

SOLUTION OF REVERSE AND INVERSE PROBLEMS
OF THERMAL PROCESSES IN METALLURGY BY
ELECTRICAL SIMULATION

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Methods of electrical simulation of problems of solidification within a temperature range are presented. Unique features in solutions of reverse and inverse problems are noted. Certain thermophysical properties of the crystallizing "steel ingot-gray iron mold" system are obtained.

Methods and examples of electrical simulation on ohmic-resistance grids (R-grids) of temperature fields in molds and ingots during crystallization with the heat of crystallization (L) released at constant temperature are given in [1, 2]. Solution of the solidification (melting) problem with the inner heat L released in the liquidus-solidus temperature range ($\Delta T_{cr} = T_{liq} - T_{sol} \neq 0$) is of considerable interest.

The electric analogy method [1, 2] is also applicable in the latter case not only for solving direct problems of defining the temperature field and the law governing translation of phase fronts under given boundary conditions, but also for solving reverse and inverse problems. In a reverse problem we derive boundary conditions from a known temperature field, while in the inverse problem, thermophysical properties of materials, including L, are determined.

Let us investigate by electrical simulation the following mathematical model of the solidification of an ingot in a mold:

$$\frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) - c \rho \frac{\partial T}{\partial \tau} + w = 0. \quad (1)$$

For simplicity, let us consider a one-dimensional problem and relate the equations to a rectangular system of coordinates. Equation (1) defines the nonsteady process of heat conduction in the mold, in the solid and liquid phases, and in the two-phase region of the ingot. In direct problems the thermophysical parameters λ , c , ρ , and w are given functions of coordinates and temperature. Neither in the mold nor in the solid and liquid phase does w have any effect, i.e., we neglect internal heats, except the heat of solidification L released in the two-phase region.

Boundary conditions which together with (1) constitute the mathematical model are of the following form (see Fig. 1).

- a) Boundary conditions of the IIIrd kind are specified for the external surface of the mold, where α_{em} takes into account convection and radiation.
- b) Boundary conditions of the IIIrd kind are specified for the inner surface of the mold and the outer surface of the ingot, with α_g taking into account the thermal resistance ($R_g = 1/\alpha_g$) in the gap. The temperature of the [external] medium is represented for the ingot by the temperature of the mold inner surface, and for the mold by that of the outer surface of the ingot.
- c) Boundary conditions of the IVth kind are specified for the interface of the solid and liquid phases (in the two-phase zone), i.e., temperatures and heat fluxes at related phase fronts are equal.
- d) The problem is symmetric, i.e., at the ingot center line $\partial T/\partial x = 0$.

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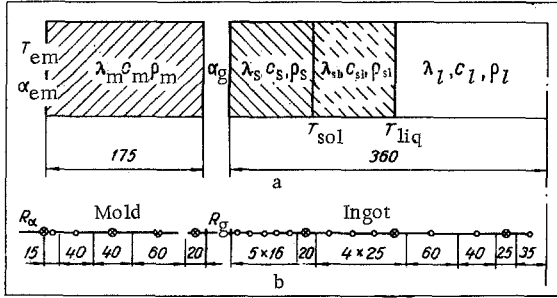


Fig. 1

Fig. 1. Diagram of the heat problem (a) and of the resistance grid (b). Resistances R_T and R_W at the input to the nodes are not shown.

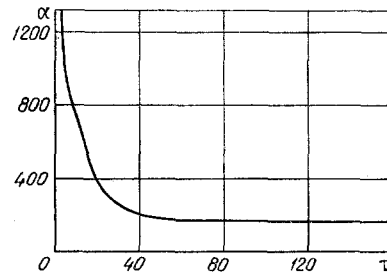


Fig. 2

Fig. 2. Dependence of the heat-transfer coefficient ($1/R_g$ in $W/m^2 \cdot \text{deg}$) of the gap on solidification time τ (min) derived by the solution of the reverse problem.

The initial condition presupposes a given temperature distribution in the ingot and in the mold at the reference instant of time. The latter makes it possible to specify and to take into account in the electrical analog the superheating of the molten metal.

This analog admits of the assumption of heat transfer by conduction in the liquid-phase and in the two-phase zones. Heat transfer by forced or natural convection in the liquid and in the two-phase zones can be taken into account by the introduction of an effective (or equivalent) thermal-conductivity coefficient.

Since a sufficiently detailed description of the computation method for parameters of the R-grid electrical analogs or of combined analogs (R-grid plus conductive paper) is given in [2, 4], we pause to consider only the features of simulating the internal heat released in the ΔT_{CR} temperature range.

In considering solidification (melting) at constant temperature T_{CR} , it was assumed in [1, 2, 5] that

$$w = \frac{L\rho}{\delta\tau} \quad (2)$$

The finite-difference equation approximating (1) is of the form

$$2 \frac{\lambda_1 \frac{T_{1,n} - T_{0,n}}{h_1} + \lambda_2 \frac{T_{2,n} - T_{0,n}}{h_2}}{h_1 + h_2} + c\rho \frac{T_{0,n-1} - T_{0,n}}{\delta\tau} + \frac{L\rho}{\delta\tau} = 0 \quad (3)$$

We write the second and third terms of Eq. (3) as

$$\left(c + \frac{L}{T_{0,n-1} - T_{0,n}} \right) \rho \frac{T_{0,n-1} - T_{0,n}}{\delta\tau} \quad (4)$$

When $\Delta T_{CR} \neq 0$, the expression in parentheses is called the effective specific heat capacity c_{eff} , and $L / (T_{0,n-1} - T_{0,n})$ the spectral heat of solidification (L_{sh}) when L is released according to a linear law in the $T_{0,n-1} - T_{0,n}$ range.

Although we are now considering the case of $\Delta T_{CR} = 0$, the derived characteristics c_{eff} and L_{sh} relate to $\Delta T_{CR} \neq 0$. Obviously, the method of simulation used in [1, 2] assumes that the release of L occurs in the temperature range $T_{0,n-1} - T_{0,n}$. During solidification and melting $T_{0,n-1} = T_{CR}$, while $T_{0,n}$ during solidification becomes lower, and during melting higher, than T_{CR} .

The smaller $T_{0,n-1} - T_{0,n}$, which is related to the shortening of the time interval $\delta\tau$, the more completely satisfied is the condition of phase transition at $\Delta T_{CR} = 0$ and the higher the overall accuracy of the solution [2].

Thus the method of [1, 2] assumes that L is released within a range of temperatures, while, in fact, it is released at $\Delta T_{CR} = 0$.

If it is assumed that L is released in the range $\Delta T_{CR} = T_{liq} - T_{sol} \neq 0$, Eq. (1) may then be written as

$$\frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) - c\rho \frac{\partial T}{\partial \tau} + \rho \frac{\partial L}{\partial T} \frac{\partial T}{\partial \tau} = 0 \quad (5)$$

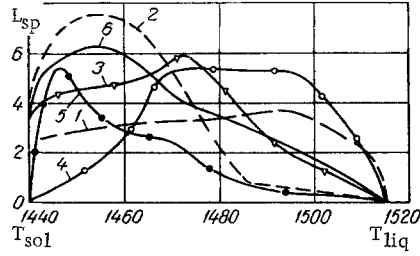


Fig. 3

Fig. 3. Dependence of the spectral heat of crystallization (kJ/kg·deg) on temperature (°K) in the interval ΔT_{CR} of solidification and on the position of the two-phase zone, derived by solving the inverse problem. Curves 1, 2, 3, 4, and 5 relate to L_{sh} at points lying, respectively, at 48, 64, 100, and 260 mm from the ingot surface. Curve 6 shows the dependence of the mean L_{sh} on temperature.

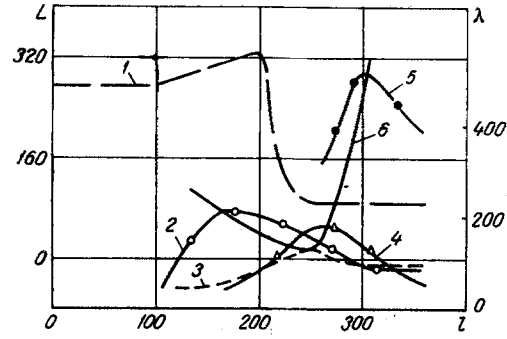


Fig. 4

Fig. 4. Variation of the total heat of crystallization (kJ/kg) and of the effective thermal-conductivity coefficient (W/m·deg) of the liquid phase across the ingot section l (mm): 1) total heat of crystallization; 2, 3, 4, and 5) λ_l at instants of time 15, 25, 45, and 70 min, respectively; 6) variation of maximum λ_l with time across the ingot section.

or

$$\frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) - \rho (c + L_{sh}) \frac{\partial T}{\partial \tau} = 0. \quad (6)$$

We know that

$$L = \int_{T_{sol}}^{T_{liq}} L_{sh} dT, \quad L_{sh} = \frac{\partial L}{\partial T}. \quad (7)$$

After suitable transformation, as in [2], we obtain

$$R_{\tau} = \frac{\delta \tau R_N}{(c + L_{sh}) \rho (h_1 + h_2)}, \quad (8)$$

for the one-dimensional problem and, respectively,

$$R_{\tau} = \frac{\delta \tau R_N}{(c + L_{sh}) \rho (h_1 + h_2) (h_3 + h_4)}; \quad (9)$$

$$R_{\tau} = \frac{\delta \tau R_N}{(c + L_{sh}) \rho (h_1 + h_2) (h_3 + h_4) (h_5 + h_6)}.$$

for the two-, and three-dimensional problems. The remaining grid parameters are obtained as in [2].

For electrical simulation it is necessary to know the function $L_{sh}(T)$ which makes it possible to introduce corrections to R_{τ} in the range $T_{liq} - T_{sol}$, and this permits us to take into account at each step of solution that L_{sh} is a function of temperature.

If

$$L_{sh} = \frac{L}{T_{liq} - T_{sol}},$$

is assumed, the mean integral spectral heat of solidification is, by the same token, defined and it is constant throughout the $T_{liq} - T_{sol}$ range.

Thus the first variant of the analog takes into consideration L in c_{eff} , when the problem is solved in the absence of heat sources, but with c_{eff} entering R_{τ} .

The second variant of the analog of Eq. (5) is the one in which

$$\rho \frac{\partial L}{\partial T} \frac{\partial T}{\partial \tau} = w, \quad (10)$$

i.e., the last term of (5) is considered to be an internal heat source of power w .

When simulating the transition through the $T_{\text{liq}} - T_{\text{sol}}$ range, w must be calculated at each step of solution by the expression

$$w = \rho \frac{\int_{T_{0,n}}^{T_{0,n-1}} L_{\text{sh}} dT}{\delta \tau}. \quad (11)$$

The limits of integration in the numerator of (11) relate to solidification. In the case of melting, the lower and upper limits are transposed.

The resistances R_w through which flow the currents simulating heat sources (sinks) of power w are determined by relationships given, for example, in [2].

If a node of the R-grid is supplied directly by current, the latter is defined (in a three-dimensional problem) by the expression

$$I_w = w(h_1 + h_2)(h_3 + h_4)(h_5 + h_6)/kR_N. \quad (12)$$

Experiment has shown that the amount of work involved in the solution is smaller, if the first variant of the analog with c_{eff} is used. In the second case it becomes necessary to make a second approximation to obtain a more accurate definition of the $T_{0,n}$ appearing in w as the integration limit and in R_w as a separate term.

The first variant of direct-problem simulation was used to solve the reverse and inverse problems. The process was repeated at each step of the solution until coincidence of the experimental and electrical analog temperature fields was reached. This was achieved by suitably varying resistances R_α , R_q , R_λ , R_τ , and R_w , or currents I_w which contain the unknown magnitudes.

Temperature distributions in the mold, in the solid and liquid phases, and in the two-phase zone, needed for solving the reverse and the inverse problems, were obtained by thermocouple measurement of the temperature of a rectangular ingot of grade 17 MnSi killed steel weighing 13 tons, whose cross section at mid-height was 1150×720 mm.

Temperature measurements were carried out simultaneously in three cross sections. No temperature gradients were observed over a considerable part of the ingot height, which made possible the solution of the reverse and inverse problems as one-dimensional in first approximation.

A diagram of the heat problem and the corresponding R-grid is shown in Fig. 1 in which the small circles denote nodes of the R-grid and the crosses indicate those nodes whose coordinates coincide with the coordinates of thermocouple ends.

Parameters T_{em} , α_{em} , c_m , ρ_m , c_s , ρ_s , T_{sol} , T_{liq} , c_l , and ρ_l appearing in Fig. 1 were assumed to be given. The thermal-conductivity coefficient of the two-phase zone was assumed to be equal to λ_s and its volumetric specific heat equal to c_{vl} . This is due to $c_{vs} \approx c_{vl}$ and $\lambda_s \neq \lambda_l$, since in the liquid phase λ_l is the effective λ mentioned above.

The sought unknowns were α_{eff} , L_{sh} , λ_m , and λ_l .

If the principle of local effect [6] is taken into consideration, it becomes possible to try to obtain at each stage of solution all of the unknown magnitudes with the aid of one model.

In our case the principle of local effect manifests itself, for example, by the fact that a change in the thermal resistance $1/\alpha_g$ of the gap affects mainly the temperature in the region of the inner surface of the mold and of the solid-phase outer surface, or by the importance in the determination of λ_m of the correspondence with experimentally defined temperatures in the mold and in the region of the ingot surface, and so on.

In the iteration process which this method of solution of reverse and inverse problems involves, a thorough analysis of results of each iteration, comparison of obtained data with their possible limit values,

consideration of the properties of curves representing the variation of unknown magnitudes, etc., are obviously important.

The results of solution of the reverse problem – determination of the coefficient of heat transfer in the the gap – are shown in Fig. 2. The comparison of data derived by electrical simulation with those obtained in experiments on a 12-ton ingot [7] shows a very satisfactory qualitative and quantitative correlation.

The dependence of L_{Sh} on temperature is shown in Fig. 3.

It became clear that the law of release of L_{Sh} does not only depend on temperature, but also on the position of the front of the phases. The dependence of the mean L_{Sh} on temperature is also shown in Fig. 3, while Fig. 4 shows the dependence of total L , as defined in [7], on the position of the two-phase zone.

It should be noted that integration with respect to T along curves 1, 2, and 3 yields like values of L , and along curves 4 and 5 it yields values which are lower than those obtained along curves 1, 2, and 3. This shows that the quantity of heat released in the two-phase zone diminishes with diminishing distance from the ingot center.

This may be explained by the sinking of the solid phase from higher layers, i.e., in a given section the quantity of the liquid phase during solidification diminishes not only owing to solidification but, also, because of an intake of solid phase from upper layers – in other words, owing to crystallization of upper layers and sinking from upper layers, and not from the crystallization of liquid metal in that section.

Hence in solving direct problems it is necessary to use curves similar to those in Fig. 3, where the described effect is taken into account.

If an actual heat problem were one-dimensional, the pattern of curves 4 and 5 (see Fig. 3) would be the same as that of curves 1, 2, and 3, and it would appear that L would have remained unchanged during solidification.

Hence a sufficient justification for treating this problem as one-dimensional is given not only by the small temperature gradients in the vertical direction but, also, by the law $L_{Sh}(T, x)$ which takes into account the variation of L in the motion of the two-phase zone.

A check solution of a direct two-dimensional problem for values of L_{Sh} quoted above and a comparison of experimental data with those of electrical analog computation confirm this assumption.

The dependence of λ_m on T obtained in the solution of an inverse problem is given in Table 1. It will be seen that in the interval of 923–973°K λ_m changes abruptly. This can be explained by changes in the structure of the gray iron at these temperatures. The pattern of variation of λ_m in the 293–873°K range conforms to published data on the variation of λ of pig irons with temperature.

A check has shown the necessity of taking $\lambda_m(T)$ into account only when the temperature field of the mold itself is to be determined with sufficient accuracy. In investigations of the temperature field of an ingot and for determining the pattern of motion of the two-phase zone λ_m can be taken at its mean value given by the relationship

$$\lambda_{m\text{ av}} = \frac{\int_{T_1}^{T_2} \lambda_m(T) dT}{T_2 - T_1} . \quad (13)$$

The mean integral $\lambda_{m\text{ av}}$ can be derived from the tabulated data.

Curves showing the dependence of the effective coefficient of thermal conductivity in the liquid phase on the position of the two-phase zone, obtained in the course of solving an inverse problem, are given in Fig. 4. It will be noted that all curves (only a few of the obtained curves are shown in Fig. 4) have a characteristic maximum approximately midway between the liquidus line and the ingot center line. The curve of

TABLE 1. The Dependence of the λ of the Mold Material on Temperature

$T, ^\circ K$	293	373	473	573	672	773	873	953	1023	1073
λ_m	53,6	52,5	51,5	50,5	49	48	46,5	45,5	34	24,5

maximum λ_l has a characteristic minimum, i.e., λ_l first increases and then decreases with the translation of the two-phase zone.

These peculiarities of the variation in λ_l may be explained by convection in the liquid phase, resulting from the characteristic temperature drop across that phase and by the translation of this drop during solidification of the ingot.

Thus, the electrical model – the R-grid – used in conjunction with the method proposed by Libmann [2] makes possible the solution of direct, reverse, and inverse problems of solidification (melting) with inner heat release either at constant temperature or in a range of temperatures. Solutions of reverse and inverse problems provide fairly accurate means for selecting optimum conditions for casting and for designing molds.

NOTATION

λ	is the coefficient of thermal conductivity;
c	is the specific heat;
ρ	is the density;
w	is the volumetric specific power of internal heat sources;
c_v	is the volumetric specific heat ($c\rho$);
α	is the heat-transfer coefficient;
$\delta\tau$	is the time interval;
h	is a space interval;
R_T, R_W	are resistances of the R-grid simulating, respectively, heat capacities and w ;
K	is the conversion factor from temperature to voltage;
R_N	is the conversion factor from thermal to electric resistance;
I	is the electric current.

Subscripts

em	denotes external medium;
m	denotes mold;
s	denotes solid phase;
l	denotes liquid phase;
g	denotes gap;
sh	denotes spectral heat of solidification;
cr	denotes crystallization;
sol	denotes solidus;
liq	denotes liquidus;
sl	denotes solid liquid (two-phase);
av	denotes mean (average).

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