and  $A_2(x, \eta)$ , we introduce the distance  $R(x, \eta)$ , measured in  $K_0$ , to a point on  $S^2$  with coordinates  $(\varphi, \eta, x)$ ,  $R(\varphi, \eta) = r(\varphi, \eta) + xh(\eta)N(\eta)$ . Then two basis vectors on  $S^2$  will be:

$$(17) \quad R_{,\varphi} = r_{,\varphi} + xhN_{,\varphi}; \quad R_{,\eta} = r_{,\eta} + xhN_{,\eta} + xh_{,\eta}N.$$

From (5)÷(7) we obtain:

$$(18) \quad \begin{aligned} N_{,\varphi} &= (N + Br_{,\eta})/(1 + B^2) \\ N_{,\eta} &= -NB\dot{B}/(1 + B^2)^{3/2} + B\dot{B}(BN - r_{,\eta})/(1 + B^2). \end{aligned}$$

It follows from (6) and (7) that  $r_{,\varphi} \times r_{,\eta} = |r|N$ ;  $r_{,\varphi} \times N = |r|r_{,\eta}$ ;  $r_{,\eta} \times N = |r|r_{,\varphi}$ . For the normal vector  $n$  to the surface  $S^2$  we deduce that:

$$(19) \quad \begin{aligned} R_{,\varphi} \times R_{,\eta} &= (1 - xh\dot{B}/(1 + B^2))|r|N - x(h + hB\dot{B}/(1 + B^2) + \dot{h})|r|r_{,\eta} \\ n &= \frac{R_{,\varphi} \times R_{,\eta}}{|R_{,\varphi} \times R_{,\eta}|} = [h(1 - xh\dot{B}/(1 + B^2))N - x\dot{h}r_{,\eta}]/G_{22}^2. \end{aligned}$$

Now the flux of the vector  $\nabla T$  across  $S^2$  can be computed:

$$(20) \quad \frac{\partial T}{\partial n}|_{S^2} = [G^{33}h(1 - xh\dot{B}/(1 + B^2))T_{,x} - G^{22}x\dot{h}T_{,\eta}]/(G_{22}^2)^{\frac{1}{2}}.$$

It follows from (9):

$$(21) \quad \begin{aligned} G_{22} &= (1 - xh\dot{B}/(1 + B^2)) + G_{23}^2/G_{33} \\ \beta_x &= (1 - xh\dot{B}/(1 + B^2))/G_{22}^{\frac{1}{2}} \\ x\dot{h}/G_{22}^{\frac{1}{2}} &= (1 - \beta_x^2)^{\frac{1}{2}}. \end{aligned}$$

The derivative  $\frac{\partial T}{\partial n}|_{S^2}$  could be determined from (20), (21):

$$(22) \quad \frac{\partial T}{\partial n}|_{S^2} = G^{33}h\beta_x T_{,x} - G^{22}(1 - \beta_x^2)^{\frac{1}{2}} T_{,\eta}.$$

When the relations  $G^{23} = \frac{1}{G_{33}\beta_x^2}$  and  $G^{22} = \frac{1}{G_{22}\beta_x^2}$  are applied to (22) we come to the expres-

sion for the boundary condition of the III kind on  $S^2$ :

$$(23) \quad \lambda(G^{33})^{\frac{1}{2}} \frac{\partial T}{\partial x} \Big|_{S^2} + \alpha_1 T \Big|_{S^2} = \alpha_0 T^1 + \lambda G_{33}^{\frac{1}{2}} G^{23} \frac{\partial T}{\partial \eta} \Big|_{S^2}.$$

Now the temperature on  $S^2$  can be computed:

$$T^S(J) \Big|_{S^2} = \left[ \alpha_0 T^1 + \lambda (G_{33})^{\frac{1}{2}} G^{23} T_{,n} - \lambda (G^{33})^{\frac{1}{2}} \frac{4T(J, K) - T(J, K-I)}{2\Delta x} \Big|_{S^2} \right] / \left( \alpha_1 T(J, K) - \frac{3\lambda (G^{33})^{\frac{1}{2}}}{2\Delta x} \right)$$

## 5. Description of the process of crystallization

In the present work the process of crystallization is described by the method of equivalent heat capacity. Let  $L$  be the latent heat of crystallization and  $\kappa_s$  — the solidified volume fraction in the two phase region. From (4) follows:

$$(24) \quad c\rho \frac{\partial T}{\partial t} = \nabla \lambda \cdot \nabla T + \rho L \frac{\partial \kappa_s}{\partial t}$$

$$\rho \left( c - L \frac{\partial \kappa_s}{\partial T} \right) \frac{\partial T}{\partial t} = \nabla \lambda \cdot \nabla T.$$

Consequently the equivalent heat capacity is (12):

$$C_E = C - L \frac{\partial \kappa_s}{\partial T}.$$

In order to obtain an expression for  $\kappa_s(t, T)$ , we use Kolmogorov's formula:

$$(25) \quad \kappa_s(t) = 1 - \exp \left( - \int_0^t J(\tau) \omega(t-\tau) d\tau \right),$$

where  $J(t)$  is the velocity of appearance of new nuclei of crystallization, and  $\omega(t)$  — the volume of the solid phase, [5]. Let  $T_c$  is the temperature of crystallization and  $\delta T = T_c - T$  is the temperature of overcooling. In (5) the dependence of  $J(t)$  and  $\omega(t)$  on  $\delta T$  was determined. To the first term of the power series expansion of  $\kappa_s(T)$  in respect to  $\delta T$ :

$$(26) \quad \kappa_s = \beta J(\delta T) \delta T \varphi(\Delta t_k)$$

$$J(\delta T) = \begin{cases} 0 & |\delta T| > \Delta T \\ A \delta T^2 & |\delta T| \leq \Delta T \end{cases},$$

where  $\Delta t_k$  is the time from the beginning of crystallization,  $\beta$  and  $A$  are constants. We suppose that the process of crystallization is over at temperature  $T = T_c - \Delta T$ ,  $\Delta T$  is determined in the experiment and the constants  $A$  and  $\beta$  — from the requirement of energy conservation. The expression for  $C_E$  is derived from (26):

$$C_E = C + 6L(\Delta T + \delta T) \delta T / \Delta T^3 \quad T_c - \Delta T < T < T_c$$

$$C_E = C \quad T > T_c; \quad T < T_c - \Delta T$$

## 6. Results

A computer program for the numerical solution of (4) was realized. Solutions were obtained for some cases. The model example of cooling of a ball, Fig. 2, is interesting because it demonstrates the coordinate effects, described in section 4. The

solution without the additional terms differs from the exact one by scores of per cents. When these terms are accounted for, the accuracy rises and becomes comparative to that of the solution for a cylinder (orthogonal coordinates and trivial metric). The diagram on Fig. 2 gives the relative errors of the solution. On the surface of the ball the solution practically does not differ from the analytical one, and near the axis  $Oz$ , where the grid is rarefied, the error rises to 1%. Fig. 3 and 4 illustrate the solution of the thermophysical problem in the case of a bell. On the left picture the fronts of crystallization are drawn at different times from the beginning of the process (in seconds) and on the right one — the isothermic curves at the end of the process of crystallization. The coefficient of heat transfer is designated by  $\alpha$ , where  $\alpha = \alpha_0 = \alpha_1$  from (14) and (23). On Fig. 3 and 4 the effects of different coefficients on the solution

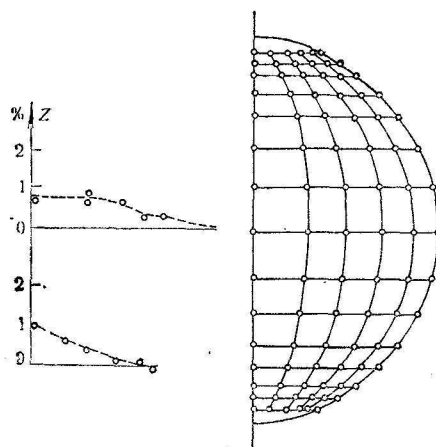


Fig. 2

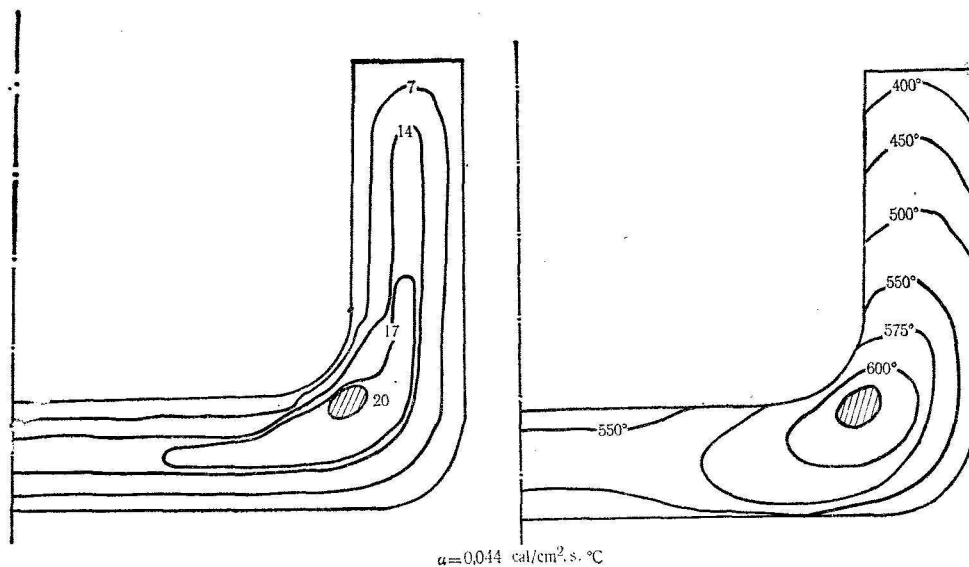


Fig. 3

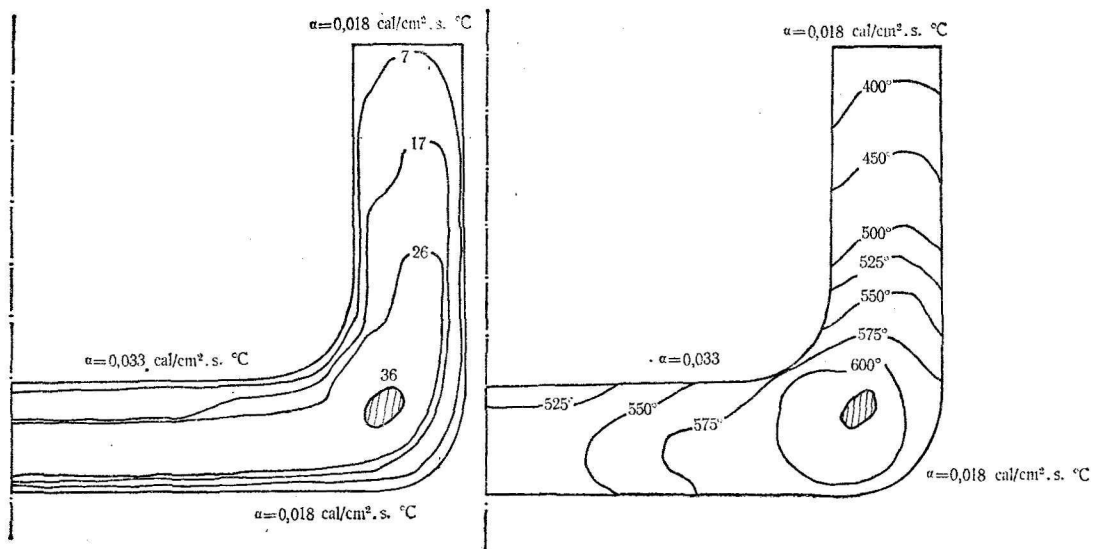


Fig. 4

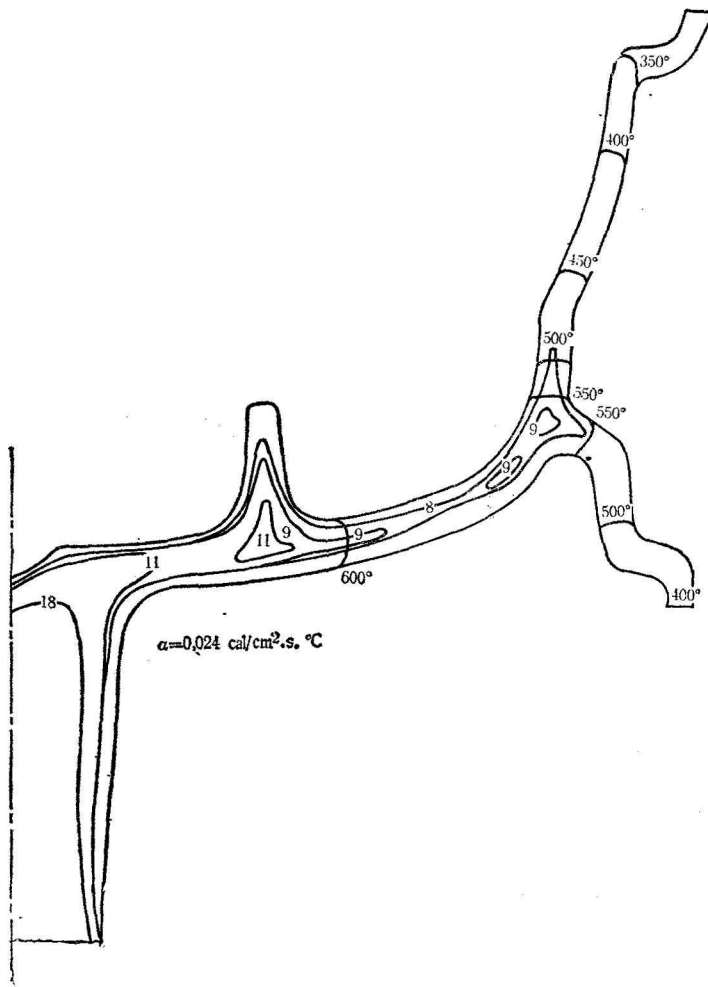


Fig. 5

are seen. On fig. 5 the solution of the problem for a wheel is given. The fronts of crystallization up to the 18 th second from the start of the process, and the isothermic curves at the end, are drawn. One can follow the formation of cavities with molten metal, where usually the defects emerge. In both cases the metal is conventional, with  $T_c=660^\circ\text{C}$ , latent heat of crystallization  $L=95\text{ cal/g}$ , with initial temperature  $T_{in}=700^\circ\text{C}$  and external temperature  $T^L=0^\circ\text{C}$ .

## 7. Conclusions

Many authors treating the problems of mass and heat transfer, have suggested more or less complicated methods of construction of boundary fitted curvilinear coordinate systems (2, 7, 9, 10, 11). Most frequently these coordinates are obtained as equipotential solutions of an elliptic differential system with Dirichlet boundary conditions (9, 10). The shortcomings of such an approach are: a) the coordinate system does not reflect the peculiarities of the treated differential equations, b) when the boundaries of the region alter in the process, the problem of updating them becomes too cumbersome.

In the present work we have demonstrated another approach, in which the coordinate system is generated by algebraic means in the Riemannian space in order to geometrize the continuity equations. We have shown that it can be applied to the thermophysical problem. We shall note that greater variety of problems of heat and mass transfer can be treated in the framework of this approach.

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*Received 18. 09. 1985*