

## NUMERICAL MODELLING OF SOLIDIFICATION PROCESS USING INTERVAL FINITE DIFFERENCE METHOD

*Alicja Piasecka Belkhat*

*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 ( $\Omega_1$ ) and mould ( $\Omega_2$ ) (see Figure 1).

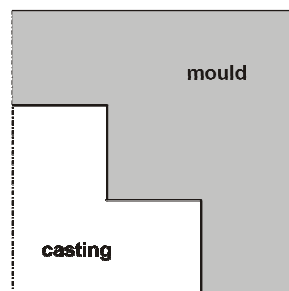


Fig. 1. Domain considered

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

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

where  $\tilde{C}_1(T)$  is the directed interval substitute thermal capacity [2],  $\lambda_1$  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]

$$\tilde{C}_1(T) = \begin{cases} c_L, & T_1 > T_L \\ c_p + \frac{\tilde{Q}}{T_L - T_S}, & T_S \leq T_1 \leq T_L \\ c_S, & T_1 < T_S \end{cases} \quad (2)$$

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)

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

The considered equation (1) is supplemented by the energy equation concerning a mould sub-domain  $\Omega_2$

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

where  $c_2$  is the mould volumetric specific heat,  $\lambda_2$  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

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

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

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

## 2. Interval finite difference method

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

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

where

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

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

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

Using the mean quotient definition, we can write

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

while

$$R_{01} = \frac{h}{2\lambda_{ij}} + \frac{h}{2\lambda_1} \quad R_{02} = \frac{h}{2\lambda_{ij}} + \frac{h}{2\lambda_2} \quad (11)$$

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).

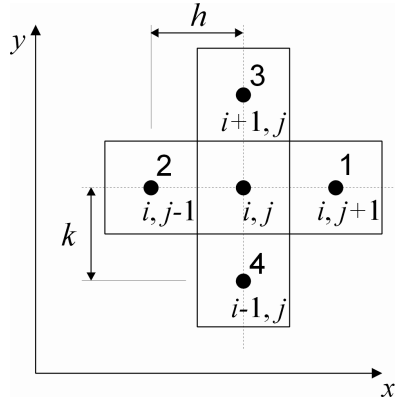


Fig. 2. 5-point star

Analogically

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

while

$$R_{03} = \frac{h}{2\lambda_{ij}} + \frac{h}{2\lambda_3} \quad R_{04} = \frac{h}{2\lambda_{ij}} + \frac{h}{2\lambda_4} \quad (13)$$

are the thermal resistances from the node 'ij' 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

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

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

$$\Phi_1 = \Phi_2 = \frac{1}{h} \quad \Phi_3 = \Phi_4 = \frac{1}{k} \quad (15)$$

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

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

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

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

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

So, one obtains the following formula

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

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

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

where

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

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  $\Gamma$  the approximation of operator  $\nabla(\lambda \nabla \tilde{T})_{ij}$  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  $T_L = 1505^\circ\text{C}$ , solidus temperature  $T_S = 1470^\circ\text{C}$ , pouring temperature  $T_{10} = 1550^\circ\text{C}$ , initial mould temperature  $T_{20} = 20^\circ\text{C}$ ,  $\lambda_1 = 30 \text{ W/mK}$ ,  $c_L = 5.904 \text{ MJ/m}^3\text{K}$ ,  $c_S = 4.875 \text{ MJ/m}^3\text{K}$ ,  $\tilde{Q} = \langle 1885.275, 2083.725 \rangle \text{ MJ/m}^3$ ,  $\lambda_2 = 1 \text{ W/mK}$ ,  $c_2 = 1.75 \text{ MJ/m}^3\text{K}$ .

The problem considered has been solved using the explicit scheme of interval FDM. The regular mesh created by  $30 \times 30$  nodes with constant step  $h = 0.002 \text{ m}$  has been introduced, time step  $\Delta t = 0.1 \text{ s}$ .

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.

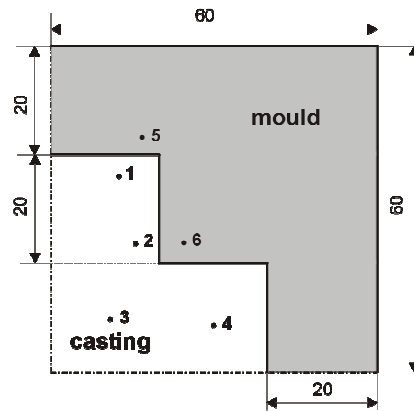


Fig. 3. Casting-mould system

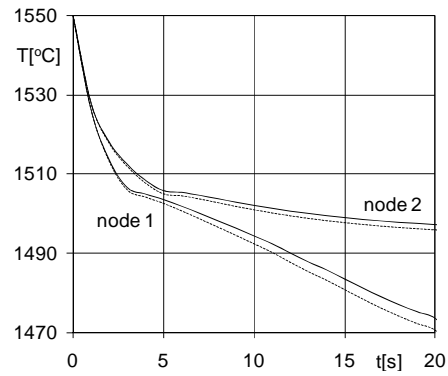


Fig. 4. Cooling curves at nodes 1 and 2 from the casting

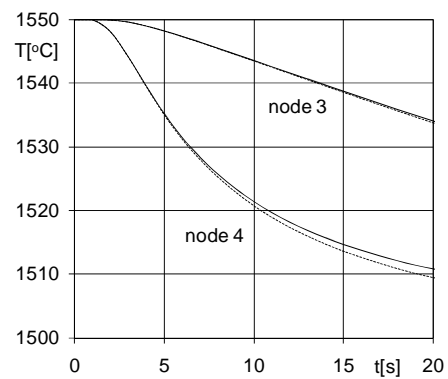


Fig. 5. Cooling curves at nodes 3 and 4 from the casting

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

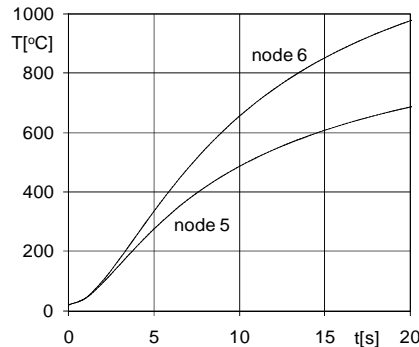


Fig. 6. Heating curves at nodes from the mould

## 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

- [1] Mochnacki B., Suchy J.S., Numerical methods in computations of foundry processes, PFTA, Cracow 1995.
- [2] Mochnacki B., Majchrzak E., Suchy J.S., Thermal theory of foundry processes - a base of numerical simulation of casting solidification, [in:] Casting Simulation. Background and Examples, Zurich, World Foundrymen Organization, International Commission 3.3, 2000, 31-66.
- [3] Markov S.M., On directed interval arithmetic and its applications, Journal of Universal Computer Science 1995, 1, 514-526.
- [4] Popova E.D., Multiplication Distributivity of Proper and Improper Intervals, Reliable Computing 2001, 7, 129-140.
- [5] Piasecka Belkhat A., Mendakiewicz J., *Application of interval arithmetic for numerical modeling of solidification process*, EUROGEN 2009, Extended Abstracts, Cracow/Gliwice, 2009, 87-88.
- [6] Piasecka Belkhat A., *Numerical modelling of solidification process using interval boundary element method*, Archives of Foundry Engineering 2008, 8, 4, 171-176.
- [7] Moore R.E., Bierbaum F., Methods and applications of interval analysis, SIAM, 1979.
- [8] Neumaier A., *Interval methods for system of equations*, Cambridge University Press, Cambridge, New York, Port Chester, Melbourne, Sydney 1990.

## APPENDIX

### Directed interval arithmetic

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

$$\tilde{a} = \langle a^-, a^+ \rangle := \{ \tilde{a} \in \mathbf{D} \mid a^-, a^+ \in \mathbf{R} \} \quad (21)$$

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

$$++ = -- = + \quad +- = -+ = - \quad (22)$$

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

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

$$\mathbf{Z}_p = \{ \tilde{a} \in \mathbf{P} \mid a^- \leq 0 \leq a^+ \} \quad \mathbf{Z}_I = \{ \tilde{a} \in \mathbf{I} \mid a^+ \leq 0 \leq a^- \} \quad (23)$$

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

$$\tau(\tilde{a}) = \begin{cases} +, & \text{if } a^- \leq a^+ \\ -, & \text{if } a^- > a^+ \end{cases} \quad \sigma(\tilde{a}) = \begin{cases} +, & \text{if } a^- > 0, a^+ > 0 \\ -, & \text{if } a^- < 0, a^+ < 0 \end{cases}, \quad \tilde{a} \in \mathbf{D} \setminus \mathbf{Z} \quad (24)$$

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

$$\tilde{a} + \tilde{b} = \langle a^- + b^-, a^+ + b^+ \rangle, \quad \tilde{a}, \tilde{b} \in \mathbf{D} \quad (25)$$

The difference is of the form

$$\tilde{a} - \tilde{b} = \langle a^- - b^+, a^+ - b^- \rangle, \quad \tilde{a}, \tilde{b} \in \mathbf{D} \quad (26)$$

The product of the directed intervals is described by the formula



$$\tilde{a} \cdot \tilde{b} = \begin{cases} \langle a^{-\sigma(\tilde{b})} \cdot b^{-\sigma(\tilde{a})}, a^{\sigma(\tilde{b})} \cdot b^{\sigma(\tilde{a})} \rangle, & \tilde{a}, \tilde{b} \in \mathbf{D} \setminus \mathbf{Z} \\ \langle a^{\sigma(\tilde{a})\tau(\tilde{b})} \cdot b^{-\sigma(\tilde{a})}, a^{\sigma(\tilde{a})\tau(\tilde{b})} \cdot b^{\sigma(\tilde{a})} \rangle, & \tilde{a} \in \mathbf{D} \setminus \mathbf{Z}, \tilde{b} \in \mathbf{Z} \\ \langle a^{-\sigma(\tilde{b})} \cdot b^{\sigma(\tilde{b})\tau(\tilde{a})}, a^{\sigma(\tilde{b})} \cdot b^{\sigma(\tilde{b})\tau(\tilde{a})} \rangle, & \tilde{a} \in \mathbf{Z}, \tilde{b} \in \mathbf{D} \setminus \mathbf{Z} \\ \langle \min(a^- \cdot b^+, a^+ \cdot b^-), \max(a^- \cdot b^-, a^+ \cdot b^+) \rangle, & \tilde{a}, \tilde{b} \in \mathbf{Z}_p \\ \langle \max(a^- \cdot b^-, a^+ \cdot b^+), \min(a^- \cdot b^+, a^+ \cdot b^-) \rangle, & \tilde{a}, \tilde{b} \in \mathbf{Z}_l \\ 0, & (\tilde{a} \in \mathbf{Z}_p, \tilde{b} \in \mathbf{Z}_l) \cup (\tilde{a} \in \mathbf{Z}_l, \tilde{b} \in \mathbf{Z}_p) \end{cases} \quad (27)$$

The quotient of two directed intervals can be written as

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

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

$$-_{\mathbf{D}} \tilde{a} = \langle -a^-, -a^+ \rangle, \quad \tilde{a} \in \mathbf{D} \quad (29)$$

and inversion of multiplication

$$1 /_{\mathbf{D}} \tilde{a} = \langle 1 / a^-, 1 / a^+ \rangle, \quad \tilde{a} \in \mathbf{D} \setminus \mathbf{Z} \quad (30)$$

So, two additional mathematical operations can be defined as follows

$$\tilde{a} -_{\mathbf{D}} \tilde{b} = \langle a^- - b^-, a^+ - b^+ \rangle, \quad \tilde{a}, \tilde{b} \in \mathbf{D} \quad (31)$$

and

$$\tilde{a} /_{\mathbf{D}} \tilde{b} = \begin{cases} \langle a^{-\sigma(\tilde{b})} / b^{-\sigma(\tilde{a})}, a^{\sigma(\tilde{b})} / b^{\sigma(\tilde{a})} \rangle, & \tilde{a}, \tilde{b} \in \mathbf{D} \setminus \mathbf{Z} \\ \langle a^{-\sigma(\tilde{b})} / b^{\sigma(\tilde{b})}, a^{\sigma(\tilde{b})} / b^{\sigma(\tilde{b})} \rangle, & \tilde{a} \in \mathbf{Z}, \tilde{b} \in \mathbf{D} \setminus \mathbf{Z} \end{cases} \quad (32)$$

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