NUMERICAL MODELLING OF SOLIDIFICATION PROCESS USING INTERVAL FINITE DIFFERENCE METHOD

Alicja Piasecka Belkhayat

Department of Strength of Materials and Computational Mechanics
Silesian University of Technology, Poland, alicja.piasecka@polsl.pl

Abstract. The numerical modelling of steel cast solidification process in sand mould is considered. The problem analyzed is described by the system of partial differential equations supplemented by adequate boundary and initial conditions. The latent heat appearing in the model of a casting sub-domain is treated as directed interval value. The problem formulated has been solved by means of interval finite difference method with the approach of directed interval arithmetic. In the final part of the paper, results of numerical computations are shown.

1. Governing equations

Let us consider the solidification process in heterogeneous domain of the casting (Ω_1) and mould (Ω_2) (see Figure 1).

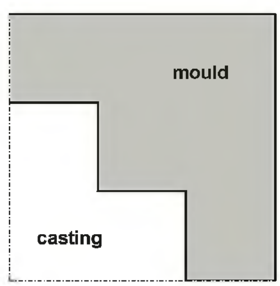

Fig. 1. Domain considered

The energy equation describing the casting solidification has the form [1]

$$X \in \Omega_1 : \quad \tilde{C}_1(T)\frac{\partial T_1(x,t)}{\partial t} = \lambda_1 \nabla^2 T_1(x,t) \tag{1}$$

where $\tilde{C}_1(T)$ is the directed interval substitute thermal capacity [2], λ_1 is the thermal conductivity, T_1, $X = \{x, y\}$, t denote the temperature, geometrical coordinates and time of the casting sub-domain, respectively.

In the case of steel cast solidification the following approximation of directed interval substitute thermal capacity can be taken into account [2]

$$\tilde{C}_1(T)=\begin{cases} c_L, & T_1>T_L \\ c_P+\dfrac{\tilde{Q}}{T_L-T_S}, & T_S\le T_1\le T_L \\ c_S, & T_1<T_S \end{cases} \tag{2}$$

where T_L, T_S correspond to the liquidus and solidus temperatures, $\tilde{Q}$ is the directed interval latent heat, c_L, c_S are the volumetric specific heats of molten metal and solid state, respectively, while $c_P=0.5(c_L+c_S)$.

For example, for $c_P=5.3895$, $T_S=1470$, $T_L=1505$ and the interval latent heat $\tilde{Q}=\langle 1885.275,\ 2083.725\rangle$, the directed interval substitute thermal capacity for $T_1\in\langle T_S,\ T_L\rangle$ is computed according to the rules of the directed interval arithmetic [3, 4] (see Appendix)

$$\begin{gathered}\tilde{C}_1(T)=c_P+\frac{\tilde{Q}}{T_L-T_S}=5.3895+\frac{\langle 1885.275,\ 2083.725\rangle}{35}=\\ \langle 5.3895,\ 5.3895\rangle+\langle 53.865,\ 59.535\rangle=\langle 59.2545,\ 64.9245\rangle\end{gathered} \tag{3}$$

The considered equation (1) is supplemented by the energy equation concerning a mould sub-domain Ω_2

$$X\in\Omega_2:\qquad c_2\frac{\partial T_2(x,t)}{\partial t}=\lambda_2\nabla^2T_2(x,t) \tag{4}$$

where c_2 is the mould volumetric specific heat, λ_2 is the mould thermal conductivity and T_2 is the mould temperature.

The energy equations for both sub-domains must be supplemented by the boundary-initial conditions

$$\begin{cases} X\in\Gamma_\infty: & q_2(x,\ t)=-\lambda_2\dfrac{\partial T_2(,\ t)}{\partial n}=0 \\ t=0: & T_e(x,\ 0)=T_{e0}(x), \qquad e=1,\ 2 \end{cases} \tag{5}$$

and the continuity condition on the contact surface between the casting and mould

$$X\in\Gamma:\qquad \begin{cases} -\lambda_1\dfrac{\partial T_1(x,\ t)}{\partial n}=-\lambda_2\dfrac{\partial T_2(x,\ t)}{\partial n} \\ T_1(x,\ t)=T_2(x,\ t) \end{cases} \tag{6}$$

2. Interval finite difference method

The energy equations (1) and (4) for directed interval latent heat can be written in the form [1]

$$X \in \Omega: \quad \tilde{c}\frac{\partial \tilde{T}(X,t)}{\partial t} = \nabla\left[\lambda \nabla \tilde{T}(X,t)\right] \tag{7}$$

where

$$\begin{aligned} X \in \Omega_1: &\quad \tilde{c} = \tilde{C}_1(T), \quad \lambda = \lambda_1 \\ X \in \Omega_2: &\quad \tilde{c} = c_2, \quad \lambda = \lambda_2 \end{aligned} \tag{8}$$

The right-hand side of the interval equation (7) can be expressed as follows [1, 5]

$$\nabla\left[\lambda \nabla \tilde{T}(X,t)\right] = \frac{\partial}{\partial x}\left(\lambda \frac{\partial \tilde{T}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda \frac{\partial \tilde{T}}{\partial y}\right) \tag{9}$$

Using the mean quotient definition, we can write

$$\left(\frac{\partial}{\partial x}\lambda\frac{\partial\langle T^-, T^+\rangle}{\partial x}\right)_{ij} = \frac{1}{h}\frac{\langle T^-, T^+\rangle_1 - \langle T^-, T^+\rangle_{ij}}{R_{01}} + \frac{1}{h}\frac{\langle T^-, T^+\rangle_{ij} - \langle T^-, T^+\rangle_2}{R_{02}} \tag{10}$$

while

$$R_{01} = \frac{h}{2\lambda_{ij}} + \frac{h}{2\lambda_1} \qquad R_{02} = \frac{h}{2\lambda_{ij}} + \frac{h}{2\lambda_2} \tag{11}$$

are the thermal resistances from the node '$i\,j$' to the nodes '1' and '2', respectively, h is the grid step in the direction of x axis (see Figure 2).

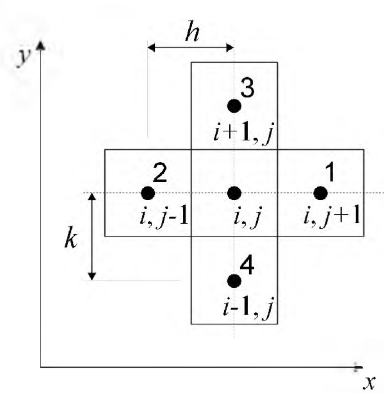

Fig. 2. 5-point star

Analogically

$$\left(\frac{\partial}{\partial y}\lambda\frac{\partial\left\langle T^-,T^+\right\rangle}{\partial y}\right)_{ij}=\frac{1}{k}\frac{\left\langle T^-,T^+\right\rangle_3-\left\langle T^-,T^+\right\rangle_{ij}}{R_{03}}+\frac{1}{k}\frac{\left\langle T^-,T^+\right\rangle_{ij}-\left\langle T^-,T^+\right\rangle_4}{R_{04}} \tag{12}$$

while

$$R_{03}=\frac{h}{2\lambda_{ij}}+\frac{h}{2\lambda_3} \qquad\qquad R_{04}=\frac{h}{2\lambda_{ij}}+\frac{h}{2\lambda_4} \tag{13}$$

are the thermal resistances from the node '$i\,j$' to the nodes '3' and '4', respectively, k is the grid step in the direction of y axis.

Finally, for the time t^{f-1}, the right-hand side of the interval equation (7) can be written as

$$\begin{gathered}\nabla\left[\lambda\nabla\tilde{T}(X,t)\right]^{f-1}=\frac{\Phi_1}{R_{01}}\left(\left\langle T^-,T^+\right\rangle_1^{f-1}-\left\langle T^-,T^+\right\rangle_{ij}^{f-1}\right)+\\ \frac{\Phi_2}{R_{02}}\left(\left\langle T^-,T^+\right\rangle_{ij}^{f-1}-\left\langle T^-,T^+\right\rangle_2^{f-1}\right)+\frac{\Phi_3}{R_{03}}\left(\left\langle T^-,T^+\right\rangle_3^{f-1}-\left\langle T^-,T^+\right\rangle_{ij}^{f-1}\right)+\\ \frac{\Phi_4}{R_{04}}\left(\left\langle T^-,T^+\right\rangle_{ij}^{f-1}-\left\langle T^-,T^+\right\rangle_4^{f-1}\right)\end{gathered} \tag{14}$$

where $\tilde{T}_{ij}^{f-1}$ are the directed interval temperatures in the central node at the beginning of the time interval Δt, Φ_e $(e=1,2,3,4)$ are called the shape functions and are defined as follows

$$\Phi_1=\Phi_2=\frac{1}{h} \qquad\qquad \Phi_3=\Phi_4=\frac{1}{k} \tag{15}$$

The left-hand side of the energy equation will be substituted by a differential quotient

$$\left(\left\langle c^-,c^+\right\rangle\frac{\partial\left\langle T^-,T^+\right\rangle}{\partial t}\right)_{ij}^{f-1}=\left\langle c^-,c^+\right\rangle_{ij}^{f-1}\frac{\left\langle T^-,T^+\right\rangle_{ij}^{f}-\left\langle T^-,T^+\right\rangle_{ij}^{f-1}}{\Delta t} \tag{16}$$

where $\tilde{T}_{ij}^{f}$ are the directed interval temperatures in the central node at the end of the considered time interval Δt.

For example, for $\tilde{T}_1\in\left\langle T_S,T_L\right\rangle$, $\tilde{C}_{1ij}^{f-1}=\left\langle 59.2545,\,64.9245\right\rangle$ (see eq.3) and $\tilde{T}_{1ij}^{f}=\left\langle 1499.48,\,1501.23\right\rangle$ the sign variables are of the form

$\sigma(\tilde{C}_{1ij}^{f-1}) = +$, $\sigma(\tilde{T}_{1ij}^{f}) = +$, so the product of $\tilde{C}_{1ij}^{f-1}$ and $\tilde{T}_{1ij}^{f}$ is computed as follows (see Appendix)

$$\begin{gathered}\tilde{C}_{1ij} \cdot \tilde{T}_{1ij} = \left\langle C_{1ij}^{-\sigma(\tilde{T}_{1ij})} \cdot T_{1ij}^{-\sigma(\tilde{C}_{1ij})},\ C_{1ij}^{\sigma(\tilde{T}_{1ij})} \cdot T_{1ij}^{\sigma(\tilde{C}_{1ij})} \right\rangle = \\ \left\langle C_{1ij}^{-+} \cdot T_{1ij}^{-+},\ C_{1ij}^{+} \cdot T_{1ij}^{+} \right\rangle = \left\langle C_{1ij}^{-} \cdot T_{1ij}^{-},\ C_{1ij}^{+} \cdot T_{1ij}^{+} \right\rangle = \\ \left\langle 59.2545 \cdot 1499.48,\ 64.9245 \cdot 1501.23 \right\rangle \approx \left\langle 88851,\ 97466 \right\rangle\end{gathered} \tag{17}$$

So, one obtains the following formula

$$\tilde{c}_{ij}^{f-1} \frac{\tilde{T}_{ij}^{f} - \tilde{T}_{ij}^{f-1}}{\Delta t} = \sum_{e=1}^{4} \frac{\left(\tilde{T}_{e}^{f-1} - \tilde{T}_{ij}^{f-1}\right)\Phi_e}{R_{0e}} \tag{18}$$

where e denotes the main direction (e = 1, 2, 3, 4).

At last the approximate form of the energy equation is of the following form

$$\left\langle T^-,\ T^+ \right\rangle_{ij}^{f} = \left\langle A_0^-,\ A_0^+ \right\rangle \left\langle T^-,\ T^+ \right\rangle_{ij}^{f-1} + \sum_{e=1}^{4} \left\langle A_e^-,\ A_e^+ \right\rangle \left(\left\langle T^-,\ T^+ \right\rangle_{e}^{f-1} - \left\langle T^-,\ T^+ \right\rangle_{ij}^{f-1} \right) \tag{19}$$

where

$$\tilde{A}_e = \frac{\Phi_e \Delta t}{R_{0e}^{f-1} \left\langle c^-,\ c^+ \right\rangle_{ij}^{f-1}} \qquad \tilde{A}_0 = 1 - \sum_{e=1}^{4} \tilde{A}_e \tag{20}$$

All this interval values must be calculated according to the rules of the directed interval arithmetic [3, 4].

It should be pointed out that for the nodes in the vicinity of the boundary Γ the approximation of operator $\nabla\left(\lambda \nabla \tilde{T}\right)_{ij}$ is formally the same.

3. Numerical examples

As an example, the 2D casting-mould system shown in Figure 3 is considered.

The following input data have been introduced: liquidus temperature T_L = 1505°C, solidus temperature T_S = 1470°C, pouring temperature T_{10} = 1550°C, initial mould temperature T_{20} = 20°C, λ_1 = 30 W/mK, c_L = 5.904 MJ/m^{3}K, c_S = 4.875 MJ/m^{3}K, $\tilde{Q} = \left\langle 1885.275,\ 2083.725 \right\rangle$ MJ/m^3, λ_2 = 1 W/mK, c_2 = 1.75 MJ/m^{3}K.

The problem considered has been solved using the explicit scheme of interval FDM. The regular mesh created by 30×30 nodes with constant step h = 0.002 m has been introduced, time step Δt = 0.1 s.

Figures 4 and 5 present the cooling curves at the nodes from the casting sub-domain. The dashed and solid lines denote the lower and the upper bounds of the temperature intervals, respectively. We can see that the temperature intervals are narrow and their width does not increase in the time considered.

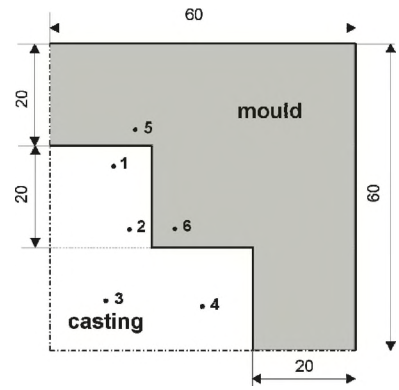

Fig. 3. Casting-mould system

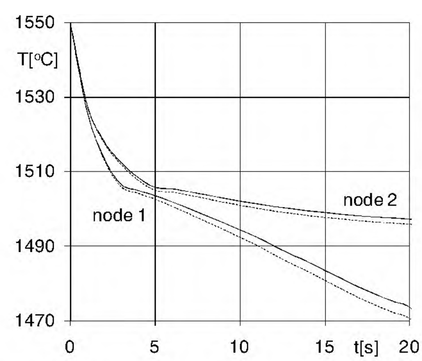

Fig. 4. Cooling curves at nodes 1 and 2 from the casting

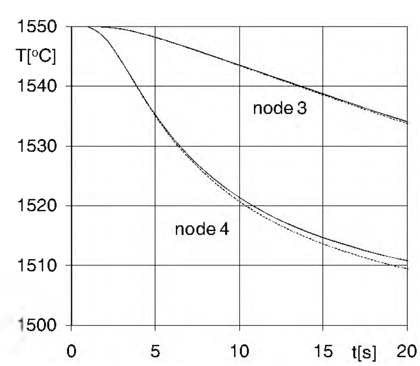

Fig. 5. Cooling curves at nodes 3 and 4 from the casting

Figure 6 illustrates the heating curves at the nodes from the mould sub-domain. The temperature intervals' width is very small.

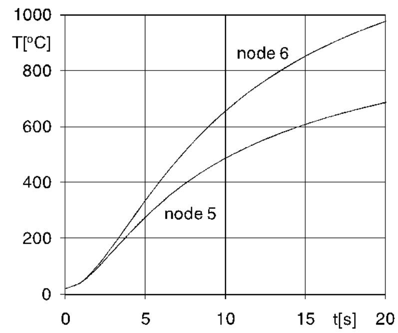

Fig. 6. Heating curves at nodes from the mould

Conclusions

In this paper the solidification process of the casting proceeding in the mould is analysed. The latent heat appearing in the approximation of the substitute thermal capacity has been assumed as interval value. The problem discussed has been solved using the interval finite difference method.

Directed interval arithmetic allows one to obtain narrow and convergent temperature intervals, while classical interval arithmetic gives large and divergent temperature intervals [5, 6].

References

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APPENDIX

Directed interval arithmetic

Let us consider a directed interval $\tilde{a}$ which can be defined as a set $\boldsymbol{D}$ of all directed pairs of real numbers defined as follows [3, 4, 7]

$$\tilde{a} = \left\langle a^-, a^+ \right\rangle := \left\{ \tilde{a} \in \boldsymbol{D} \,\middle|\, a^-, a^+ \in \boldsymbol{R} \right\} \tag{21}$$

where a^- and a^- denote the beginning and the end of the interval, respectively. The left or the right endpoint of the interval $\tilde{a}$ can be denoted as a^s, $s \in \{+, -\}$, where s is a binary variable. This variable can be expressed as a product of two binary variables and is defined as

$$++ = -- = + \qquad\qquad +- = -+ = - \tag{22}$$

An interval is called proper if $a^- \le a^+$, improper if $a^- \ge a^+$ and degenerate if $a^- = a^+$. The set of all directed interval numbers can be written as $\boldsymbol{D} = \boldsymbol{P} \cup \boldsymbol{I}$, where $\boldsymbol{P}$ denotes a set of all directed proper intervals and $\boldsymbol{I}$ denotes a set of all improper intervals.

Additionally a subset $\boldsymbol{Z} = \boldsymbol{Z}_P \cup \boldsymbol{Z}_I \in \boldsymbol{D}$ should be defined, where

$$\boldsymbol{Z}_P = \left\{ \tilde{a} \in \boldsymbol{P} \,\middle|\, a^- \le 0 \le a^+ \right\} \qquad\qquad \boldsymbol{Z}_I = \left\{ \tilde{a} \in \boldsymbol{I} \,\middle|\, a^+ \le 0 \le a^- \right\} \tag{23}$$

For directed interval numbers two binary variables are defined. The first of them is the direction variable and the other is the sign variable

$$\tau(\tilde{a}) = \begin{cases} +, & if \;\; a^- \le a^+ \\ -, & if \;\; a^- > a^+ \end{cases} \qquad\qquad \sigma(\tilde{a}) = \begin{cases} +, & if \;\; a^- > 0,\, a^+ > 0 \\ -, & if \;\; a^- < 0,\, a^+ < 0 \end{cases}, \quad \tilde{a} \in \boldsymbol{D} \setminus \boldsymbol{Z} \tag{24}$$

The sum of two directed intervals $\tilde{a} = \left\langle a^-, a^+ \right\rangle$ and $\tilde{b} = \left\langle b^-, b^+ \right\rangle$ can be written as

$$\tilde{a} + \tilde{b} = \left\langle a^- + b^-,\, a^+ + b^+ \right\rangle, \quad \tilde{a}, \tilde{b} \in \boldsymbol{D} \tag{25}$$

The difference is of the form

$$\tilde{a} - \tilde{b} = \left\langle a^- - b^+,\, a^+ - b^- \right\rangle, \quad \tilde{a}, \tilde{b} \in \boldsymbol{D} \tag{26}$$

The product of the directed intervals is described by the formula

$$\tilde{a} \cdot \tilde{b} = \begin{cases} \left\langle a^{-\sigma(\tilde{b})} \cdot b^{-\sigma(\tilde{a})}, a^{\sigma(\tilde{b})} \cdot b^{\sigma(\tilde{a})} \right\rangle, & \tilde{a}, \tilde{b} \in \boldsymbol{D} \setminus \boldsymbol{Z} \\ \left\langle a^{\sigma(\tilde{a})\tau(\tilde{b})} \cdot b^{-\sigma(\tilde{a})}, a^{\sigma(\tilde{a})\tau(\tilde{b})} \cdot b^{\sigma(\tilde{a})} \right\rangle, & \tilde{a} \in \boldsymbol{D} \setminus \boldsymbol{Z}, \tilde{b} \in \boldsymbol{Z} \\ \left\langle a^{-\sigma(\tilde{b})} \cdot b^{\sigma(\tilde{b})\tau(\tilde{a})}, a^{\sigma(\tilde{b})} \cdot b^{\sigma(\tilde{b})\tau(\tilde{a})} \right\rangle, & \tilde{a} \in \boldsymbol{Z}, \tilde{b} \in \boldsymbol{D} \setminus \boldsymbol{Z} \\ \left\langle \min\left(a^- \cdot b^+, a^+ \cdot b^-\right), \max\left(a^- \cdot b^-, a^+ \cdot b^+\right) \right\rangle, & \tilde{a}, \tilde{b} \in \boldsymbol{Z}_P \\ \left\langle \max\left(a^- \cdot b^-, a^+ \cdot b^+\right), \min\left(a^- \cdot b^+, a^+ \cdot b^-\right) \right\rangle, & \tilde{a}, \tilde{b} \in \boldsymbol{Z}_I \\ 0, & \left(\tilde{a} \in \boldsymbol{Z}_P, \tilde{b} \in \boldsymbol{Z}_I\right) \cup \left(\tilde{a} \in \boldsymbol{Z}_I, \tilde{b} \in \boldsymbol{Z}_P\right) \end{cases} \tag{27}$$

The quotient of two directed intervals can be written as

$$\tilde{a} / \tilde{b} = \begin{cases} \left\langle a^{-\sigma(\tilde{b})} / b^{\sigma(\tilde{a})}, a^{\sigma(\tilde{b})} / b^{-\sigma(\tilde{a})} \right\rangle, & \tilde{a}, \tilde{b} \in \boldsymbol{D} \setminus \boldsymbol{Z} \\ \left\langle a^{-\sigma(\tilde{b})} / b^{-\sigma(\tilde{b})\tau(\tilde{a})}, a^{\sigma(\tilde{b})} / b^{-\sigma(\tilde{b})\tau(\tilde{a})} \right\rangle, & \tilde{a} \in \boldsymbol{Z}, \tilde{b} \in \boldsymbol{D} \setminus \boldsymbol{Z} \end{cases} \tag{28}$$

In the directed interval arithmetic two extra operators are defined, inversion of summation

$$-_D \tilde{a} = \left\langle -a^-, -a^+ \right\rangle, \quad \tilde{a} \in \boldsymbol{D} \tag{29}$$

and inversion of multiplication

$$1 /_D \tilde{a} = \left\langle 1 / a^-, 1 / a^+ \right\rangle, \quad \tilde{a} \in \boldsymbol{D} \setminus \boldsymbol{Z} \tag{30}$$

So, two additional mathematical operations can be defined as follows

$$\tilde{a} -_D \tilde{b} = \left\langle a^- - b^-, a^+ - b^+ \right\rangle, \quad \tilde{a}, \tilde{b} \in \boldsymbol{D} \tag{31}$$

and

$$\tilde{a} /_D \tilde{b} = \begin{cases} \left\langle a^{-\sigma(\tilde{b})} / b^{-\sigma(\tilde{a})}, a^{\sigma(\tilde{b})} / b^{\sigma(\tilde{a})} \right\rangle, & \tilde{a}, \tilde{b} \in \boldsymbol{D} \setminus \boldsymbol{Z} \\ \left\langle a^{-\sigma(\tilde{b})} / b^{\sigma(\tilde{b})}, a^{\sigma(\tilde{b})} / b^{\sigma(\tilde{b})} \right\rangle, & \tilde{a} \in \boldsymbol{Z}, \tilde{b} \in \boldsymbol{D} \setminus \boldsymbol{Z} \end{cases} \tag{32}$$

Now, it is possible to obtain the number zero by subtraction of two identical intervals $\tilde{a} -_D \tilde{a} = 0$ and the number one as the result of the division $\tilde{a} /_D \tilde{a} = 1$, which was impossible when applying classical interval arithmetic [8].