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Application of the dual reciprocity boundary element method for numerical modelling of solidification process

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Abstract

The dual reciprocity boundary element method is applied for numerical modelling of solidification process. This variant of the BEM is connected with the transformation of the domain integral to the boundary integrals. In the paper the details of the dual reciprocity boundary element method are presented and the usefulness of this approach to solidification process modelling is demonstrated. In the final part of the paper the examples of computations are shown.

Keywords: Application of information technology to the foundry industry, Solidification process, Numerical techniques, Dual reciprocity boundary element method

1. Introduction

The thermal processes proceeding in the casting domain are described by the energy equation (Fourier-Kirchhoff equation) and boundary initial conditions resulting from the technology considered [1, 2, 3]. In the case of solidification process modelling this energy equation is strongly non-linear because the evolution of latent heat has been taken into account (one domain approach). There are the several numerical methods which allow to solve the problem discussed. Most popular are finite difference method (FDM) [1, 4, 5] and finite element method (FEM) [1, 6, 7], but the boundary element method (BEM) [8, 9] is also applied. All of these methods require the discretization of boundary and interior of the casting domain.

During the past decade the meshless methods basing on the boundary element approach have been developed. One of them is the dual reciprocity boundary element method (DRBEM) [10]. In this variant of the BEM only the boundary is discretized, additionally the collocation points distinguished in the interior of the domain considered should be introduced.

In the paper the DRBEM is adapted to solve the solidification problem. The time stepping approach is applied and next the algorithm basing on the boundary integral equation for Poisson one written for transition $t^{f-1} \rightarrow t^{f}$ is used. The source function corresponds to the time derivative multiplied by substitute thermal capacity corresponding to the moment t^f. Next, the domain integral is transformed to the boundary integrals. In this way the discretization of the interior of the domain is needless.

In the paper the mathematical model of solidification process is presented, the DRBEM algorithm is discussed and finally the results of computations are shown.

2. Governing equations

A transient temperature field in a casting domain is described by the following equation

$$x \in \Omega: \quad C(T)\frac{\partial T(x,\,t)}{\partial t} = \lambda \nabla^2 T(x,\,t) \tag{1}$$

where λ is the thermal conductivity, $C(T)$ is the substitute thermal capacity [1], $T = T(x, t)$, $x = (x_1, x_2)$, t denote temperature, spatial co-ordinates and time, respectively.

The substitute thermal capacity for cast steel can be defined as follows [11] – Figure 1

$$C(T) = \begin{cases} c_L, & T > T_L \\ c_1 + c_2 T + c_3 T^2 + c_4 T^3 + c_5 T^4, & T_S \le T \le T_L \\ c_S, & T < T_S \end{cases} \tag{2}$$

where the temperatures T_L, T_S correspond to the beginning and the end of the solidification process, respectively, c_L, c_S are the constant volumetric specific heats of liquid and solid state. The coefficients c_e, $e = 1, 2, ..., 5$ have been found on the basis of conditions assuring the continuity of C^1 class and physical correctness of approximation [11].

The equation (1) is supplemented by adequate boundary and initial condition resulting from the technology considered.

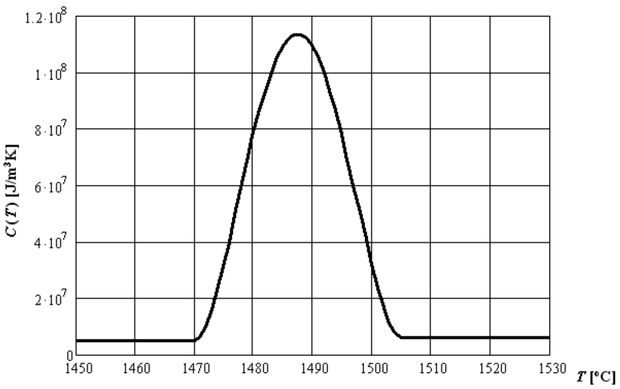


Fig. 1. Substitute thermal capacity

3. Dual reciprocity boundary element method

To solve the equation (1) the dual reciprocity boundary element method has been used. So, the time grid is introduced

$$0 = t^0 < t^1 < ... < t^{f-1} < t^f < ... < t^F \tag{3}$$

with constant time step $\Delta t = t^f - t^{f-1}$.

The equation (1) should be written for time $t = t^f$

$$\lambda \nabla^2 T(x,\,t^f) - \left[C(T)\frac{\partial T(x,\,t)}{\partial t} \right]_{t=t^f} = 0 \tag{4}$$

The standard boundary element method algorithm leads to the following integral equation [9, 12]

$$B(\xi)\,T(\xi,\,t^f) + \int_\Gamma T^*(\xi,\,x)\,q(x,\,t^f)\,\mathrm{d}\Gamma = \int_\Gamma q^*(\xi,\,x)\,T(x,\,t^f)\,\mathrm{d}\Gamma - \int_\Omega \left[C(T)\frac{\partial T(x,t)}{\partial t} \right]_{t=t^f} T^*(\xi,\,x)\mathrm{d}\Omega \tag{5}$$

where ξ is the observation point, $B(\xi) \in (0,\ 1]$, $T^*(\xi,\ x)$ is the fundamental solution, $q(x, t^f) = -\lambda\, \partial T(x, t^f)/\partial n$ is the heat flux, $q^*(\xi, x) = -\lambda\, \partial T^*(\xi, x)/\partial n$ is the heat flux resulting from the fundamental solution, Γ is the boundary of domain Ω.
Fundamental solution has the following form

$$T^*(\xi,\,x) = \frac{1}{2\pi\lambda}\ln\frac{1}{r} \tag{6}$$

where r is the distance between the points ξ and x. Heat flux resulting from the fundamental solution can be calculated analytically, namely

$$q^*(\xi,\ x) = \frac{d}{2\pi r^2} \tag{7}$$

where

$$d = (x_1 - \xi_1)\cos\alpha_1 + (x_2 - \xi_2)\cos\alpha_2 \tag{8}$$

while $\cos\alpha_1$, $\cos\alpha_2$ are the directional cosines of the boundary normal vector n.

It should be pointed out that the function $T^*(\xi,\ x)$ fulfills the equation

$$\lambda \nabla^2 T^*(\xi,\,x) = -\delta(\xi,\,x) \tag{9}$$

where $\delta(\xi, x)$ is the Dirac function.

In the dual reciprocity method the following approximation is proposed [10]

$$\left[C(T)\frac{\partial T(x,\,t)}{\partial t} \right]_{t=t^f} = \sum_{k=1}^{N+L} a_k(t^f)\,P_k(x) \tag{10}$$

where $a_k(t^f)$ are unknown coefficients, $P_k(x)$ are approximating functions fulfilling the equations

$$P_k(x) = \lambda \nabla^2 U_k(x) \tag{11}$$

In equation (10) $N + L$ corresponds to the total number of nodes, where N is the number of boundary nodes and L is the number of internal nodes.

Putting (11) into (10) one has

$$\left[C(T)\frac{\partial T(x,\,t)}{\partial t}\right]_{t=t^f}=\sum_{k=1}^{N+L}\lambda\,a_k(t^{\,f})\nabla^2 U_k(x) \tag{12}$$

and then the last integral in equation (5) takes a form

$$D=-\int_\Omega \left[C(T)\frac{\partial T(x,\,t)}{\partial t}\right]_{t=t^{\,f}} T^*(\xi,\,x)\;\mathrm{d}\Omega=$$
$$-\int_\Omega \sum_{k=1}^{N+L}\lambda\,a_k(t^{\,f})\nabla^2 U_k(x)T^*(\xi,\,x)\;\mathrm{d}\Omega \tag{13}$$

Using the second Green formula [9, 12] one has

$$D=-\sum_{k=1}^{N+L}a_k(t^f)\int_\Omega \left[\lambda\nabla^2 T^*(\xi,\,x)\right]U_k(x)\;\mathrm{d}\Omega-$$
$$\sum_{k=1}^{N+L}\lambda\,a_k(t^f)\int_\Gamma \left[T^*(\xi,\,x)\frac{\partial U_k(x)}{\partial n}-U_k(x)\frac{\partial T^*(\xi,\,x)}{\partial n}\right]\mathrm{d}\Gamma \tag{14}$$

Because (c. f. formula (9))

$$\int_\Omega \left[\lambda\nabla^2 T^*(\xi,\,x)\right]U_k(x)\;\mathrm{d}\Omega=$$
$$-\iint_\Omega \delta(\xi,\,x)U_k(x)\;\mathrm{d}\Omega=-B(\xi)U_k(\xi) \tag{15}$$

therefore

$$D=\sum_{k=1}^{N+L}a_k(t^{\,f})\,B(\xi)U_k(\xi)+$$
$$\sum_{k=1}^{N+L}a_k(t^{\,f})\int_\Gamma \left[T^*(\xi,\,x)W_k(x)-U_k(x)\,q^*(\xi,\,x)\right]\mathrm{d}\Gamma \tag{16}$$

where

$$W_k(x)=-\lambda\frac{\partial U_k(x)}{\partial n} \tag{17}$$

Taking into account the formula (16) the equation (5) can be written in the form

$$B(\xi)\;T(\xi,\,t^{\,f})+\int_\Gamma T^*(\xi,\,x)\;q(x,\,t^{\,f})\;\mathrm{d}\Gamma=$$
$$\int_\Gamma q^*(\xi,\,x)\;T(x,\,t^{\,f})\;\mathrm{d}\Gamma+\sum_{k=1}^{N+L}a_k(t^{\,f})\Big[B(\xi)\;U_k(\xi)+$$
$$\int_\Gamma T^*(\xi,\,x)\;W_k(x)\;\mathrm{d}\Gamma-\int_\Gamma q^*(\xi,\,x)\;U_k(x)\;\mathrm{d}\Gamma\Big] \tag{18}$$

In this way one obtains the integral equation in which only the boundary integrals appear. It should be pointed out that this equation can be successfully solved under the assumption that the functions $U_k(x)$ are known.

4. Numerical realisation

To solve the equation (18), the boundary Γ is divided into N boundary elements and in the interior of the domain L internal nodes are distinguished. In the case of constant boundary elements it is assumed that

$$x\in\Gamma_j:\quad \begin{cases} T(x,\,t^{\,f})=T(x_j,\,t^{\,f})=T_j^f \\ q(x,\,t^{\,f})=q(x_j,\,t^{\,f})=q_j^f \end{cases} \tag{19}$$

and

$$x\in\Gamma_j:\quad \begin{cases} U_k(x)=U_k(x_j)=U_{jk} \\ W_k(x)=W_k(x_j)=W_{jk} \end{cases} \tag{20}$$

So the following approximation of equation (18) can be taken into account (i = 1, 2, …, N, N + 1, …, N + L)

$$B_iT_i^{\,f}+\sum_{j=1}^{N}q_j^f\int_{\Gamma_j}T^*(\xi_i,\,x)\;\mathrm{d}\Gamma_j=\sum_{j=1}^{N}T_j^f\int_{\Gamma_j}q^*(\xi_i,\,x)\;\mathrm{d}\Gamma_j+$$
$$\sum_{k=1}^{N+L}a_k^f\left[B_i\,U_{ik}+\sum_{j=1}^{N}W_{jk}\int_{\Gamma_j}T^*(\xi_i,\,x)\;\mathrm{d}\Gamma_j-\right.$$
$$\left.\sum_{j=1}^{N}U_{jk}\int_{\Gamma_j}q^*(\xi_i,\,x)\;\mathrm{d}\Gamma_j\right] \tag{21}$$

or

$$\sum_{j=1}^{N}G_{ij}\,q_j^f=\sum_{j=1}^{N}H_{ij}T_j^f+$$
$$\sum_{k=1}^{N+L}a_k^f\left(\sum_{j=1}^{N}G_{ij}W_{jk}-\sum_{j=1}^{N}H_{ij}U_{jk}\right) \tag{22}$$

where

$$G_{ij}=\int_{\Gamma_j}T^*(\xi_i,\,x)\;\mathrm{d}\Gamma_j \tag{23}$$

and

$$H_{ij} = \begin{cases} \int_{\Gamma_j} q^*(\xi_i, x)\, d\Gamma_j, & i \neq j \\ \int_{\Gamma_j} q^*(\xi_i, x)\, d\Gamma_j - B_i & i = j \end{cases} \tag{24}$$

while $B_i = B(\xi_i)$.

The following matrices of dimensions $N + L \times N + L$ can be defined

$$\mathbf{G} = \begin{bmatrix} G_{11} & G_{12} & \cdots & G_{1N} & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ G_{N,1} & G_{N,2} & \cdots & G_{N,N} & 0 & \cdots & 0 \\ G_{N+1,1} & G_{N+1,2} & \cdots & G_{N+1,N} & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ G_{N+L,1} & G_{N+L,2} & \cdots & G_{N+L,N} & 0 & \cdots & 0 \end{bmatrix} \tag{25}$$

$$\mathbf{H} = \begin{bmatrix} H_{11} & H_{12} & \cdots & H_{1N} & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ H_{N,1} & H_{N,2} & \cdots & H_{N,N} & 0 & \cdots & 0 \\ H_{N+1,1} & H_{N+1,2} & \cdots & H_{N+1,N} & -1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ H_{N+L,1} & H_{N+L,2} & \cdots & H_{N+L,N} & 0 & \cdots & -1 \end{bmatrix} \tag{26}$$

and

$$\mathbf{U} = \begin{bmatrix} U_{11} & U_{12} & \cdots & U_{1N} & U_{1,N+1} & \cdots & U_{1,N+L} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ U_{N,1} & U_{N,2} & \cdots & U_{N,N} & U_{N,N+1} & \cdots & U_{N,N+L} \\ U_{N+1,1} & U_{N+1,2} & \cdots & U_{N+1,N} & U_{N+1,N+1} & \cdots & U_{N+1,N+L} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ U_{N+L,1} & U_{N+L,2} & \cdots & U_{N+L,N} & U_{N+L,N+1} & \cdots & U_{N+L,N+L} \end{bmatrix} \tag{27}$$

$$\mathbf{W} = \begin{bmatrix} W_{11} & W_{12} & \cdots & W_{1N} & W_{1,N+1} & \cdots & W_{1,N+L} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ W_{N,1} & W_{N,2} & \cdots & W_{N,N} & W_{N,N+1} & \cdots & W_{N,N+L} \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \end{bmatrix} \tag{28}$$

So, the system of equations (22) can be written in the matrix form

$$\mathbf{G}\,\mathbf{q}^f = \mathbf{H}\,\mathbf{T}^f + (\mathbf{G}\,\mathbf{W} - \mathbf{H}\,\mathbf{U})\mathbf{a}^f \tag{29}$$

where

$$\mathbf{T}^f = \begin{bmatrix} T_1^f \\ \cdots \\ T_N^f \\ T_{N+1}^f \\ \cdots \\ T_{N+L}^f \end{bmatrix}, \quad \mathbf{q}^f = \begin{bmatrix} q_1^f \\ \cdots \\ q_N^f \\ 0 \\ \cdots \\ 0 \end{bmatrix} \tag{30}$$

We define [10, 13, 14]

$$U_{jk} = \frac{r_{jk}^2}{4} + \frac{r_{jk}^3}{9} \tag{31}$$

where (Figure 2)

$$r_{jk}^2 = (x_{1k} - x_{1j})^2 + (x_{2k} - x_{2j})^2 \tag{32}$$

Using the formula (17) one obtains

$$W_{jk} = -\lambda \left[\cos\alpha_{1j} \;\; \cos\alpha_{2j}\right] \begin{bmatrix} \dfrac{\partial U_{jk}}{\partial x_{1j}} \\ \dfrac{\partial U_{jk}}{\partial x_{2j}} \end{bmatrix} = \lambda\, d_{jk} \left(\frac{1}{2} + \frac{1}{3} r_{jk}\right) \tag{33}$$

where

$$d_{jk} = (x_{1k} - x_{1j})\cos\alpha_{1j} + (x_{2k} - x_{2j})\cos\alpha_{2j} \tag{34}$$

Because

$$\nabla^2 U_{sk} = \frac{\partial^2 U_{sk}}{\partial x_{1k}^2} + \frac{\partial^2 U_{sk}}{\partial x_{2k}^2} = 1 + r_{sk} \tag{35}$$

so on the basis of equation (11) one has

$$P_{sk} = P_k(x_s) = \lambda(1 + r_{sk}) \tag{36}$$

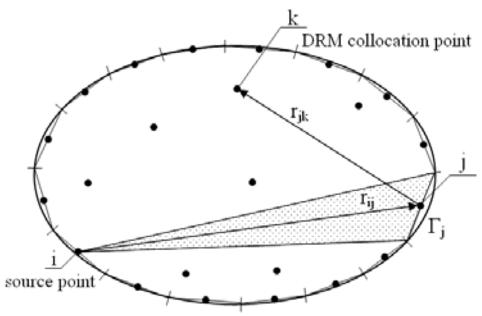


Fig. 2. Illustration of r_{ij} and r_{jk}

A time derivative is approximated as follows

$$\left[C(T)\frac{\partial T(x,\,t)}{\partial t}\right]_{t=t^f} = C(T^{\,f-1})\,\frac{T(x,\,t^f)-T(x,\,t^{f-1})}{\Delta t} \tag{37}$$

and then the equation (12) takes a form

$$C(T_s^{\,f-1})\,\frac{T_s^{\,f}-T_s^{\,f-1}}{\Delta t} = \sum_{k=1}^{N+L} a_k^f\,P_{s\,k} \tag{38}$$

or

$$\frac{T_s^{\,f}-T_s^{\,f-1}}{\Delta t} = \sum_{k=1}^{N+L} a_k^f\,\frac{P_{s\,k}}{C(T_s^{\,f-1})} \tag{39}$$

where $s = 1, 2, \ldots, N, N+1, \ldots, N+L$

The system of equations (39) can be written in the matrix form

$$\frac{1}{\Delta t}\begin{bmatrix} T_1^{\,f}-T_1^{\,f-1} \\ \ldots \\ T_N^{\,f}-T_N^{\,f-1} \\ T_{N+1}^{\,f}-T_{N+1}^{\,f-1} \\ \ldots \\ T_{N+L}^{\,f}-T_{N+L}^{\,f-1} \end{bmatrix} =$$

$$\begin{bmatrix} \dfrac{P_{1,1}}{C(T_1^{\,f-1})} & \dfrac{P_{1,2}}{C(T_1^{\,f-1})} & \ldots & \dfrac{P_{1,N+L}}{C(T_1^{\,f-1})} \\ \ldots & \ldots & \ldots & \ldots \\ \dfrac{P_{N,1}}{C(T_N^{\,f-1})} & \dfrac{P_{N,2}}{C(T_N^{\,f-1})} & \ldots & \dfrac{P_{N,N+L}}{C(T_N^{\,f-1})} \\ \dfrac{P_{N+1,1}}{C(T_{N+1}^{\,f-1})} & \dfrac{P_{N+1,2}}{C(T_{N+1}^{\,f-1})} & \ldots & \dfrac{P_{N+1,N+L}}{C(T_{N+1}^{\,f-1})} \\ \ldots & \ldots & \ldots & \ldots \\ \dfrac{P_{N+L,1}}{C(T_{N+L}^{\,f-1})} & \dfrac{P_{N+L,2}}{C(T_{N+L}^{\,f-1})} & \ldots & \dfrac{P_{N+L,N+L}}{C(T_{N+L}^{\,f-1})} \end{bmatrix} \begin{bmatrix} a_1^f \\ \ldots \\ a_N^f \\ a_{N+1}^f \\ \ldots \\ a_{N+L}^f \end{bmatrix} \tag{40}$$

or

$$\frac{1}{\Delta t}\left(\mathbf{T}^{f}-\mathbf{T}^{f-1}\right) = \mathbf{Z}^{f-1}\mathbf{a}^{f} \tag{41}$$

From (41) results that

$$\mathbf{a}^{f} = \frac{1}{\Delta t}(\mathbf{Z}^{f-1})^{-1}\left(\mathbf{T}^{f}-\mathbf{T}^{f-1}\right) \tag{42}$$

Putting (41) into (29) one obtains

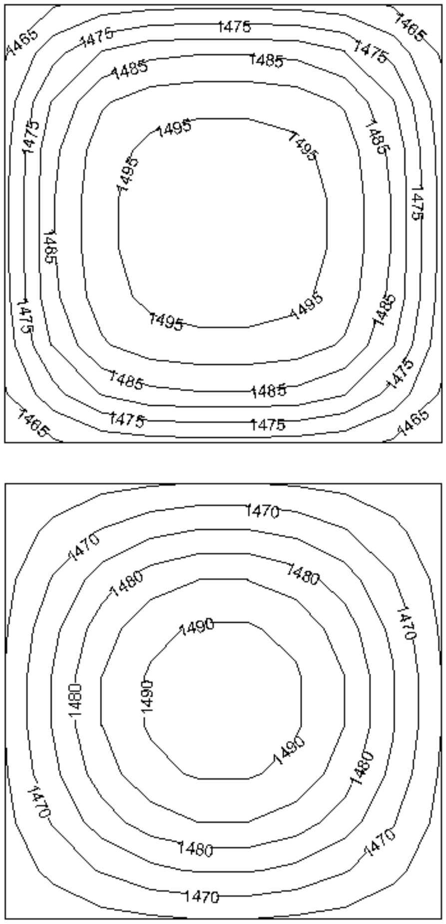
$$\mathbf{G}\,\mathbf{q}^{f} = \mathbf{H}\mathbf{T}^{f} + \frac{1}{\Delta t}(\mathbf{G}\mathbf{W}-\mathbf{H}\mathbf{U})\left(\mathbf{Z}^{f-1}\right)^{-1}\left(\mathbf{T}^{f}-\mathbf{T}^{f-1}\right) \tag{43}$$

This system of equations allows to determine the temperatures at the boundary and internal nodes.

5. Example of computations

The casting domain of dimensions 0.04 m × 0.04 m has been considered. On the casting boundary the Dirichlet condition $T(x_1, x_2) = 1460\ ^{\mathrm{o}}\mathrm{C}$ has been assumed, the pouring temperature equals $T_0 = 1550\ ^{\mathrm{o}}\mathrm{C}$. The following input data have been introduced: thermal conductivity $\lambda = 35$ W/(mK), liquidus temperature $T_L = 1505\ ^{0}\mathrm{C}$, solidus temperature $T_S = 1470\ ^{\mathrm{o}}\mathrm{C}$. The coefficients c_e, $e = 1, 2, \ldots, 5$ appearing in the substitute thermal capacity definition (c. f. equation (2)) are taken from [11].

The boundary is divided into $N = 40$ constant boundary elements, in the interior of the domain $L = 100$ internal points have been distinguished, time step: $\Delta t = 2$ s. In Figure 3 the temperature distribution for times 60, 120 and 180 s is shown.



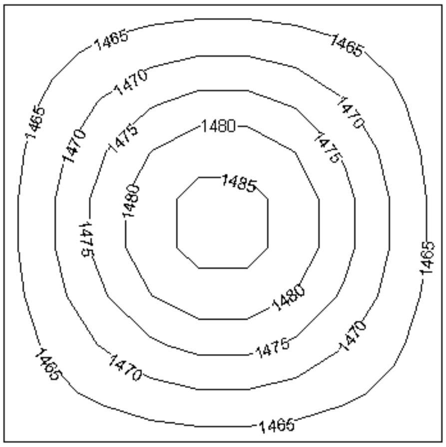


Fig. 3. Temperature distribution (60, 120, 180 s)

Figure 4 illustrates the course of cooling curves at the points 1 (0.002, 0.002), 2 (0.006, 0.006), 3 (0.01, 0.01), 4 (0.014, 0.014) and 5 (0.018, 0.018).

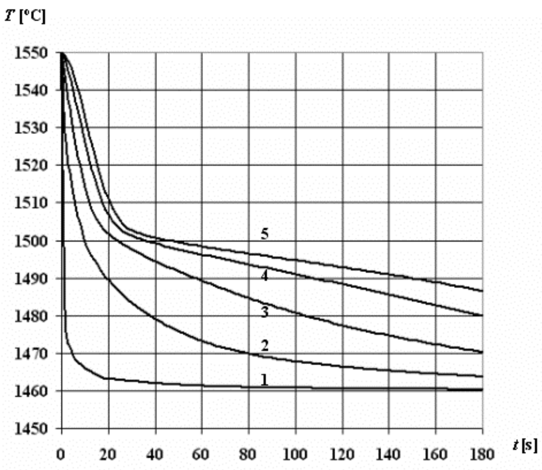


Fig. 4. Cooling curves

6. Conclusions

The dual reciprocity method has been applied to solve the solidification problem. This method requires only the discretization of the boundary of the domain considered. In future the algorithm presented should be extended on the numerical modelling of the heat transfer processes proceeding in the system casting-mould-environment.

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