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Formation of castings with complex geometry. Thermomechanical effects, growth and influence of the air gap

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Abstract—In previous works we have proposed a method for mathematical modelling of the processes of heat and mass transfer in castings, which includes the construction of a boundary fitted coordinate system in a Riemannian coordinate space. Within this approach we obtain the deformations, stresses and strains in the casting-mould system within a linear thermoelastic model. The equations for the stresses and deformations are derived from the corresponding laws of conservation in the coordinate space. Secondly, we consider the problem of heat transfer between the casting and the mould, while the boundary conditions change during the crystallization and formation of the crust due to the thermomechanical interaction there. We describe the evolution of the air gap and consider its influence on the process of crystallization. Some consequences from this model, which may allow a more subtle description of the casting formation, like the segregation behaviour in the two-phase region, are also discussed.

INTRODUCTION

A PRINCIPAL difficulty in the mathematical modelling of casting formation is the simultaneous treatment of hydrodynamic, thermoelastic, crystallization processes in castings with complex shapes. The problem becomes even more complicated when the shape is not stationary, e.g. when the solidification begins during the filling of the mould.

In refs. [1, 2] we proposed a method for treating such problems—they are written and numerically solved in a Riemannian coordinate space, obtained through a metric mapping from the space of the real process. The mapping is constructed in such a way, that: (1) a boundary fitted coordinate system is obtained and (2) under certain conditions the hydrodynamic equations, describing a laminar filling of the mould, can be factorized over a family of coordinate surfaces $\hat{S}$ [1, 3]. In this coordinate system various problems of casting formation could be treated simultaneously—in refs. [2, 3] we demonstrated some results from hydrodynamics, cooling and crystallization of castings, including the case with nonstationary geometry. In addition, the coordinate system is generated by algebraic methods, which makes more feasible the problem of its updating in cases with non-stationary metrics. (A review of the different methods for generation of boundary fitted coordinate systems can be found in ref. [4].)

The essential steps in the construction of the metric are shown in Fig. 1. The coordinate system consists of a congruence of surfaces $\hat{S}$ with a metric on them, and a transverse vector field, parametrized by the variable x^3, $0 \leqslant x^3 \leqslant 1$. The two metric forms on S^1, $g_{ab}(t, x^1, x^2)$ and $b_{ab}(t, x^1, x^2)$, are obtained as:

$$g_{ab}(t, x^1, x^2) = (r_a, r_b)$$
$$b_{ab}(t, x^1, x^2) = -(r_a, n_b)$$

where r_a are vectors in S^1, tangent to the coordinate curves x^a: $r_{aQ} = \partial R/\partial x^a$, where R is the vector from a concurrent coordinate system K_0 to a point Q in S^1; n_Q is the unit normal vector at the same point Q, and the scalar product (,) is defined by the external

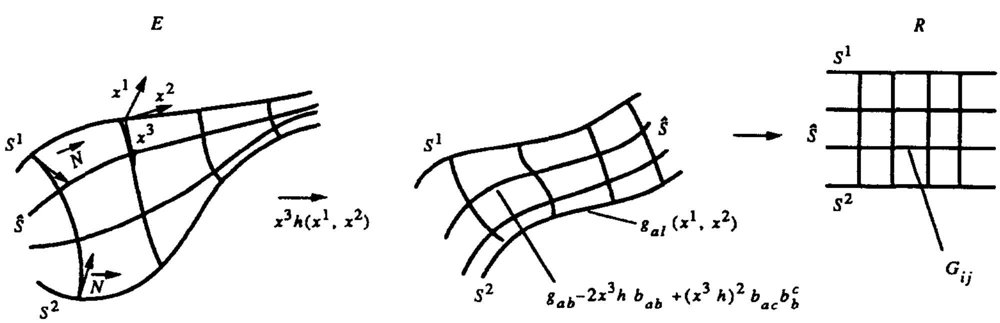

FIG. 1. Stages of the construction of the metric mapping to the coordinate space R.

NOMENCLATURE

$a, b, \ldots$ indexes, running over 1, 2
c heat capacity coefficient
$\partial_i f = f_{,i} = \partial f/\partial x^i$ partial derivative along x^i
$\nabla_i F = F_{;i}$ covariant derivatives along x^i
F density of the external volume force
$G^{ij}(t, x^1, x^2, x^3)$ components of the metric tensor
$G(t, x^1, x^2, x^3)$ determinant of the metric tensor
$g_{ab}(t, x^1, x^2)$ components of the metric on the basic surface S^1
$h(t, x^1, x^2)$ transverse distance along n
$i, j, \ldots$ indexes, running over 1, 2, 3
L latent heat of crystallization
n unit vector field, normal to S^1
q heat flux vector, $q_i = -\kappa\nabla_i T$
S^1 one of the boundaries, chosen as a basic surface
$\hat{S}$ coordinate surfaces
t time parameter
T temperature field
T_0 external temperature
T_c temperature of the liquid phase
δT $T - T_0$
ΔT temperature interval of crystallization
$t^{ij}(t, r)$ stress tensor
U density of the internal energy
V velocity of a volume element.

Greek symbols
$\alpha(t)$ heat transfer coefficient
α_0 initial value of $\alpha(t)$
β thermal expansion coefficient
Γ^i_{jk} affine connection coefficients
$\theta^{ij}(t, r)$ velocity of deformation tensor
κ heat conductivity coefficient of metal
κ_g heat conductivity coefficient of air
λ, μ Lamé's coefficients
ρ specific density
ω_s volume ratio of solid phase.

euclidean metric in K_0. The components of the metric tensor are obtained in ref. [1]:

$$G_{ab}(t, x^1, x^2, x^3) = g_{ab} - 2x^3 h b_{ab} + (x^3 h)^2 [b_{ac} b^c_b + (\nabla_a r_a)(\nabla_b r_b)]$$

$$G_{a3}(t, x^1, x^2, x^3) = -x^3 h(\nabla h, r_a)/G^{1/2}_{ab}$$

$$G_{33}(t, x^1, x^2) = h^2. \quad (1)$$

The family of surfaces $\hat{S}$ and the vector field n, normal to S^1, with geometry defined by (1), form a boundary fitted coordinate system. The equations of heat and mass transfer in metric (1) should be derived in a covariant way in order to account for the effects of boundary curvature and nonstationarity. We obtain them from the laws of conservation of mass, momentum and energy, defined in the coordinate space [1]. The corresponding equations are:

(a) mass:

$$(1/\sqrt{G})\partial_t(\sqrt{G}\rho) + \nabla\cdot(\rho V) = 0 \quad (2)$$

(b) momentum:

$$\rho(V^i_{,t} + V^k\nabla_k V^i + 2\Gamma^i_{tk}V^k) - \nabla_k t^{ik} = \rho F^i \quad (3)$$

(c) energy:

$$\rho(U_{,t} + U\partial_t \ln G + V^i U_{,i}) = t_{ij}\theta^{ij} - \nabla_j q^j + \rho V^k F_k. \quad (4)$$

THE THERMOELASTIC MODEL

We shall use a linear thermoelastic model, defined by the stress tensor:

$$t^{ik} = A(T)G^{ik}\delta T + B(T)(\nabla\cdot\xi)G^{ik} + C(T)(\nabla^i\xi^k + \nabla^k\xi^i).$$

The coefficients A, B and C are obtained on the assumption of adiabatic initial conditions [5]:

$$A = \Lambda\beta/(1+Z\Lambda); \quad B = \lambda - Z\Lambda^2/(1+Z\Lambda); \quad C = \mu$$

where $Z = T_0\beta^2/c$; $\Lambda = \lambda + 2/3\mu$.

With the use of the expression $G^{ij}\Gamma^k_{jl} + G^{ik}\Gamma^i_{jl} = -G^{ik}_{,l}$, the stress tensor is written down in partial derivatives:

$$t^{ik} = AG^{ik}\delta T + BG^{ik}(\xi^l_{,l} + (\ln\sqrt{G})_{,l}\xi^l) + C(G^{il}\xi^k_{,l} + G^{kl}\xi^i_{,l} - G^{ik}_{,l}\xi^l). \quad (5)$$

In the case, when the inertia and convective terms can be neglected, equation (3) is presented in the form:

$$\rho F^i + 2\rho\Gamma^i_{tk}\xi^k_{,t} = \nabla_k t^{ik} = AG^{ki}\nabla_k\delta T + (B+C)G^{ki}\nabla_k\nabla_i\xi^i + C\Delta\xi^i + CR^i_k\xi^k \quad (6)$$

where R_{ik} is the curvature tensor of the surface $\hat{S}$.

Let us consider a region with axial symmetry and designate $x^1 = \phi$, $x^2 = \eta$, $x^3 = x$. If ϕ, r, z are the variables of an orthogonal cylindrical coordinate system and $r = r(z)$ is a coordinate line in S^1, which in fact is the distance from a certain point of S^1 to the symmetry axis, and $B(z) = \partial_z r$, then $d\eta = (1+B^2)^{1/2}dz$. The components of the metric are derived from (1):

$$G_{11} = [r + xh/(1+B^2)^{1/2}]^2$$

$$G_{22} = [1 - xh\partial_\eta B/(1+B^2)]^2 + (x\partial_\eta h)^2$$

$$G_{33} = h^2; \quad G_{23} = xh\partial_\eta h. \quad (7)$$

When equations (7) are substituted into (6), the thermoelasticity equations in terms of the displacement ξ^i are represented in the specific metric and coordinate system. With regard to the symmetry of the problem in $x^1 = \phi$, we obtain for the terms $\nabla_i t^{ij}$:

$$\begin{aligned}\nabla_i t^{i2} = {} & (B+2C)G^{22}\xi^2_{,22}+(B+3C)G^{23}\xi^2_{,23} \\ & +CG^{33}\xi^2_{,33}+(B+C)G^{22}\xi^3_{,32} \\ & +[C/\sqrt{G}(G^{22}\sqrt{G})_{,2}+(G^{23}\sqrt{G})_{,3} \\ & +(B+C)G^{22}(\ln\sqrt{G})_{,2}+2C(G^{22}\Gamma^2 \\ & +G^{23}\Gamma^2)]\xi^2_{,2}+[C/\sqrt{G}(G^{32}\sqrt{G})_{,2} \\ & +(G^{33}\sqrt{G})_{,3}+(B+C)G^{23}(\ln\sqrt{G})_{,2} \\ & +2C(G^{33}\Gamma^2_{32}+G^{23}\Gamma^2_{22})]\xi^2_{,3} \\ & +[(B+C)G^{22}(\ln\sqrt{G})_{,3} \\ & +2C(G^{22}\Gamma^2+G^{23}\Gamma^2)]\xi^3_{,2} \\ & +[(B+C)G^{23}(\ln\sqrt{G})_{,3} \\ & +2C(G^{33}\Gamma^2_{33}+G^{23}\Gamma^2_{23})]\xi^3_{,3} \\ & +[(B+C)G^{22}(\ln\sqrt{G})_{,22}+G^{23}(\ln\sqrt{G})_{,23} \\ & +CG^{ij}\Gamma^2_{ij,2}]\xi^2+[(B+C)G^{22}(\ln\sqrt{G})_{,23} \\ & +G^{23}(\ln\sqrt{G})_{,33}+CG^{ij}\Gamma^2_{ij,s}]\xi^3 \\ & +A(G^{22}T_{,2}+G^{23}T_{,3}) \end{aligned} \quad (8a)$$

$$\begin{aligned}\nabla_i t^{i3} = {} & (B+2C)G^{22}\xi^2_{,22}+(B+3C)G^{23}\xi^2_{,23} \\ & +CG^{33}\xi^2_{,33}+(B+C)G^{22}\xi^3_{,32} \\ & +[C/\sqrt{G}(G^{22}\sqrt{G})_{,2}+(G^{23}\sqrt{G})_{,3} \\ & +(B+C)G^{22}(\ln\sqrt{G})_{,2}+2C(G^{22}\Gamma^2_{22} \\ & +G^{23}\Gamma^2)]\xi^2_{,2}+[C/\sqrt{G}(G^{32}\sqrt{G})_{,2} \\ & +(G^{33}\sqrt{G})_{,3}+(B+C)G^{23}(\ln\sqrt{G})_{,2} \\ & +2C(G^{33}\Gamma^2_{32}+G^{23}\Gamma^2_{22})]\xi^2_{,3} \\ & +[(B+C)G^{22}(\ln\sqrt{G})_{,3} \\ & +2C(G^{22}\Gamma^2_{23}+G^{23}\Gamma^2)]\xi^3_{,2} \\ & +[(B+C)G^{23}(\ln\sqrt{G})_{,3} \\ & +2C(G^{33}\Gamma^2_{33}+G^{23}\Gamma^2_{23})]\xi^3_{,3} \\ & +[(B+C)G^{22}(\ln\sqrt{G})_{,22} \\ & +G^{23}(\ln\sqrt{G})_{,23}+CG^{ij}\Gamma^2_{ij,2}]\xi^2 \\ & +[(B+C)G^{22}(\ln\sqrt{G})_{,23} \\ & +G^{23}(\ln\sqrt{G})_{,33}+CG^{ij}\Gamma^2_{ij,3}]\xi^3 \\ & +A(G^{32}T_{,2}+G^{33}T_{,3}). \end{aligned} \quad (8b)$$

The metric coefficients and the terms, included in the figure brackets in equation (8) are derived only at the beginning of the calculations or when the metric is updated. For that reason equation (8) is of the same numerical difficulty as the problems, conventionally treated in a Cartesian coordinate system. The difference between the two coordinate systems will come in the way in which the boundary conditions are defined.

The initial conditions, imposed on the unknown functions $\xi^2(\eta, x)$ and $\xi^3(\eta, x)$, depend on the way the casting is formed. If the mould is filled with molten metal with temperature T_0 and pressure p_0 at the beginning, only the isotropic part of the stress tensor (5) differs from zero and the initial values are:

$$\xi^2(t=0) = (p_0/2B\sqrt{G})\int\sqrt{G}\,\mathrm{d}\eta$$

$$\xi^3(t=0) = (p_0/2B\sqrt{G})\int\sqrt{G}\,\mathrm{d}x. \quad (9)$$

When the pressure p in the liquid phase does not change (because of a permanent feeding up), expressions (9) will hold in the melt throughout the process of cooling and crystallization. A different pattern of casting formation is realized, when the molten metal is enclosed within a solid crust and the feeding is ceased. Then the pressure changes during the process—in the case considered here it rises initially, and afterwards, due to the thermal contraction, it drops sharply. In such regions defects like pores and cracks will appear. The evolution of the isothropic part of the stress tensor in this case is shown in Fig. 6.

The boundary conditions for equation (6) vary during the process. The vector $\mathbf{N}$, normal to $\hat{S}$, Fig. 1, can be obtained from (7), [2]:

$$\mathbf{N} = \sigma n-(1-\sigma^2)^{1/2}r_\eta;\quad \sigma = (G^{22}G_{22})^{-1/2}. \quad (10)$$

The components of the normal stress on a surface $\hat{S}$ will be:

$$P^i = t^i_j\mathbf{N}^j = (A\delta T+B(\xi^l_{,l}+(\ln\sqrt{G})_{,l}\xi^l))N^i + C(G^{il}G_{kn}\xi^n_{,l}+\xi^i_{,k}+G^{ij}_{l}G_{jk}\xi^l)N^k. \quad (11)$$

The scalar $P = P^i\mathbf{N}_i$ measures the normal stress on the walls of the form S^k. Initially it equals the pressure p_0, but after a crust is formed, it diminishes because of the shrinkage. While $P>0$, the boundary conditions are $\xi^i_{|s} = 0$. When P becomes zero, the boundary conditions are determined from the expression $P = 0$, which links the magnitudes and the derivatives of the displacement at the boundary according to (11). The air gap, which appears, is determined as the sum of the boundary displacements of the casting and mould:

$$\delta(t,z) = (\xi^i(t,z),N_i)_c+(\xi^i(t,z),N_i)_m.$$

In this case the heat transfer between the mould and the casting will change significantly:

$$\alpha(t,z) = \alpha_0\kappa_g/(\kappa_g+\alpha_0\delta(t,z)) \quad (12)$$

where α_0 is the heat transfer coefficient at the beginning of the process, when the contact between the boundary surfaces is fast. The dependence of α_0 on the value of the pressure P while $\xi_{|s} = 0$ will not be accounted here.

The heat problem is described in ref. [2]. It is solved in two regions, with solid and molten metal, where the equation is:

$$\rho(c+L\partial_T\omega_s)\partial_t T = \nabla\cdot\kappa\nabla T$$

This problem is treated in the same coordinate system. After the substitution of the metric components from (7) we obtain:

$$c\rho\partial_t T = [\kappa(G^{22}T_{,22}+G^{33}T_{33}+2G^{23}T_{,23}) + G^{22}T_{,2}\kappa_{,2}+G^{33}T_{,3}\kappa_{,3}+G^{23}(T_{,3}\kappa_{,2}+T_{,2}\kappa_{,3}) + \kappa((\sqrt{G}G^{22})_{,2}T_{,2}+(\sqrt{G}G^{23})_{,3}T_{,2} + (\sqrt{G}G^{23})_{,2}T_{,3}+(\sqrt{G}G^{33})_{,3}T_{,3})]/\sqrt{G}. \quad (13)$$

The boundary conditions of II and III kind follow from $\partial_n T = N \cdot \nabla T$:

$$\kappa(G^{33})^{1/2}\partial_3 T_{|s} = \alpha(t)(T_c - T_{|s}) + \kappa(G_{33})^{1/2}G^{23}\partial_2 T_{|s} \quad (14)$$

where N is obtained from equation (10) and $\alpha(t)$ from (12). On the boundary between mould and casting T_c is respectively the surface temperature of casting and mould.

The crystallization is described by the method of equivalent heat capacity $C_E = c + L\partial_T\omega_s$. A simple equilibrium model for ω_s is used:

$$C_E = c - 2L\delta T/\Delta T^2 \quad T_c - \Delta T \leqslant T \leqslant T_c$$

$$C_E = c \quad T > T_c \quad \text{or} \quad T < T_c - \Delta T.$$

NUMERICAL RESULTS AND DISCUSSION

The system (6), written in metric (7), is solved jointly with the problem for cooling and crystallization (13) with initial and boundary conditions, settled above. The interaction between the heat and the mechanical problems takes place through the boundary conditions: while the normal stress, by which the casting acts on the walls of the mould is positive, $\xi_{ls} = 0$, and the coefficient of heat transfer is α_0; when a gap appears, $|\xi_{ls}| > 0$, and the heat transfer

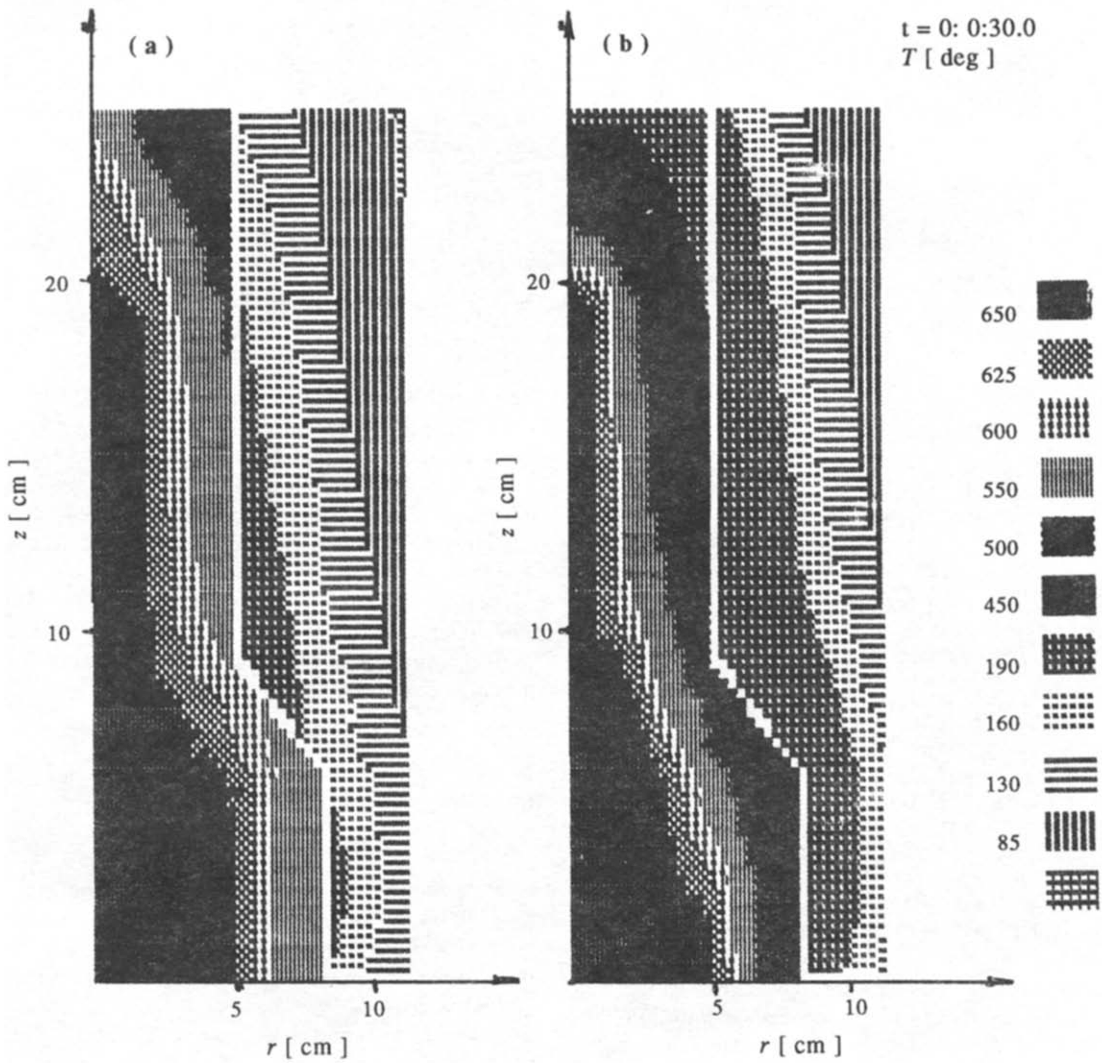

Fig. 2. Formation of a cylindrical casting with a permanent feed-up. (a) The influence of the air gap is accounted for. (b) The air gap is not accounted for. The surfaces of crystallization and several isothermic curves at 30 s are shown. The cooling rate α_0 at $t = 0$ is 5000 W m^{-2} grad^{-1}.

Table 1. Parameter values

c	1088 J kg^{-1} grad^{-1}
L	4×10^5 J kg^{-1}
T_c	660°C
ΔT	5°C
α_0	1500 W m^{-2} grad^{-1}
β	$\beta_0+\beta_1 T$; $\beta_0=0.7\times10^{-4}$; $\beta_1=10^{-8}$ grad^{-1}
λ	0.49×10^7 N m^{-2}
μ	$\mu_0+\mu_1 T+\mu_2 T^2$; $\mu_0=0.25\times10^7$ N m^{-2}; $\mu_1=0.246\times10^4$ N m^{-2} grad^{-1}; $\mu_2=2$ N m^{-2} grad^{-2}
κ	200 W m^{-1} grad^{-1}
κ_g	0.04 W m^{-1} grad^{-1}
ρ	2700 kg m^{-3}

changes according to (12). Calculations were carried out for a conventional metal with parameters, listed in Table 1.

The problem was solved numerically for castings with different shapes. In Fig. 2 we present results from the solution for axially symmetric castings with a permanent feed up with a molten metal. A solution for the air gap is obtained, and its influence on the crystallization is shown. The evolution of the heat transfer coefficient $\alpha(t)$ is shown on Fig. 3. As seen from (12), the air gap $\delta(t)=\kappa_g(\alpha^{-1}-\alpha_0^{-1})$. The surface temperature at Fig. 4 sharply rises after the appearance of the air gap, because the heat transfer coefficient diminishes according to (12), and the rearrangement of the temperature gradient field inside the casting lags behind. Figure 5 illustrates the magnitude of the displacements $|\xi|$.

In the next figure we demonstrate another solution for the same configuration, this time without a feed up of the two-phase region. This is shown in Fig. 6, where the evolution of the isotropic part of the stress tensor $1/3t_{ii}=A\delta T+(B+2/3C)\xi^l_{,l}+B(\ln\sqrt{g})_{,l}\xi^l$ is presented for an element with $x=0.6$. After the formation of a solid core the molten metal remains

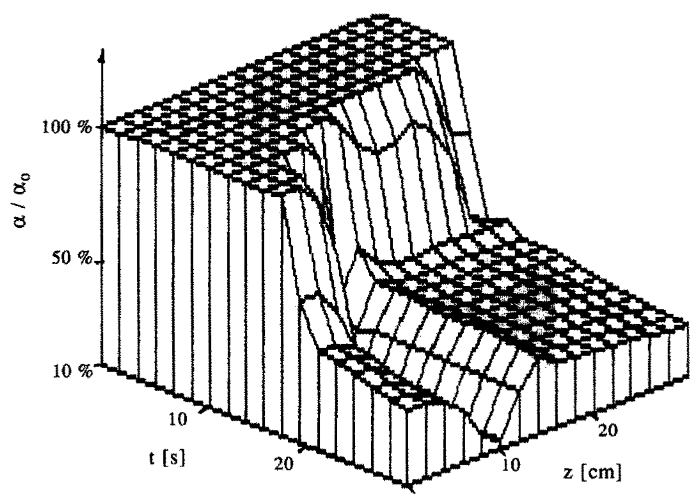

FIG. 3. Evolution of the coefficient of heat transfer $\alpha(t, z)$. According to equation (12) the air gap $\delta(t)=\kappa_g(\alpha^{-1}-\alpha_0^{-1})$ is easily derived from here.

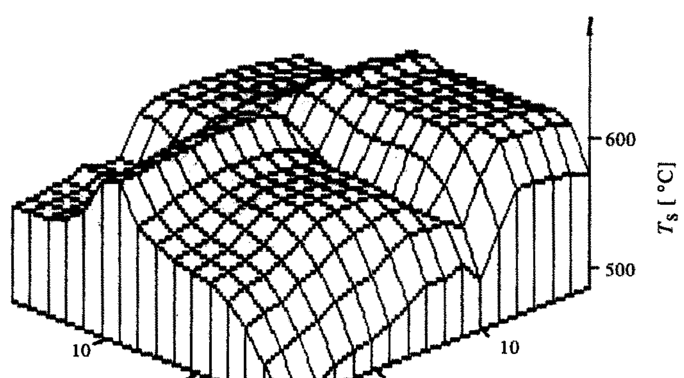

FIG. 4. Surface temperature T_{ls} of the casting. When the crystallization of the layers immediately below the surface is completed, T_{ls} falls sharply. After the appearance of the air gap, the temperature on the surface may rise again, which is due to the rearrangement of the thermal fluxes inside the casting.

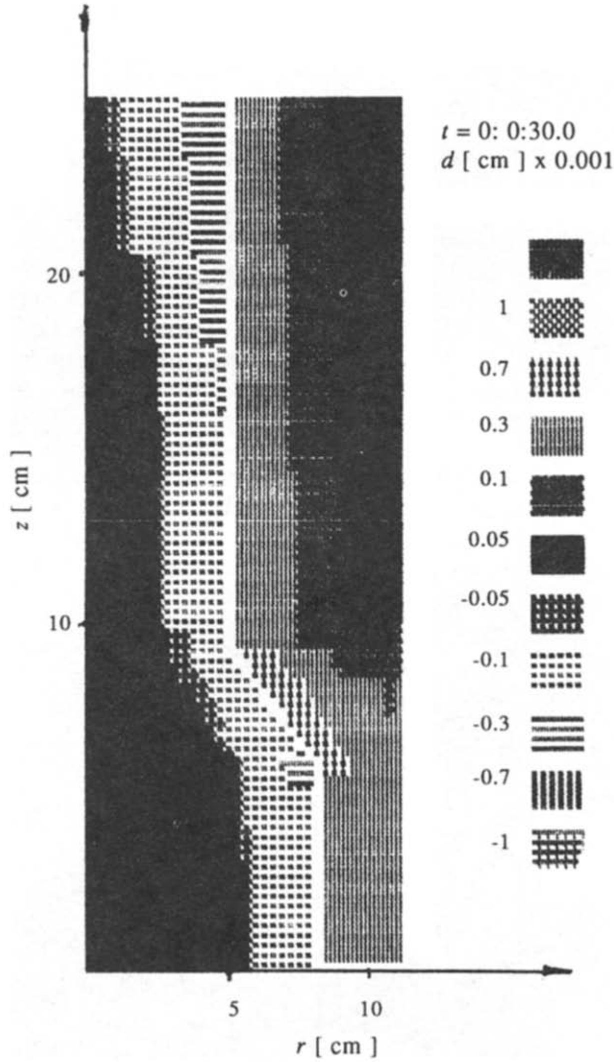

Fig. 5. Field of the deformations $|\xi(x, z)|$.

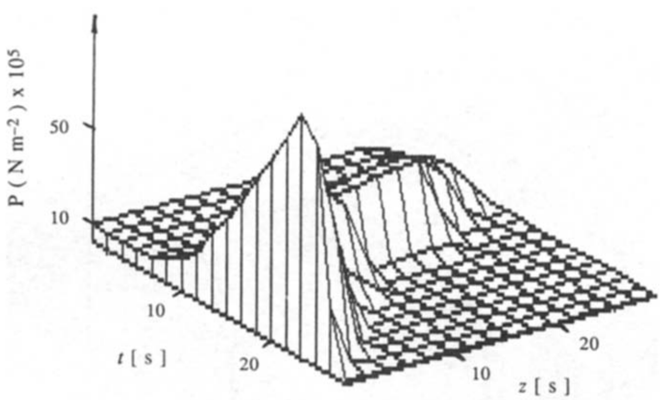

Fig. 6. Evolution of the isotropic part of the stress tensor t_{ii} for a layer from the casting with $x^3 = 0.6$. In this case the feeding is ceased and the pressure depends on the progress of the crystallization in outer layers of the casting.

enclosed, and the pressure there depends on the progress of crystallization in the outer layers. Initially the pressure rises, because the outer layers are shrinking (ρ is considered to be constant during the phase transition). An important aspect here is the possibility to judge the quality of the casting—when crystallization takes place in the considered volume, the pressure there falls to zero, and pores and hot cracks will be imminent—in addition, it provides the initial conditions which are needed to treat such problems as segregation, pores, stress relaxation near T_c. To describe these problems simultaneously with crystallization and deformation becomes feasible in this context.

The considered problems constitute only a part of a whole complex of processes, which take place during the casting. Their modelling is important for the correct description of the casting formation. The advantage of the described method is, that it treats uniformly and simultaneously the different problems of heat and mass transfer in castings with complicated and even non-stationary shapes.

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