

# Calculation of Phase-Change Boundary Position in Continuous Casting

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# Abstract

The problem of determination of the phase-change boundary position at the mathematical modeling of continuous ingot temperature field is considered. The description of the heat transfer process takes into account the dependence of the thermal physical characteristics on the temperature, so that the mathematical model is based on the nonlinear partial differential equations. The boundary position between liquid and solid phase is given by the temperatures equality condition and the Stefan condition for the two-dimensional case. The new method of calculation of the phase-change boundary position is proposed. This method based on the finite-differences with using explicit schemes and on the iteration method of solving of non-linear system equations. The proposed method of calculation is many times faster than the real time. So that it amenable to be used for model predictive control of continuous semifinished product solidification.

**Keywords:** Solidification Process, Application of Information Technology to the Foundry Industry, Mathematical Modeling of Temperature Distribution, Stefan Conditions for Phase-change Boundary, Continuous Casting.

# 1. Introduction

To develop new casting technology it is need to estimate the relation between the continuous casting process parameters and semifinished product quality. But almost all measurements in continuous casting are very difficult and expensive. Therefore we turn to development of enough precise mathematical models to investigate these relations as more accurately as possible [1].

To deal with the high variability of the described problem the heat and mass phenomenon must also be taken into account, and therefore the employed numerical model has to cover all the phase and structural changes [2].

A temperature field of steel slab in continuous casting process must be described as a heat transfer problem involving solidification. The phase transformation phenomenon is dominant in such technological process. Additionally the knowledge about position of the phase-change boundary is very important for technology and control of continuous casting process.

One of the simplest methods of the phase-change position determination is the engineering method of the square root [3], which in some cases gives a sufficiently close to the reality of the data. Nevertheless, it cannot be always considered as enough reliable.

So the next step in improvement of mathematical model of continuous ingot crystallization is the consideration of Stefan condition. In [4], the classical and the generalized formulation of Stefan problem are given, as well as the basic mathematical results on the existence and uniqueness of analytical solutions are presented. The numerical solution of this problem was a purpose of the work a lot of researchers. Many authors use the so-called method of spreading [5], which consists in the introduction of the Dirac delta function with the aim of defining the heat transfer inside a continuous medium. Then the Dirac delta function is replaced of a simple approximation. At the same time

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the thermal physical characteristics also are replaced of some effective values. But recent researches showed that in reality there is not so called jump of the thermal physical parameters at the phase-change boundary.

In [6] authors suggest the boundary element method to solve this problem for one-dimensional case. In [7] authors consider the quasi-stationary process in two-dimension. Then they turn to onedimensional model and also simplify the Stefan condition to onedimensional case to provide the analytic-numerical method for solving the problem of the moving boundary in continuous casting.

In this paper, we propose a fairly simple to understand and implement method for the determination of the phase-change boundary position. The mathematical model is based on the nonlinear partial differential equations because of the description of the heat transfer process takes into account the dependence of the thermal physical characteristics on the ingot temperature. The boundary position between liquid and solid phase is given by the temperatures equality condition and the Stefan condition for the two-dimensional case. The method of calculation of the phasechange boundary position is based on the finite-differences with using explicit schemes and on the iteration method of solving of non-linear system equations. In case of the two-dimensional formulation of this problem the numerical calculations can be carried out at a rate several times higher than the real-time. Due to this the proposed mathematical model can be successfully used in the circuit of the automatic control of continuous ingot solidification using model predictive control (MPC).

# 2. The method of determination of the phase-change boundary position.

The mathematical modelling method is based on the theory of mathematical physics and partial differential equations. At the formalization of continuous casting process we make the follow assumptions.

- 1. Heat flow in the direction perpendicular to the narrow mold walls is negligible.
- 2. The continuous medium is homogeneous.
- 3. The liquid and solid phases are separated by a thin border, not a strip, and the solidification temperature is the average from liquidus solidus interval.
- 4. Stirring in the liquid phase is not considered.
- 5. Since the casting is carried out under the slag, the heat flow from the top of the metal in the mold is equal to zero.
- 6. The friction between the surfaces of the ingot and the mold is not considered.
- 7. The width of the ingot at any level is constant.
- 8. Temperature field inside the mold is symmetric respect to the axis of the ingot, so one half-plane is considered.

After the problem formulation in partial differential equations we make the transition to the finite-difference problem. We suggest the special method based on the Stefan condition to determine the position of the phase-change boundary. We use the iteration method to solve the non-linear equations system.

#### 2.1. Mathematical model

The non-steady-state mathematical model describes the convective-conductive heat transfer in a continuous casting slab. The model examines the two-dimensional field of temperature and the phase boundary in a longitudinal section of a wide slab (Figure 1).

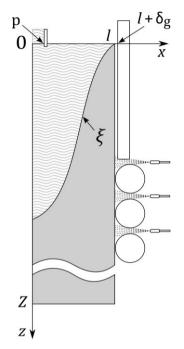


Fig. 1. Scheme of area modelled. (p is a half-thickness of poured molten steel stream,  $\xi$  is the phase boundary, l is the half-thickness of the slab)

The heat transfer in the ingot is described by the equation

$$\frac{\partial T}{\partial \tau} + v(\tau) \cdot \frac{\partial T}{\partial z} = \frac{1}{c(T)\rho(T)} \times \left\{ \frac{\partial}{\partial x} \left[ \lambda(T) \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial z} \left[ \lambda(T) \frac{\partial T}{\partial z} \right] \right\},$$
(1)

Where  $\tau$  is a time, x, z are space variables (Fig. 1),  $v(\tau)$  is the casting speed,  $T = T(\tau, x, z)$  is the temperature of ingot metal, c(T) is its specific heat,  $\rho(T)$  is its density, and  $\lambda(T)$  is its thermal conductivity.

The position of the unknown phase boundary is specified by equality condition of the temperatures and the Stefan condition for the two-dimensional case:

$$T(\tau, x, z)\Big|_{x=\xi_{-}(\tau, z)} = T(\tau, x, z)\Big|_{x=\xi_{+}(\tau, z)} = T_{cr},$$
(2)

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$$\begin{split} \lambda(T) \frac{\partial T}{\partial \overline{n}} \Big|_{\xi_{+}} &-\lambda(T) \frac{\partial T}{\partial \overline{n}} \Big|_{\xi_{-}} = \\ &= \mu \rho(T_{\kappa p}) \bigg( \frac{d\xi}{d\tau} + v(\tau) \frac{d\xi}{dz} \bigg), \end{split}$$
(3)

where  $\xi$  is the phase boundary  $x = \xi(\tau, z)$ ,  $\overline{n}$  is a normal to the phase boundary,  $\frac{\partial T}{\partial \overline{n}}\Big|_{\xi_{+/-}}$  is the left/right limit of the temperature derivative in the normal direction,  $\mu$  is the latent heat of crystallization,  $T_{cr}$  is the crystallization temperature (the

average temperature from the liquidus-solidus interval).

The boundary conditions for the ingot surface inside the mold are formulated with allowance for the presence of a gap between the surface of the ingot and the wall of the mold:

$$\begin{split} \lambda(T) \frac{\partial T}{\partial x} \bigg|_{x=l} &= \frac{\lambda_g}{\delta_g} \Big[ T_m(\tau, z) - T(\tau, l, z) \Big] + \\ &+ \sigma_m \Big[ T_m(\tau, z)^4 - T^4(\tau, l, z) \Big], \end{split} \tag{4}$$

where l is the half-thickness of the ingot,  $\lambda_g$  is an effective value of thermal conductivity of the slag crust in the gap with allowance for surface roughness,  $\delta_g$  is an effective value of the gap between the surface of the ingot and the given wall of the mold,  $T_m(\tau, z)$  is the temperature of the inner side of mold surface,  $\sigma_m$  is reduced radiation coefficient between the surface of the ingot and the inner side of mold surface.

After the mold zone the ingot moves into the secondary cooling zone (SCZ).

The boundary conditions in the SCZ account for the convective and radiative components of the heat transfer, the dependence of ambient temperature and the heat-transfer coefficients on the locations of the nozzles and water discharge in them:

$$\begin{split} \lambda(T) \frac{\partial T}{\partial x} \bigg|_{x=l} &= \alpha(\vec{t}, \vec{k}, \vec{G}, \vec{P}) [T_A - T(\tau, l, z)] + \\ &+ \sigma_n [T_A^{\ 4} - T^4(\tau, l, z)], \end{split} \tag{5}$$

where  $\alpha$  is convective heat transfer coefficient,  $(\vec{t}, \vec{k}, \vec{G}, \vec{P})$  is the vector of type, coordinate, water discharge, and air pressure in the nozzles respectively,  $\sigma_n$  is reduced radiation coefficient,

#### $T_A$ is an ambient temperature.

The boundary conditions at the meniscus level, at the center and at the end of ingot are:

$$T\Big|_{z=0} = T_p, \ 0 \le x \le p,$$
  
$$\frac{\partial T}{\partial z}\Big|_{z=0} = 0, \ p < x \le l,$$
(6)

$$\left. \frac{\partial T}{\partial x} \right|_{x=0} = 0, \left. \frac{\partial T}{\partial z} \right|_{z=Z} = 0$$

where  $T_p$  is the temperature of molten steel poured into the casting mould.

The initial condition for temperature field is:

$$T(0, x, z) = T_0(x, z).$$
<sup>(7)</sup>

And since (3) is also a non-stationary differential equation we have to set for it a boundary condition

$$\xi(\tau, 0) = l \tag{8}$$

and an initial condition

$$\xi(0,z) = \xi_0(z). \tag{9}$$

This problem is a nonlinear non-stationary (time-dependent) boundary problem for partial differential equations. Such problem isn't amenable to analytical solution but it can be solved numerically.

#### **2.2.** Finite-difference approximation

To solve the above problem we use the method of finite differences. Briefly, this method for the Stefan problem in similar formulation is described in [8]. It consists of the following.

- Region of the continuous variation of the argument is replaced by a finite set of points, called a finite-difference grid;
- Instead of the function of a continuous argument we consider the function of a discrete argument defined in the grid and called grid functions;
- All derivatives in the differential equations are replaced (approximated) using the corresponding difference relations, i.e. linear combinations of the values of the grid function in several nodes;
- The differential equations are replaced by algebraic equations (we get a system of algebraic equations);
- Initial and boundary conditions also are replaced by differences of initial and boundary conditions for the grid function.

So, let us consider the next uniform rectangular finite-

difference grid  $\omega_{q,h}$  with space steps  $q = \frac{l}{N}$  and  $h = \frac{Z}{M}$  on the ingot area  $(0, l) \times (0, Z)$  (see Fig. 2).





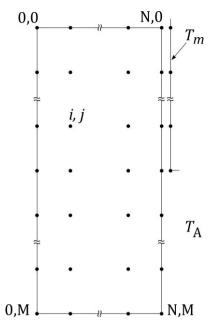
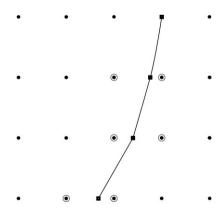


Fig. 2. The finite-difference grid

Additionally we consider the set of nodes to determine the phase-change boundary (or in other words free-boundary) position (Fig.3). We will call a node of the finite-difference grid "irregular node" if the distance between it and a phase-change node less than q.



- regular node
- irregular node
- phase-change node
- phase-change boundary

Fig. 3. The phase-change boundary nodes in the finite-difference grid

The heat transfer equation (1) in the not-divergence form:

$$\frac{\partial T}{\partial \tau} + v(\tau) \cdot \frac{\partial T}{\partial z} = \frac{1}{c(T)\rho(T)} \times \left\{ \frac{\partial \lambda}{\partial x} \cdot \frac{\partial T}{\partial x} + \lambda(T) \frac{\partial^2 T}{\partial x^2} + \frac{\partial \lambda}{\partial z} \cdot \frac{\partial T}{\partial z} + \lambda(T) \frac{\partial^2 T}{\partial z^2} \right\}.$$
<sup>(10)</sup>

Using a five-point pattern (Fig. 4), we can construct the finitedifference analogue of (10):

$$\begin{split} \frac{T_{i,j}^{k+1} - T_{i,j}^{k}}{\Delta \tau} + v_{k} \frac{T_{i,j}^{k} - T_{k,i,j-1}}{h} &= \\ &= \frac{1}{c_{i,j}^{k} \rho_{i,j}^{k}} \Biggl\{ \lambda_{i,j}^{k} \frac{T_{i+1,j}^{k} - 2T_{i,j}^{k} + T_{i-1,j}^{k}}{q^{2}} + \\ &+ \frac{\lambda_{i,j}^{k} - \lambda_{i-1,j}^{k}}{q} \cdot \frac{T_{i,j}^{k} - T_{i-1,j}^{k}}{q} + \\ &+ \lambda_{i,j}^{k} \frac{T_{i,j+1}^{k} - 2T_{i,j}^{k} + T_{i,j-1}^{k}}{h^{2}} + \\ &+ \frac{\lambda_{i,j}^{k} - \lambda_{i,j-1}^{k}}{h} \cdot \frac{T_{i,j}^{k} - T_{i,j-1}^{k}}{h} \Biggr\}, \end{split}$$

where k is the time-index, and i,j are the space-nodes indexes (see Fig.3 and Fig.4),  $\Delta \tau$  is a time step,  $T_{i,j}^k$  is the temperature in the *i,j* node in a time moment numbered k, and  $v_k$  is the casting speed at the moment of k.

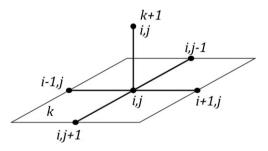


Fig. 4. Five-point pattern of explicit scheme

This is so called explicit finite-difference scheme. It is conditionally stable. The stable condition for it is

$$\Delta \tau \le \frac{c_{\min}\rho_{\min}q^2h^2}{2\lambda_{\max}(q^2+h^2) + v_k q^2 h c_{\max}\rho_{\max}}$$
(12)

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We can use (11) only for regular nodes (see Fig.3).

The finite-difference approximation for boundary conditions (4)-(6) also must take into account the position of the phasechange boundary position. For instance at the top of slab the solid shell is very thin and we have an irregular node in boundary condition (4). Therefore in the case  $\xi_j^k > l-q$  the finitedifference approximation of (4) is

$$\lambda_{N,j}^{k} \frac{T_{N,j}^{k} - T_{kr}}{l - \xi_{j}^{k}} = \frac{\lambda_{g}}{\delta_{g}} \left( T_{mj}^{k} - T_{N,j}^{k} \right) + \sigma_{m} \left[ (T_{mj}^{k})^{4} - (T_{N,j}^{k})^{4} \right]$$
(13)

and for  $\xi_j^k \leq l-q$ 

$$\lambda_{N,j}^{k} \frac{T_{N,j}^{k} - T_{N-1,j}^{k}}{q} = \frac{\lambda_{g}}{\delta_{g}} \left( T_{mj}^{k} - T_{N,j}^{k} \right) + \sigma_{m} \left[ (T_{mj}^{k})^{4} - (T_{N,j}^{k})^{4} \right]$$
(14)

After the calculation of the temperature in all boundary nodes and in all regular nodes the re-calculation of the phase-change boundary position follows.

# **2.3.** Re-calculation of the phase-change boundary position.

To recalculate the position of the phase-change boundary we use the finite-difference approximation of Stefan condition (3) on the uniform pattern (Fig.5)

$$\begin{split} \lambda \Biggl( \sqrt{\Biggl(\frac{U_2 - T_{kr}}{q}\Biggr)^2 + \Biggl(\frac{U_4 - T_{kr}}{h}\Biggr)^2} - \\ - \sqrt{\Biggl(\frac{U_1 - T_{kr}}{q}\Biggr)^2 + \Biggl(\frac{U_3 - T_{kr}}{h}\Biggr)^2} \Biggr) = (15) \\ = \mu \rho \Biggl(\frac{\xi_j^{k+1} - \xi_j^k}{\Delta t} + v_{k+1}\frac{\xi_j^{k+1} - \xi_{j-1}^{k+1}}{h}\Biggr). \end{split}$$

The temperature in  $\xi_j^{k+1}$  is equal  $T_{kr}$ . Therefore the temperature  $U_1$  in the special node x can be approximated by the Lagrange polynomial of 2nd degree:

$$U_{1} = T_{kr} \cdot \frac{(x - x_{i+1,j})(x - x_{i+2,j})}{(\xi_{j}^{k+1} - x_{i+1,j})(\xi_{j}^{k+1} - x_{i+2,j})} + T_{i+1,j} \cdot \frac{(x - \xi_{j}^{k+1})(x - x_{i+2,j})}{(x_{i+1,j} - \xi_{j}^{k+1})(x_{i+1,j} - x_{i+2,j})} + T_{i+2,j} \cdot \frac{(x - \xi_{j}^{k+1})(x - x_{i+1,j})}{(x_{i+2,j} - \xi_{j}^{k+1})(x_{i+2,j} - x_{i+1,j})}$$
(16)

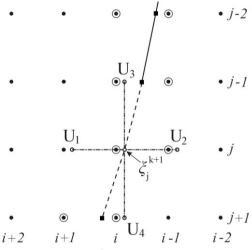
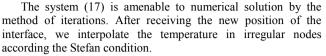


Fig. 5. Pattern for Stefan condition finite-difference approximation

Similarly we define the temperature  $U_2, U_3, U_4$  in the rest of the special nodes. After substitution these expressions in the finite-difference analog of the Stefan condition (15), we obtain the following system of nonlinear equations for the unknown boundary:

$$\begin{aligned} \xi_{j}^{k+1} &= \xi_{j}^{k} + \\ &+ \Delta t \Biggl\{ \frac{\lambda}{\mu \rho} \Biggl( \sqrt{\left(\frac{U_{2} - T_{kr}}{q}\right)^{2} + \left(\frac{U_{4} - T_{kr}}{h}\right)^{2}} - \\ &- \sqrt{\left(\frac{U_{1} - T_{kr}}{q}\right)^{2} + \left(\frac{U_{3} - T_{kr}}{h}\right)^{2}} \Biggr) - \nu \frac{\xi_{j}^{k+1} - \xi_{j-1}^{k+1}}{h} \Biggr\} \end{aligned}$$
(17)



There are also two singular cases: near the meniscus level and at the point of final solidification of the ingot. Behind the point of final solidification only the solid phase presents, and the coordinates of this point are the characteristic of the liquid phase depth (or in other words, it defines the metallurgical length). In these places there are not enough internal nodes in the solid or in the liquid phases. For re-calculation of the phase-change boundary position at these points we use special patterns. These patterns are similar to the base (see Fig.5). They are also uniform. But if we have not enough distance to place the base pattern we use smaller value instead of q in (15) - (17).

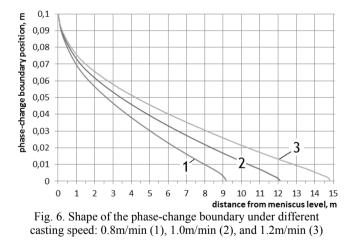
Before the start of calculations it is necessary to set the initial approximation of the phase-change boundary position and initial value of the temperature field.

# 3. Results of calculations

The numerical experiments were performed to the slab width equal to 0.2m and the steel of next chemical composition:

С	Si	Mn	Ni	S	Р	Cr	Cu
0.4	0.27	0.65	0.3	0.035	0.035	0.95	0.3

At the Fig.6 the results of calculation of the phase-change boundary position are presented. We can see that the casting speed has the greatest effect on the metallurgical length.



Additionally the model allows of the ingot temperature field estimation and prediction, to investigate the sensitivity of various operated parameters of the process to the changes of operating parameters, to make an operative estimation of the ingot thermal conditions, and to find the values of such control parameters that keep the cooling mode optimal for metal quality.

The mathematical model is able to adapt to the changing conditions of the casting process. The ways of identification of the distributed parameters of external heat exchange for initial and adaptive adjustment of convection heat transfer coefficient on the ingot surface are developed in [9].

### 4. Conclusions

The simple method of the phase-change boundary position determination is proposed. The method allows a several times higher than the real-time numerical calculations. Therefore the mathematical model can be successfully used in the circuit of the automatic control using MPC.

The method is developed under assuming that the interface between liquid and solid phases is a surface (a line in twodimensional case). Next step of research must be a development a method of calculation of phase-change boundary position for the cases when the mushy zone will be under consideration.

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