

## APPLICATION OF THE ENTHALPY APPROACH IN NUMERICAL MODELLING OF SOLIDIFICATION PROCESS

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**Abstract.** The numerical modelling of the Stefan problem using directly the typical description of the process is rather difficult. In this connection one can find in literature the models basing on the enthalpy convention and the artificial mushy zone introduction. This paper summarizes the state of the art of the enthalpy models of phase change problems. The part of the approaches discussed has been modified by the authors of the paper, we also present the new interpretations of some models.

### 1. The Stefan problem

We consider the solidification of pure metals. The typical feature of the process discussed is the constant temperature  $T^*$  of phase change. The transient temperature field in non-homogeneous domain of solidifying metal is described by the system of partial differential equations:

$$c_e \partial_t T_e(x, T) = \nabla [\lambda_e \nabla T_e(x, T)] \quad (1)$$

where  $e = 1, 2$  corresponds to the solid and liquid sub-domains,  $c_e$  [J/m<sup>3</sup> K] is the volumetric specific heat,  $\lambda_e$  [W/mK] is the thermal conductivity. On the moving boundary  $\Gamma_{12}$  between sub-domains we have the continuity condition in the form

$$\begin{cases} -\lambda_2 \partial_n T_2(x, T) = -\lambda_1 \partial_n T_1(x, T) + v_n L \\ T_2(x, T) = T_1(x, T) = T^* \end{cases} \quad (2)$$

called in literature the Stefan condition. Here  $\partial_n T$  is the normal derivative at the boundary point,  $v_n$  is the solidification rate in the normal direction,  $L$  [J/m<sup>3</sup>] is the volumetric latent heat. On the outer surface  $\Gamma_0$  of the system the boundary condition in general form

$$\Phi [T(x, T) = \partial_n T(x, T)] = 0 \quad (3)$$

is given. For time  $t = 0$  the initial distribution of temperature is known.

From the numerical point of view the model above model is not very convenient and in the next chapters the others approaches to the Stefan problem description will be presented.

## 2. Temperature recovery method

We introduce to the consideration the physical enthalpy of metal defined as follows

$$H(T) = \int_{T_r}^T c(\mu) d\mu + \eta(T)L \quad (4)$$

where for  $T > T^*$  :  $c(T) = c_2$  and for  $T < T^*$  :  $c(T) = c_1$ , while

$$\eta(T) = \begin{cases} 0 & T < T^* \\ 1 & T \geq T^* \end{cases} \quad (5)$$

The course of enthalpy function is shown in Figure 1.

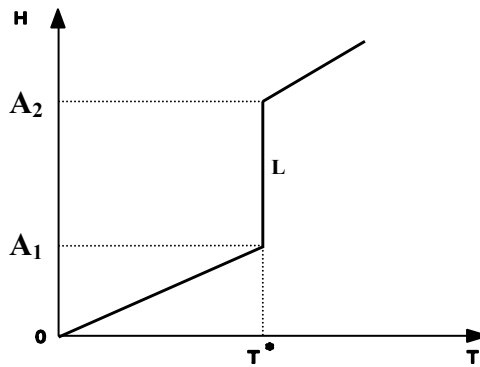


Fig. 1. Enthalpy-temperature function

Using the definition (4) one can transform the energy equations to the form

$$\partial_t H(x, T) = \nabla [\lambda \nabla T(x, T)] \quad (6)$$

It should be pointed out that for such mixed enthalpy-temperature convention the formulation of the Stefan condition is needless from the computational view point. If we use the typical numerical algorithm in which the domain is covered by the mesh (e.g. FDM, FEM, BEM, collocational methods), then if the enthalpy at the node considered  $x_i$ ,  $i = 1, 2, \dots, N$ , is from the range  $[A_1, A_2]$  then the temperature  $T(x_i, t)$  at this point equals  $T^*$ . This value is accepted until  $H(x_i, t) < A_1$ .

The idea of the temperature recovery method (TRM) is practically the same, but we consider only temperature formulation (it is more convenient on the stage of the numerical algorithm construction). So we introduce the quantity of local temperature reserve  $z_i$  defined as follows [1]

$$z_i = z(x_i, t) = \frac{L}{c_2} \quad (7)$$

Using the numerical methods we find the temperatures  $T_i^f$  at nodes  $X_i$  for successive times  $t^f, f = 0, 1, \dots, F$ . If at the moment  $t^f$  temperature  $T_i^f$  drops below  $T^*$  then we accept at this point the temperature  $T^*$ , while the temperature reserve is decreased, namely

$$z_i \rightarrow z_i - (T^* - T_i^f) \quad (8)$$

The same procedure is repeated in successive loops. If for the node  $x_i$   $z_i < 0$  we accept  $z_i = 0$  and next computations are realized without the temperature correction. The physical interpretation of TRM is the following (see Fig. 2).

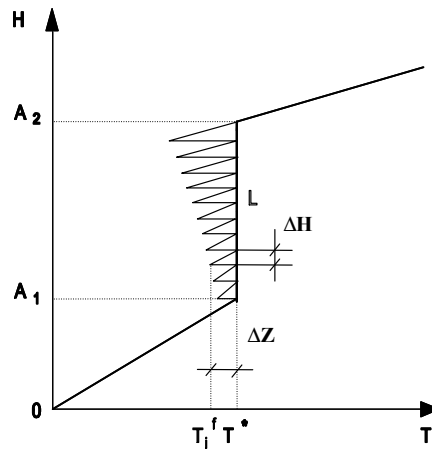


Fig. 2. Interpretation of TRM

The change of unitary enthalpy corresponding to the change of temperature from  $T^*$  to  $T_i^f$  found under the assumption that we consider the cooling of molten metal equals

$$\Delta H_i = c_2 (T^* - T_i^f) \quad (9)$$

This value we treat as the partial exhaustion of latent heat  $L$ , in particular

$$L \rightarrow L - (T^* - T_i^f) \quad (10)$$

Dividing the last formula by  $c_2$  we obtain

$$\frac{L}{c_2} \rightarrow \frac{L}{c_2} - (T^* - T_i^f) \quad (11)$$

The similar approach can be used in the case of solidification in the temperature interval [2-4].

### 3. Alternating phase truncation method

The first version of the method has been presented by Rogers, Berger and Ciment in [5, 6]. Next it was generalized by Majchrzak, Mochnacki and Kapusta [7, 8]. The essence of the method is the artificial homogenization of the domain considered. The computations concerning the transition from moment  $t$  to moment  $t + \Delta t$  are realized in two stages corresponding to the parameters of molten metal and solid state (we present the basic version of APTM concerning the Stefan problem). The mathematical description of the solidification process we formulate using the enthalpy convention. So, we consider the system of equations

$$\partial_t H_e(x, T) = \nabla [a_e \nabla H_e(x, T)] \quad (12)$$

where  $a_e$  is the diffusion coefficient. This system is supplemented by the boundary-initial conditions

$$\left. \begin{array}{l} x \in \Gamma_{1,2}(t): \quad \left\{ \begin{array}{l} -a_2 \partial_n H_2(x, T) = -a_1 \partial_n H_1(x, T) + Lv_n \\ A_2 = A_1 + L \end{array} \right. \\ x \in \Gamma_0: \quad \Phi[H, \partial_n H(x, T)] = 0 \\ t = 0: \quad H_e(x, 0) = H_{e0}(x), \quad e = 1, 2 \end{array} \right\} \quad (13)$$

The APTM algorithm for the transition from  $t = t^{f-1}$  to  $t + \Delta t = t^f$  is the following. Let us denote by  $H_i^{f-1}$  the discrete set of enthalpy values in the domain of metal at time  $t^{f-1}$ .

In the first stage of computation the domain considered is conventionally reduced to the liquid state. It corresponds to the assumption of the pseudo-initial condition in the form

$$V_1(x_i, t^{f-1}) = \max \{H_i^{f-1}, A_2\} \quad (14)$$

Next using the optional numerical method we find the solution for time  $t^f$ , this means  $V_1'(x_i, t^f)$  (the diffusion coefficient is assumed to be  $a = a_2$ ). Now we correct the obtained solution, namely

$$V_1(x_i, t^f) = V_1'(x_i, t^f) + H_i^{f-1} - V_1(x_i, t^{f-1}) \quad (15)$$

The second stage starts from the formulation of the new pseudo-initial condition for transition  $t^{f-1} \rightarrow t^f$

$$V_2(x_i, t^{f-1}) = \min \{A_1, V_1(x_i, t^f)\} \quad (16)$$

It corresponds to the conventional reduction of metal domain to the solid phase. We find the enthalpy field  $V_2'(X_i, t^f)$  (assuming  $a = a_1$ ) and we correct the result obtained using the formula

$$H_i^f = V_2'(x_i, t^f) + V_1(x_i, t^f) - V_2(x_i, t^{f-1}) \quad (17)$$

In Figures 3 and 4 the successive stages of computations are shown.

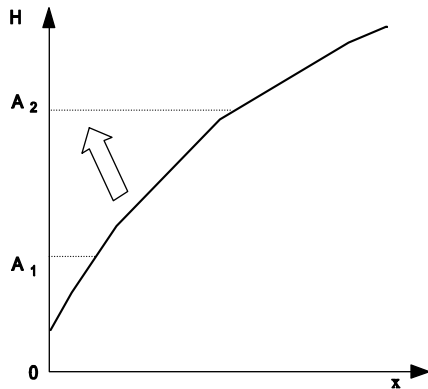


Fig. 3. Condition  $V_1(x_i, t^{f-1})$

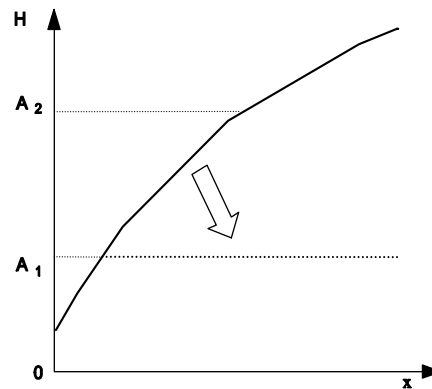


Fig. 4. Condition  $V_2(x_i, t^{f-1})$

The correctness of the algorithm discussed is proved in [6].

#### 4. The Hsiao method [9]

The method presented bases on the artificial mushy zone (AMZ) introduction. The solidification point is substituted by a temperature interval  $[T^- = T^* - \Delta T, T^+ = T^* + \Delta T]$ .

The real enthalpy-temperature diagram is transformed to the form shown in Figure 5. In this way one can define the substitute thermal capacity of AMZ sub-domain (the slope of the sector between  $T^* - \Delta T$  and  $T^* + \Delta T$ ).

So

$$T \in [T^-, T^+]: \quad c_{1,2} = \frac{L}{T^+ - T^-} = \frac{L}{2\Delta T} \quad (18)$$

If we assume the constant values of  $c_1$  and  $c_2$  then the thermal capacity of the metal is determined by the piece-wise function

$$c(T) = \begin{cases} c_2 & T > T^+ \\ c_{12} & T^- \leq T \leq T^+ \\ c_1 & T < T^- \end{cases} \quad (19)$$

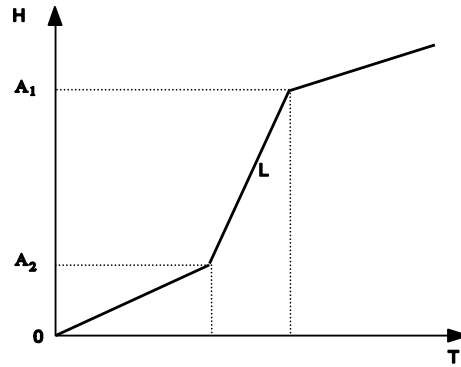


Fig. 5. Artificial mushy zone

The course of function  $c(T)$  is shown in Figure 6.

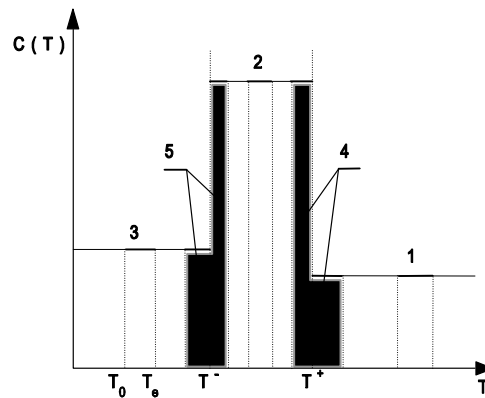


Fig. 6. Thermal capacity of metal

Let us denote by 0 and  $k$  two adjoining points resulting from the domain discretization (node 0 is a central point). We define the thermal capacity  $c_{0k}$  in the following way:

$$c_{0k} = \frac{1}{T_k - T_0} \int_{T_0}^{T_k} c(T) dT \quad (20)$$

and we obtain

$$\begin{aligned}
 T_0, T_k > T^+ : & \quad c_{0k} = c_2 \\
 T_0, T_k \in [T^-, T^+] : & \quad c_{0k} = c_{12} \\
 T_0, T_k < T^- : & \quad c_{0k} = c_1 \\
 T_0 \in [T^-, T^+], T_k > T^+ : & \quad c_{0k} = \frac{c_2(T_k - T^+) + c_{12}(T^+ - T_0)}{T_k - T_0} \quad (21) \\
 T_0 < T^-, T_k \in [T^-, T^+] : & \quad c_{0k} = \frac{c_{12}(T_k - T^-) + c_1(T^- - T_0)}{T_k - T_0} \\
 T_k > T^+, T_0 < T^- : & \quad c_{0k} = \frac{c_2(T_k - T^+) + c_{12}(T^+ - T^-) + c_1(T^- - T_0)}{T_k - T_0}
 \end{aligned}$$

The similar formulas can be found for the case  $T_k < T_0$ .

Let  $k = 1, 2, \dots, n$  denote indexes of the all adjoining nodes of node 0. Then we define the thermal capacity at the central node as

$$c_0 = \sum_{k=1}^n c_{0k} w_k \quad (22)$$

where

$$w_k = \frac{\rho_k}{\sum_{k=1}^n \rho_k} \quad (23)$$

at the same time  $\rho_k$  is the distance between points 0 and  $k$ . The numerical experiments done by Hsiao and also verified by the authors of above paper show that such approach gives quite good solution of the Stefan problem and the value of interval assumed  $[T^-, T^+]$  is not very essential.

In the version presented by Hsiao the numerical algorithm of solidification problem solution is rather complicated. In the paper [10] we present its modification and we show that the definition of  $c_{0k}$  results from the following considerations.

Because

$$\int_{T_0}^{T_k} c(T) dT = \int_0^{T_k} c(T) dT - \int_0^{T_0} c(T) dT \quad (24)$$

and next

$$\int_0^{T_k} c(T) dT - \int_0^{T_0} c(T) dT = H(T_k) - H(T_0) \quad (25)$$

Finally

$$c_{0k} = \frac{H(T_k) - H(T_0)}{T_k - T_0} \quad (26)$$

at the same time the relation  $T_e > T_0$  or  $T_e < T_0$  is here not essential. The interpretation of formula (26) is shown in Figure 7.

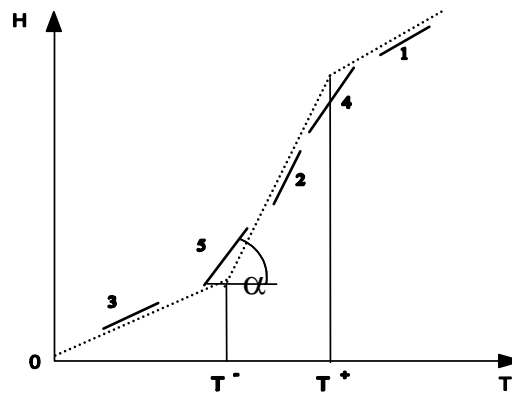


Fig. 7. Thermal capacity  $c_{0k}$

## 5. Application of the Kirchhoff function

The Kirchhoff function (Kirchhoff's transformation) linearizes the Laplace or Poisson equation in which the thermal conductivity is temperature-dependent. The Kirchhoff function is defined as follows

$$U(T) = \int_{T_r}^T \lambda(\mu) d\mu \quad (27)$$

where  $T_r$  is a reference level.

If we consider the Stefan problem using the artificial mushy zone approach then the energy equation in which the Kirchhoff function is introduced takes a form

$$\partial_t H(x, T) = \nabla[\nabla U(x, T)] \quad (28)$$



The functions  $H = H(T)$  and  $U = U(T)$  are monotonic ones and we can find the dependence  $H = \Psi(U)$ . Because

$$\frac{\partial H(x,t)}{\partial t} = \frac{dH(U)}{dU} \frac{\partial U(x,t)}{\partial t} = \Psi'(U) \frac{\partial U(x,t)}{\partial t} \quad (29)$$

therefore the energy equation can be written in the form

$$\Psi'(U) \frac{\partial U(x,t)}{\partial t} = \nabla[\nabla U(x, T)] \quad (30)$$

The function  $\Psi(U)$  and its derivative one can determine on the basis of the experimental data using the numerical methods. The knowledge of courses of the enthalpy  $H(T)$  and Kirchhoff's transformation  $U(T)$  allows to construct the function  $\Psi(U)$  - Fig. 8.

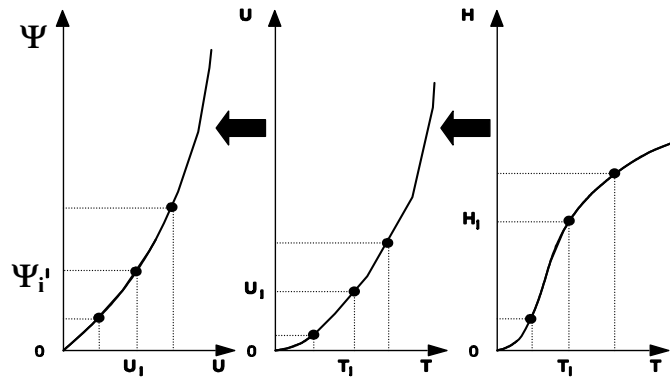


Fig. 8. Construction of  $\Psi(U)$

Such approach requires, of course, the formulation of the boundary and initial conditions using the Kirchhoff function [11].

## 6. The generalized Stefan problem

We will consider the metal for which the solidification process proceeds partially at the constant temperature and partially in the interval of temperatures. Such situation takes place, among others in the case of cast iron solidification (Fig. 9).

The example of the course of enthalpy function for generalized Stefan problem is shown in Figure 10.

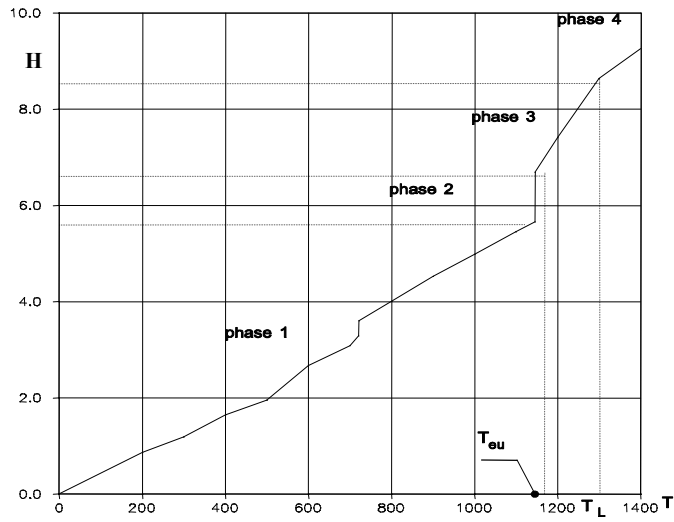


Fig. 9. Enthalpy diagram (cast iron CE = 3.95)

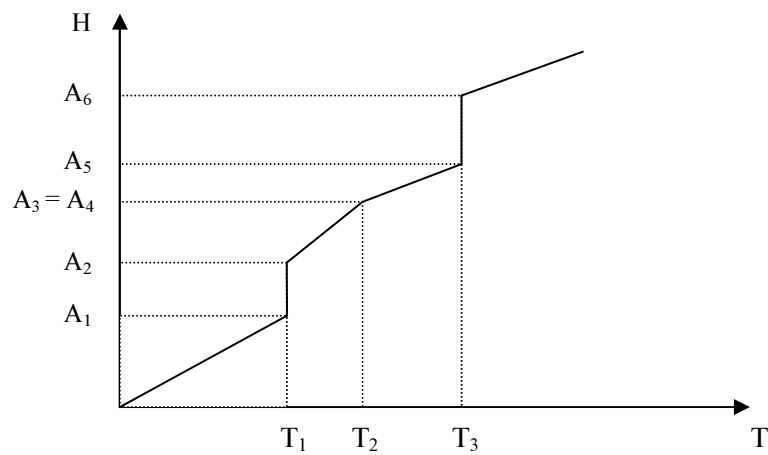


Fig. 10. Generalized course of enthalpy

In such case the function  $H(T)$  is determined by the formula

$$H(T) = \begin{cases} A_0 + c_1(T - T_0) & T < T_1 \\ A_2 + c_2(T - T_1) & T_1 \leq T < T_2 \\ \vdots & \\ A_{2n-2} + c_n(T - T_{n-1}) & T_{n-1} \leq T < T_n \end{cases} \quad (31)$$

We can find the inverse function, namely (see Fig. 11):

$$T(H) = \begin{cases} T_0 + \frac{H - A_0}{c_1} & H < A_1 \\ T_1 & A_1 \leq H < A_2 \\ T_1 + \frac{H - A_2}{c_2} & A_2 \leq H < A_3 \\ \vdots & \\ T_{n-1} & A_{2n-3} \leq H < A_{2n-2} \\ T_{n-1} + \frac{H - A_{2n-2}}{c_n} & A_{2n-2} \leq H < A_{2n-1} \end{cases} \quad (32)$$

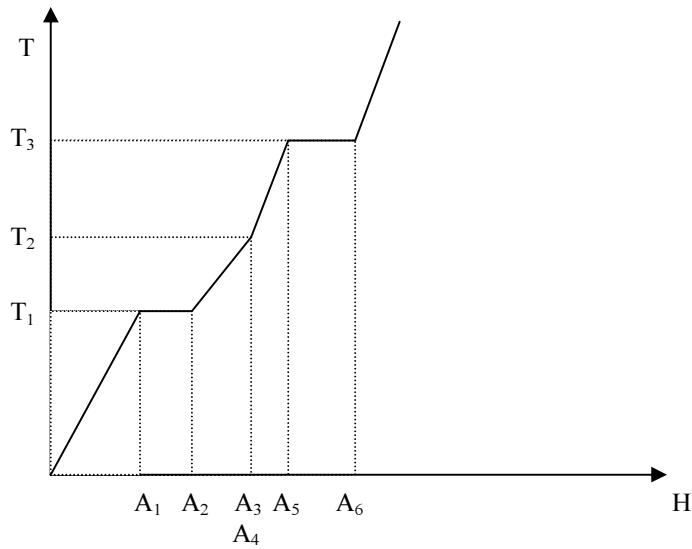


Fig. 11. The inverse function

Now we introduce the Kirchoff transformation defined as follows (Fig. 12)

$$U(T) = \begin{cases} B_0 + \lambda_1(T - T_0) & T < T_1 \\ B_1 + \lambda_2(T - T_1) & T_1 \leq T < T_2 \\ \vdots & \\ B_{n-1} + \lambda_n(T - T_{n-1}) & T_{n-1} \leq T < T_n \end{cases} \quad (33)$$

where:

$$\begin{aligned}
 B_0 &= 0 \\
 B_1 &= \lambda_1 T_1 = B_0 + \lambda_1 (T_1 - T_0) \\
 B_2 &= B_1 + \lambda_2 (T_2 - T_1) \\
 &\vdots \\
 B_{n-1} &= B_{n-2} + \lambda_{n-1} (T_{n-1} - T_{n-2})
 \end{aligned}
 \tag{34}$$

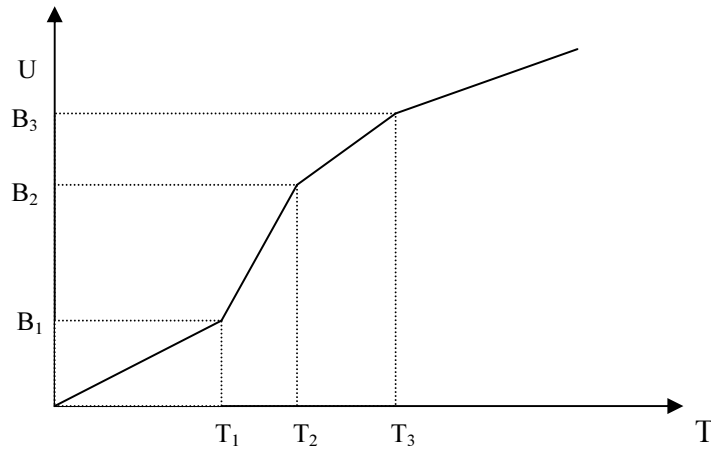


Fig. 12. The Kirchhoff function

Finally we can construct the dependence between  $U$  and  $H$  (Fig. 13) in the form

$$U(H) = \begin{cases} B_0 + a_1(H - A_0) & H < A_1 \\ B_1 & A_1 \leq H < A_2 \\ B_1 + a_2(H - A_2) & A_2 \leq H < A_3 \\ \vdots & \\ B_{n-1} & A_{2n-3} \leq H < A_{2n-2} \\ B_{n-1} + a_n(H - A_{2n-2}) & A_{2n-2} \leq H < A_{2n-1} \end{cases}
 \tag{35}$$

where

$$a_i = \frac{\lambda_i}{c_i} \quad i = 1, 2, \dots, n
 \tag{36}$$

The course of function  $U(H)$  corresponding to the previous figure shown in Figure 13. So, the energy equation written in the enthalpy convention is the following

$$\frac{\partial H(x,t)}{\partial t} = \text{div}\{\text{grad}[A(H)H + B(H)]\} \quad (37)$$

where:

$$A(H) = \begin{cases} a_1 \\ 0 \\ a_2 \\ \vdots \\ 0 \\ a_n \end{cases} \quad B(H) = \begin{cases} B_0 - a_1 A_0 \\ B_1 \\ B_1 - a_2 A_2 \\ \vdots \\ B_{n-1} \\ B_{n-1} - a_n A_{2n-2} \end{cases} \quad (38)$$

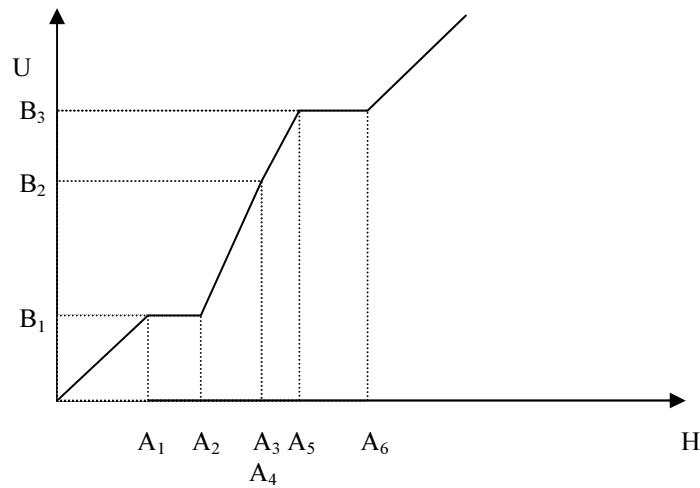


Fig. 13. The dependence between  $U$  and  $H$

Presented in this paper approach is very convenient for numerical simulation of solidification process both in the case of classical Stefan problem and also for the generalized one.

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