SOLUTION OF ENERGY EQUATION USING THE INTERVAL BOUNDARY ELEMENT METHOD

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Abstract. In the paper the 1D energy equation with an interval source function is considered. For this type of equation the 1st scheme of the interval boundary element method is presented. As an example the pure metal crystallization process is analyzed. In the final part of the paper the results of numerical computations for the cooper crystallization process with the interval source function are shown.

1. Interval boundary element method

Transient temperature field in 1D domain describes the following energy equation

$$x \in (0,\, L): \qquad c\frac{\partial T(x,t)}{\partial t} = \lambda \nabla^2 T(x,t) + \tilde{Q}(x,t) \tag{1}$$

where c is the volumetric specific heat, λ is the thermal conductivity, $\tilde{Q}(x,t)$ is the interval source function [1], T, x, t denote temperature, spatial co-ordinate and time, respectively.

The above equation must be supplemented by the following boundary-initial conditions

$$\begin{cases} x = 0: & F_1\left[T(x,\,t),\, \dfrac{\partial T(x,\,t)}{\partial x}\right] = 0 \\ x = L: & F_2\left[T(x,\,t),\, \dfrac{\partial T(x,\,t)}{\partial x}\right] = 0 \\ t = 0: & T(x,\,t) = T_0(x) \end{cases} \tag{2}$$

The 1st scheme of the boundary element method has been applied to solve the problem analyzed [2-5].

At first the time grid is introduced

$$0 = t^0 < t^1 < t^2 < \ldots < t^{f-1} < t^f < \ldots < t^F < \infty \tag{3}$$

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

The boundary interval integral equation corresponding to the transition $t^{f-1} \to t^f$ is of the form

$$\begin{aligned} &\tilde{T}(\xi, t^f) + \left[\frac{1}{c} \int_{t^{f-1}}^{t^f} T^*(\xi, x, t^f, t)\, \tilde{q}(x, t)\, \mathrm{d}t \right]_{x=0}^{x=L} = \\ &\left[\frac{1}{c} \int_{t^{f-1}}^{t^f} q^*(\xi, x, t^f, t) \tilde{T}(x, t)\, \mathrm{d}t \right]_{x=0}^{x=L} + \int_0^L T^*(\xi, x, t^f, t^{f-1}) \tilde{T}(x, t^{f-1})\, \mathrm{d}x + \\ &\frac{1}{c} \int_{t^{f-1}}^{t^f} \int_0^L \tilde{Q}(x, t) T^*(\xi, x, t^f, t)\, \mathrm{d}x\, \mathrm{d}t \end{aligned} \tag{4}$$

where ξ is the point where the concentrated heat source is applied, $T^*(\xi, x, t^f, t)$ is the fundamental solution, $q^*(\xi, x, t^f, t)$ is the heat flux corresponding to the fundamental solution, $\tilde{q}(x, t) = -\lambda\, \partial \tilde{T}(x, t) / \partial x$ is the interval boundary heat flux, $\tilde{T}(x, t)$ is the interval temperature value.

In the case of using the constant elements with respect to time the equation (4) can be written as

$$\begin{aligned} &\tilde{T}(\xi, t^f) + \left[\frac{1}{c} \tilde{q}(x, t^f) \int_{t^{f-1}}^{t^f} T^*(\xi, x, t^f, t)\, \mathrm{d}t \right]_{x=0}^{x=L} = \\ &\left[\frac{1}{c} \tilde{T}(x, t^f) \int_{t^{f-1}}^{t^f} q^*(\xi, x, t^f, t)\, \mathrm{d}t \right]_{x=0}^{x=L} + \int_0^L T^*(\xi, x, t^f, t^{f-1}) \tilde{T}(x, t^{f-1})\, \mathrm{d}x + \\ &\frac{1}{c} \int_0^L \tilde{Q}(x, t^{f-1}) \left[\int_{t^{f-1}}^{t^f} T^*(\xi, x, t^f, t)\, \mathrm{d}t \right] \mathrm{d}x \end{aligned} \tag{5}$$

The numerical approximation of this equation leads to the following interval equation

$$\begin{aligned} &\tilde{T}(\xi, t^f) + \left[g(\xi, x)\, \tilde{q}(x, t^f) \right]_{x=0}^{x=L} = \left[h(\xi, x) \tilde{T}(x, t^f) \right]_{x=0}^{x=L} + \\ &\tilde{P}(\xi, t^{f-1}) + \tilde{Z}(\xi, t^{f-1}) \end{aligned} \tag{6}$$

where

$$g(\xi, x) = \frac{1}{c}\int_{t^{f-1}}^{t^f} T^*(\xi, x, t^f, t)\,\mathrm{d}t = \frac{\sqrt{\Delta t}}{\sqrt{\lambda c}}\exp\left[-\frac{(x-\xi)^2}{4\sqrt{a(t^f - t)}}\right] - \frac{|x-\xi|}{2\lambda}\operatorname{erfc}\left(\frac{|x-\xi|}{2\sqrt{a\Delta t}}\right) \tag{7}$$

and

$$h(\xi, x) = \frac{1}{c}\int_{t^{f-1}}^{t^f} q^*(\xi, x, t^f, t)\,\mathrm{d}t = \frac{\operatorname{sgn}(x-\xi)}{2}\operatorname{erfc}\left(\frac{|x-\xi|}{2\sqrt{a\Delta t}}\right) \tag{8}$$

while $a = \lambda / c$ is the diffusion coefficient.
The interval values $\tilde{P}(\xi, t^{f-1})$ are defined as

$$\tilde{P}(\xi, t^{f-1}) = \int_0^L T^*(\xi, x, t^f, t^{f-1})\tilde{T}(x, t^{f-1})\,\mathrm{d}x = \frac{1}{2\sqrt{\pi a\Delta t}}\int_0^L \exp\left[-\frac{(x-\xi)^2}{4a\Delta t}\right]\tilde{T}(x, t^{f-1})\,\mathrm{d}x \tag{9}$$

and the interval values connected with the interval source function take the form

$$\tilde{Z}(x, t^{f-1}) = \frac{1}{c}\int_0^L \tilde{Q}(x, t^{f-1})\left[\int_{t^{f-1}}^{t^f} T^*(\xi, x, t^f, t)\,\mathrm{d}t\right]\mathrm{d}x = \int_0^L \tilde{Q}(x, t^{f-1})\, g(\xi, x)\,\mathrm{d}x \tag{10}$$

Taking into account the boundary conditions (2) the following system of interval equations is obtained

$$\begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix}\begin{bmatrix} \tilde{q}(0,\ t^f) \\ \tilde{q}(L,\ t^f) \end{bmatrix} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}\begin{bmatrix} \tilde{T}(0, t^f) \\ \tilde{T}(L, t^f) \end{bmatrix} + \begin{bmatrix} \tilde{P}(0, t^{f-1}) \\ \tilde{P}(L, t^{f-1}) \end{bmatrix} + \begin{bmatrix} \tilde{Z}(0, t^{f-1}) \\ \tilde{Z}(L, t^{f-1}) \end{bmatrix} \tag{11}$$

where

$$G_{11} = -g(0, 0) \qquad G_{12} = g(0, L)$$
$$G_{21} = -g(L, 0) \qquad G_{22} = -g(L, L) \tag{12}$$

and

$$\begin{aligned} H_{11} &= -0.5 & H_{12} &= h(0, L) \\ H_{21} &= -h(L, 0) & H_{22} &= -0.5 \end{aligned} \tag{13}$$

After determining the 'missing' boundary values the interval temperatures $\tilde{T}(\xi, t^f)$ at internal nodes of the domain considered are calculated using the formula

$$\begin{aligned} \tilde{T}(\xi, t^f) = h(\xi, L)\tilde{T}(L, t^f) - h(\xi, 0)\tilde{T}(0, t^f) - \\ g(\xi, L)\tilde{q}(L, t^f) + g(\xi, 0)\tilde{q}(0, t^f) + \tilde{P}(\xi, t^{f-1}) + \tilde{Z}(\xi, t^{f-1}) \end{aligned} \tag{14}$$

2. Interval source function

The solidification process in one-dimensional domain of pure metal is presented as an example of the interval source function appearing in the mathematical description. It is assumed that the nucleation coefficient and nuclei growth one are interval values and the both coefficients are proportional to the second power of undercooling. The driving force of crystallization is the local and temporary undercooling below solidification point T_{cr}. The nucleation and nuclei growth are proportional to the second power of undercooling [6, 7].

The interval source function can be defined using the following formula

$$\tilde{Q}(x, t) = Q_{cr} \frac{\partial \tilde{S}(x, t)}{\partial t} \tag{15}$$

where Q_{cr} is the volumetric latent heat, $\tilde{S}(x, t)$ is the interval volumetric fraction of the solid state at the neighborhood of the point considered x.

In this paper the exponential solidification model proposed by Mehl-Johnson-Avrami-Kolmogoroff is applied

$$S(x, t) = 1 - \exp\left[-\omega(x, t)\right] \tag{16}$$

or

$$\tilde{S}(x, t) = 1 - \exp\left[-\frac{4}{3}\pi \tilde{N}(x, t)\tilde{R}(x, t)^3\right] \tag{17}$$

where $\tilde{N}(x, t)$ is the interval grain density [grains/m^3], $\tilde{R}(x, t)$ is the interval value of the temporary radius of single grain.

The interval calculations of the source function connected with the crystallization process modelling require to take into account the interval values of the nucleation coefficient $\tilde{\gamma} = \langle \underline{\gamma}, \overline{\gamma} \rangle$ and the growth coefficient $\tilde{\mu} = \langle \underline{\mu}, \overline{\mu} \rangle$.

The grain density $\tilde{N}(x, t)$ and the solidification rate $\tilde{R}(x, t)$ are interval values and are defined as follows

$$\tilde{N}(x, t) = \tilde{\gamma} \Delta T(x, t)^2 \tag{18}$$

and

$$\tilde{R}(x, t) = \tilde{\mu} \Delta T(x, t)^2 \tag{19}$$

where the undercooling $\Delta T(x, t)$ is expressed as

$$\Delta T(x, t) = \begin{cases} T_{cr} - \dfrac{1}{2}\left[\underline{T}(x, t) + \overline{T}(x, t)\right], & \dfrac{1}{2}\left[\underline{T}(x, t) + \overline{T}(x, t)\right] \le T_{cr} \\ 0, & \dfrac{1}{2}\left[\underline{T}(x, t) + \overline{T}(x, t)\right] > T_{cr} \end{cases} \tag{20}$$

while $\underline{T}(x, t)$ and $\overline{T}(x, t)$ denote the first and the second endpoints of the temperature interval respectively.

The interval source function is calculated according to the rules of the interval arithmetic [6] and can be expressed as follows

$$\begin{aligned} \tilde{Q}(x, t) = \frac{4}{3}\pi Q_{cr} \left[\frac{\partial \tilde{N}(x, t)}{\partial t} \tilde{R}(x, t)^3 + 3\tilde{N}(x, t)\tilde{R}(x, t)^2 \tilde{R}(x, t) \right] \\ \times \exp\left[-\frac{4}{3}\pi \tilde{N}(x, t)\tilde{R}(x, t)^3 \right] \end{aligned} \tag{21}$$

3. Results of computations

Let us consider the crystallization process proceeding in a copper plate of dimension L = 0.01 m (one-dimensional problem). The following input data have been introduced: initial temperature T_0 = 1120°C, solidification point T_{cr} = 1083°C, thermal conductivity λ = 280 W/m·K, specific heat c = 490 J/kg·K, density ρ = 8600 kg/m^3, nuclei coefficient $\tilde{\gamma} = \langle 10^9 - 1000, 10^9 + 1000 \rangle$ 1/K^2·m^3, growth coefficient $\tilde{\mu} = \langle 2.95 \cdot 10^{-6}, 3.05 \cdot 10^{-6} \rangle$ m/s·K^2, volumetric latent heat Q_{cr} = 1754.4 MJ/m^3. On the left side of the domain considered the boundary condition of the second type is assumed: q_b = 0 W/m^2, on the right side the boundary condition of the first type is

assumed: T_b = 1070°C, the domain considered has been divided into 20 constant elements, time step Δt = 0.002 s.

Figures 1 and 2 illustrate the cooling curves obtained at the nodes 10 (x = 0.00475 m) and 12 (x = 0.00575 m) of the domain considered, where Tem L, Tem R denote the lower and the upper bounds of the temperature intervals.

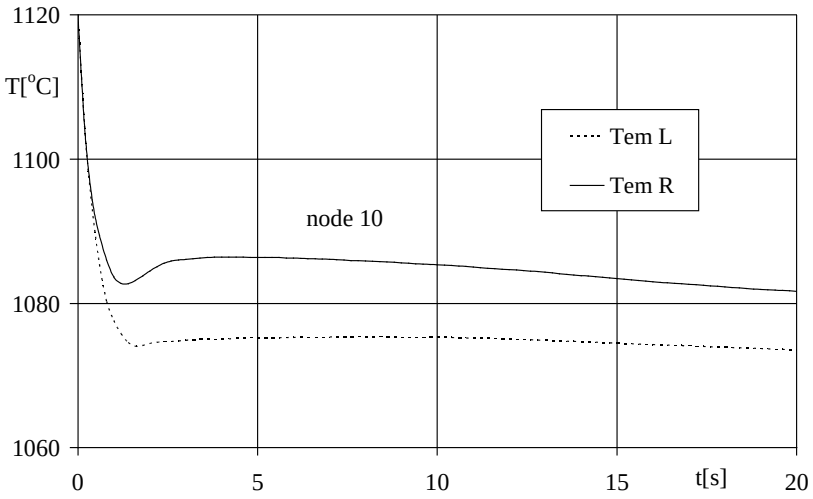

Fig. 1. Cooling curves at node 10

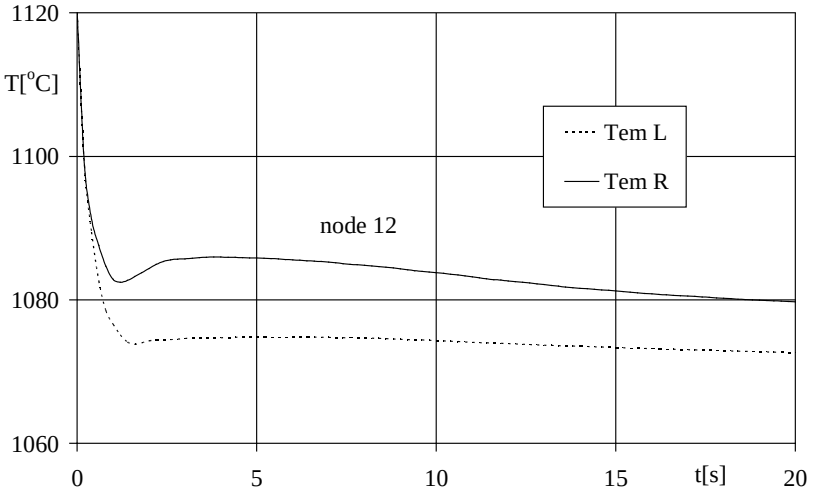

Fig. 2. Cooling curves at node 12

Figure 3 presents the courses of the source function at the same nodes, where Source L and Source R denote the first and the second endpoints of the source

interval. Figure 4 illustrates the temporary interval mean radiuses at the nodes 10 and 12.

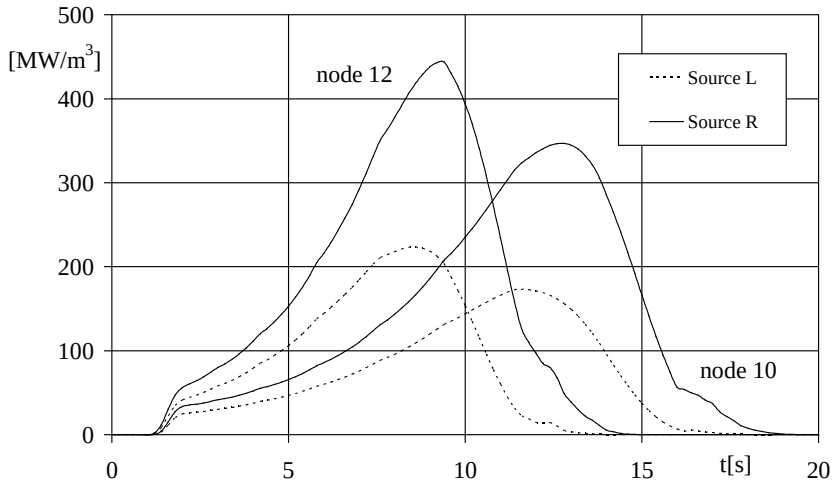

Fig. 3. The courses of the source function

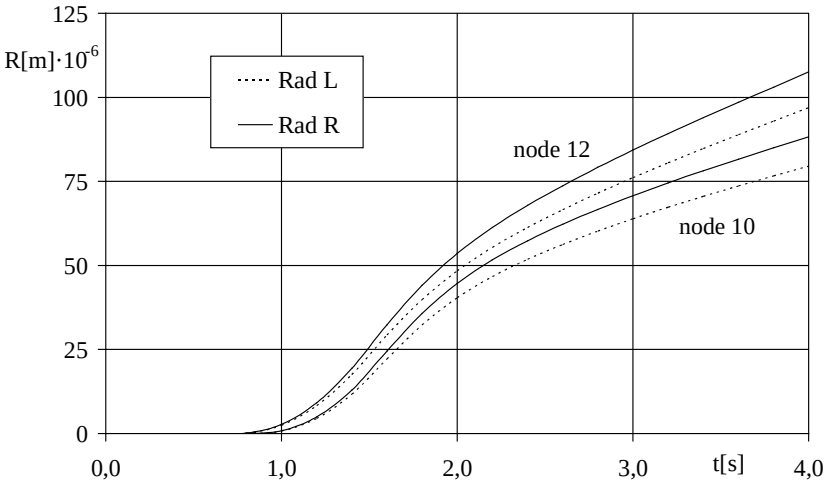

Fig. 4. The courses of the radius

Summing up, the interval boundary element method is an effective tool in numerical modelling of the problems with the interval source function.

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