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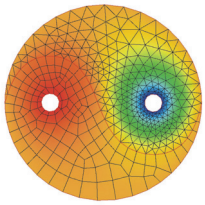

TIME-SAVING METHODS FOR CAFD MODELING OF THE MICROSTRUCTURE EVOLUTION DURING SOLIDIFICATION

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Abstract

The Cellular Automaton – Finite Difference model (CAFD) is one of the known methods of the simulation of microstructure evolution during the solidification. In the mesoscale CAFD modeling the outer shape of the growing grains is the result of the simulation and do not superimposed beforehand.

The solidification of metals and alloys is a typical example of multiphysics and multiscale engineering systems. The phenomenon of different time and spatial scales should be taken into consideration in the modeling of a microstructure formation: heat diffusion, the components diffusion in the liquid and solid phases, the thermodynamics of phase transformation under a condition of inhomogeneous chemical composition of growing and vanishing phases, phase interface kinetics and grains nucleation.

Complete numerical solution, that takes into account all above phenomena, are very time-consuming. The ability of acceleration of the implicit scheme of numerical solution was analyzed in this paper by means of the diversified number of iteration in the well-known Gauss-Seidel iterative method. For the accuracy of the proposed numerical solution the results were compared with the known exact solution of the classical one-dimension Schwarz problem.

Key words: solidification modeling, cellular automaton, time-saving calculations

1. INTRODUCTION

In the CAFD solidification models the numerical solutions were used for the modeling of temperature and/or concentration fields (Brown, 1998; Zhu at al., 2007). The parabolic nonlinear differential equations were solved by using a numerical method. The overlapping lattices with the same spatial step were used generally for concentration and temperature fields modeling and for the CA. The order of magnitude of the lattice cell size for the microstructure prediction is equal to 1 μm. Due to the above reasons the numerical CAFD experiments of the microstructure evolution are very time-consuming.

In the solidification modeling of metals and alloys the time step of the explicit numerical scheme for heat diffusion computations is about 10^4 times shorter than for mass diffusion. Very often the non-uniform temperature distribution near the solidification front is neglected in the computation experiments, and the superimposed temperature field (with uniform temperature or uniform temperature gradient) was used in the modeling (Jarvis, 2000). It is possible to streamline the heat diffusion problem solution by using another lattice with the same time step and multiple spatial step accordingly adjusted (Gurgul at al., 2010), but this method reduces the precision of solidification mapping. The aim of this work is the verification of the acceleration ability of temperature field calculation in the CAFD solidification modeling.

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2. TEMPERATURE CALCULATION IN THE CAFD SOLIDIFICATION MODELING

From a mathematical point of view, the heat transfer in the two neighbor regions of different phases with a sharp interface B between it and phase transition at the interface may be described by a linear partial differential equation (PDE Fourier equation)

$$c\frac{\partial T}{\partial \tau} = \mathrm{div}(\lambda \,\mathrm{grad}\, T) + Q \tag{1}$$

with a source term $Q = 0$ and a moving boundary condition (BC) at the trailing border B

$$\mathbf{u} \cdot L = (\lambda \,\mathrm{grad}\, T)\big|_{B-} - (\lambda \,\mathrm{grad}\, T)\big|_{B+} \tag{2}$$

where T – temperature, τ – time, c – volumetric specific heat, λ – thermal conductivity, $\mathbf{u}$ – vector of the boundary migration velocity in the positive normal direction of border B, L – volumetric latent heat.

In the numerical solution by CAFD method the linear equation is substituted by non-linear one with the source term

$$Q = L\frac{\mathrm{d}\, f_s}{\mathrm{d}\,\tau} \tag{3}$$

where f_s is a solid fraction.

According to the eq. (3), heat source is equal to zero in one-phase domains whereas it has non-zero value only in the interface cells (were grain boundary is placed).

For the numerical solution PDE (1) was substituted by a system of difference equations (one equation for one lattice nod i)

$$\sum_j d_{i,j}T_j + q_i = T_i' \tag{4}$$

where

$$d_{\substack{i,j \\ i\neq j}} = -(\lambda_{i,j}\Delta\tau)/(c_i\Delta x^2) \tag{5}$$

$$d_{i,i} = 1 + \sum_j (\lambda_{i,j}\Delta\tau)/(c_i\Delta x^2) \tag{6}$$

$$q_i = L\Delta f_i / c_i \tag{7}$$

with a summation of products $d_{i,j}T_j$ for all nods j adjoining to cell i, where T'_i is the initial temperature value from the previous time level, Δf_i is solid fraction changes during the time step $\Delta\tau$, and $\lambda_{i,j}$ is a mean heat conductivity of the material in the two neighbor cell i and j.

Using of the CAFD method for the solidification modeling was presented in details by Burbelko (2004). The temperature and concentration field predictions by using a numerical method is one of elements of the CAFD simulation. Matrix **A** of the difference equation system (5) is diagonally dominant. According to Chapra and Canale (2006) and Taler and Duda (2003), Gauss–Seidel (GS) method is an effective one used for the solution of this system. This method is an iterative technique that solves the system of equations (4) by sequentially using of forward substitution for all nods of the lattice

$$T_i^{(k+1)} = \frac{1}{d_{i,i}}\left[T_i' - q_i^{(k)} - \sum_{j<i}\left(d_{i,j}T_j^{(k+1)}\right) - \sum_{j>i}\left(d_{i,j}T_j^{(k)}\right)\right] \tag{8}$$

where upper indices k and k+1 denotes two consequent iteration steps.

The condition of the iteration process termination is inequality

$$\left\|T^{(k+1)} - T^{(k)}\right\| \le \varepsilon \tag{9}$$

where ε is the given tolerance.

Ability of the acceleration of the non-uniform temperature distribution computation by means Gauss-Seidel iterative solution with the reduced iteration number (GSRIN) of the implicit scheme was analyzed. In the proposed solution successive approximations of T_i value is excluded from the iterative loop after the iteration step m for the nodes i on condition that

$$\left|T_i^{(m)} - T_i^{(m-1)}\right| \le \varepsilon \tag{10}$$

It means, that GS iterative scheme (8) in the GSRIN was substituted by

$$T_i^{(k+1)} = \begin{cases} \dfrac{1}{d_{i,i}}\left[T_i' - q_i^{(k)} - \sum_{j<i}\left(d_{i,j}T_j^{(k+1)}\right) - \sum_{j>i}\left(d_{i,j}T_j^{(k)}\right)\right] & \text{for} \quad k \le m \\ T_i^{(k)} & \text{for} \quad k > m \end{cases} \tag{11}$$

In the test task increment of the solid fraction in the interface cells was calculated by the following equation up to time of full source face depletion:

$$\Delta f_i^{(k+1)} = \begin{cases} c_i L^{-1}\left[T_i' - T_i^{(k+1)}d_{i,i} - \sum_{j<i}\left(d_{i,j}T_j^{(k+1)}\right) - \sum_{j>i}\left(d_{i,j}T_j^{(k)}\right)\right] & \text{for} \quad k \le m \\ \Delta f_i^{(k)} & \text{for} \quad k > m \end{cases} \tag{12}$$

The accuracy of the proposed method was proved by means of the confrontation with results of

known exact solution of the classical Schwarz problem.

3. SCHWARZ MODEL OF SOLIDIFICATION

An exact mathematical solution for the problem applied to the solidification of superheated metal placed in semi-infinite one-dimensional space, having a perfect thermal contact with a semi-infinite mold, was presented by Schwarz (1931). This model can be used to calculate temperature at any point of a metal-mold system without accounting of liquid convection. It was supposed that solidification temperature T_S is constant.

The temperature distribution in the liquid metal, solid metal and in the mold in this system, without thermal resistance at the metal-mold interface can be calculated through the general solution:

$$T_i(x,\tau) = A_i + B_i \operatorname{erf}\left(\frac{x}{2\sqrt{a_i\tau}}\right) \tag{13}$$

Specific solutions for liquid metal (i = 1), solidified metal (i = 2) and mold (i = 3), accordingly:

$$T_1(x,\tau) = T_L + (T_S - T_L)\left[1-\operatorname{erf}\left(\frac{x}{2\sqrt{a_1\tau}}\right)\right]\left[1-\operatorname{erf}\left(\beta\sqrt{\frac{a_2}{a_1}}\right)\right]^{-1} \tag{14}$$

$$T_2(x,\tau) = T_C + (T_S - T_C)\operatorname{erf}\left(\frac{x}{2\sqrt{a_2\tau}}\right)(\operatorname{erf}\beta)^{-1} \tag{15}$$

$$T_3(x,\tau) = T_C + (T_M - T_C)\operatorname{erf}\left(\frac{x}{2\sqrt{a_3\tau}}\right) \tag{16}$$

were T_L and T_M are the initial temperature values of liquid metal and mold; $a = \lambda/c$ is a temperature conductivity; x and τ are a spatial coordinate and time; erf() is Gauss error function.

Constant value of the metal-mold interface temperature T_C is expressed by:

$$T_C = \left(T_S + T_M\frac{b_3}{b_1}\operatorname{erf}\beta\right)\left(\frac{b_3}{b_1}\operatorname{erf}\beta + 1`\right)^{-1} \tag{17}$$

Value of the solidification constant β can be obtained solving the following equation:

$$\frac{b_3(T_S - T_M)}{\frac{b_3}{b_1}\operatorname{erf}\beta + 1}\exp(-\beta^2) - \frac{b_1(T_L - T_S)}{1-\operatorname{erf}\beta}\exp(-\beta^2) = \sqrt{\pi a_1}\rho_1 L_1\beta \tag{18}$$

were $b = \sqrt{\lambda c}$ is a heat accumulation coefficient.

4. CALCULATION AND RESULTS

Calculation were performed on the one-dimensional lattice with 2000 nodes with a border condition calculated by equations (14) and (16). The spatial step of the lattice is equal to 1 mm. Material parameters and initial conditions are shown in the table 1.

Table 1. *Material parameters and initial conditions.*

Name	Symbol	Value for		Units
		metal	mold	
Thermal capacity	c	6026400	762840	J/(m^3·K)
Heat conductivity	λ	18	1.0	W/(m·K)
Initial temperature	$T_{L/M}$	1205	20	°C
Latent heat	L_1	267 955	-	J/kg
Solidification temperature	T_S	1200	-	°C
Solidification constant	β	0.2065		-

Temperature profile in the calculation domain after the 3600 s predicted by Schwarz solution – equation (14)-(16) – is shown in figure 1a. Differences between the analytical solution and numerical calculation are presented in figures 1b-d for three different tolerances ε: 10^{-4}, 10^{-5} and 10^{-6} K. The results of the numerical modeling with a full GS iteration process and GSRIN have the similar deviation from the exact analytical solution. When the tolerance value ε grow from 10^{-6}K to 10^{-4}K maximal deviation of both numerical scheme decreases from 0,9 to 0,6 K.

The reason of this non-typical behavior of the CAFD model may be the mode of the approximation of the heat source position in the interface cells. Solidification front has a diffuse character. It was assumed that during the solidification migration of the solid-liquid border through the cell of CA the temperature of the FD lattice node is constant and is equal to solidification temperature T_s. Changes of the front position in the CAFD model has a discrete character.

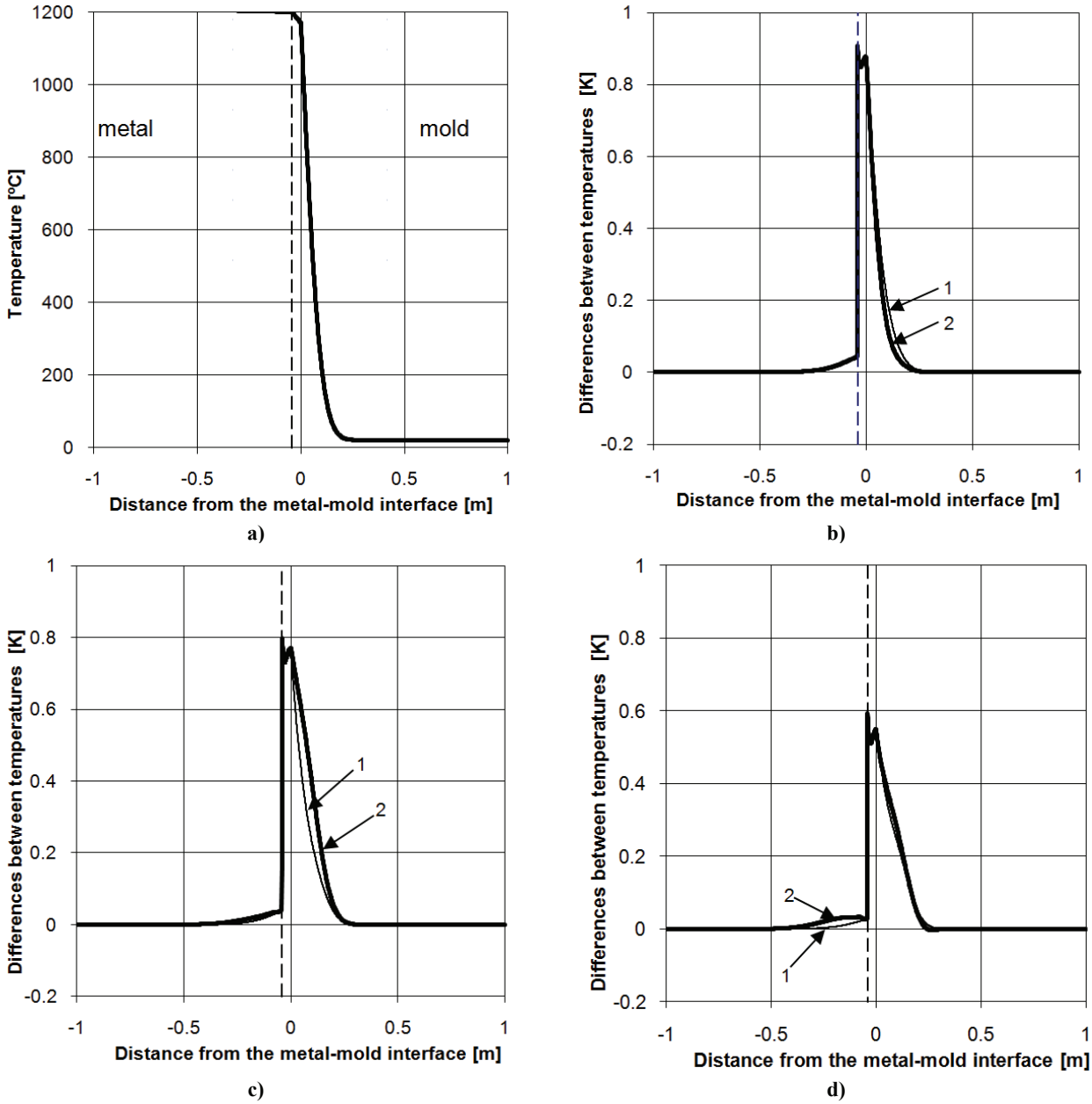

Fig. 1. *Analytical solution of the Schwarz task (a), and differences between the exact and numerical solutions as a function of the distance from the metal-mold interface for full iteration GS scheme (1) and for GSRIN (2); dashed line – position of the solid-liquid interface. Tolerances: b) $1e^{-6}$K, c) $1e^{-5}$K, d) $1e^{-4}$K. Simulation time τ = 3600 s.*

For the estimation of the numerical calculation precision the value of the mean quadrate error was used with a summation for all lattice nodes:

$$\delta = \sqrt{\frac{\sum_{i=1}^{n}\left(T_{Sch,i} - T_{N,i}\right)^2}{n}} \qquad (19)$$

where T_{Sch} is the temperature in the nodes position according to the Schwarz model, T_N is a results of numerical modeling and n is lattice nod number.

Mean quadrate error of the solution as a function of tolerance for simulation time 1800 and 3600 s was shown in figure 2. The tolerance diminishing from 10^{-4}K to 10^{-6}K have a weak influence on this value for both iterative scheme. Even the little growth of the mean quadrate error was observed.

For the evaluation of the solution rate of the GS and GSRIN schemes the value hereinafter referred to as a „solver length" was calculated. This value is equal to the number of temperature calculations by means of equation (8) for full GS method or by (11) for GSRIN realized in the all nodes of FD lattice, in the every time step and every iteration.

Solving length of both numerical solution and difference between them are shown in figure 3 for simulation time 1800 and 3600 s. Solving length is longer for less tolerance. As it is shown in fig. 3,

GSRIN scheme is near 4-times less time consuming than full GS iteration scheme.

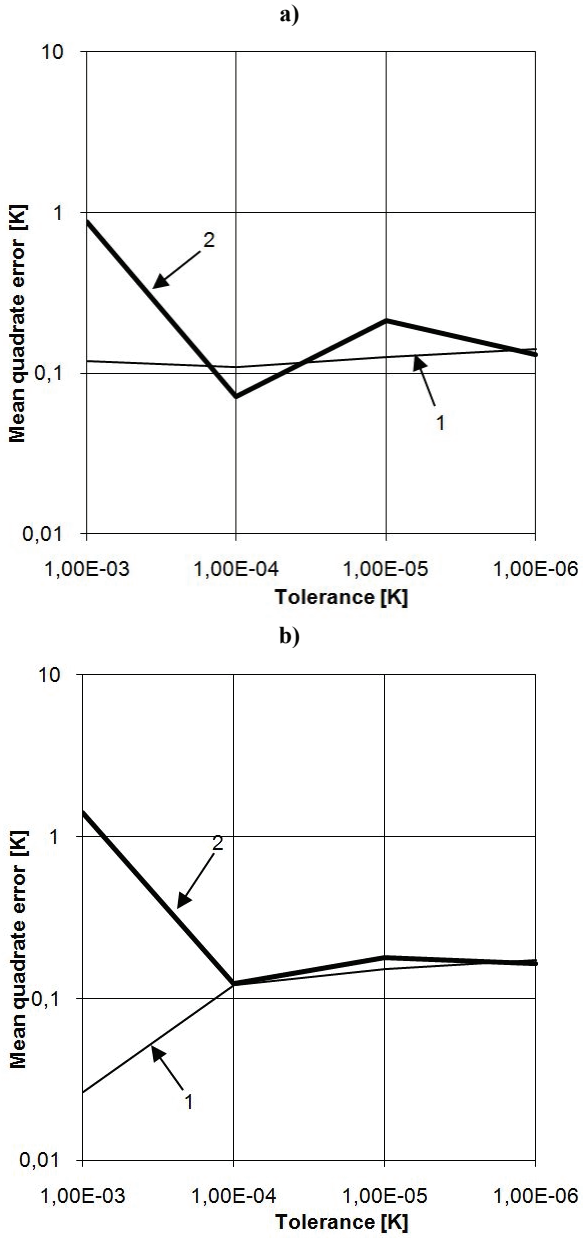

Fig. 2. Comparison of the mean square error of the GS (1) and SGRIN (2) solution as a function of the tolerance. Simulation time: a) 1800 s, b) 3600 s

5. CONCLUSIONS

The time saving calculation scheme named as GSRIN was proposed for temperature calculation in the CAFD solidification modeling. In the proposed solution the reduced and diversified number of iteration was used for different lattice nodes.

GSRIN solution gives the equivalent precision as the well-known Gauss-Seidel iterative solution. In the CAFD model with a diffusive interface the tolerance decreasing may cause the growth of the calculation error.

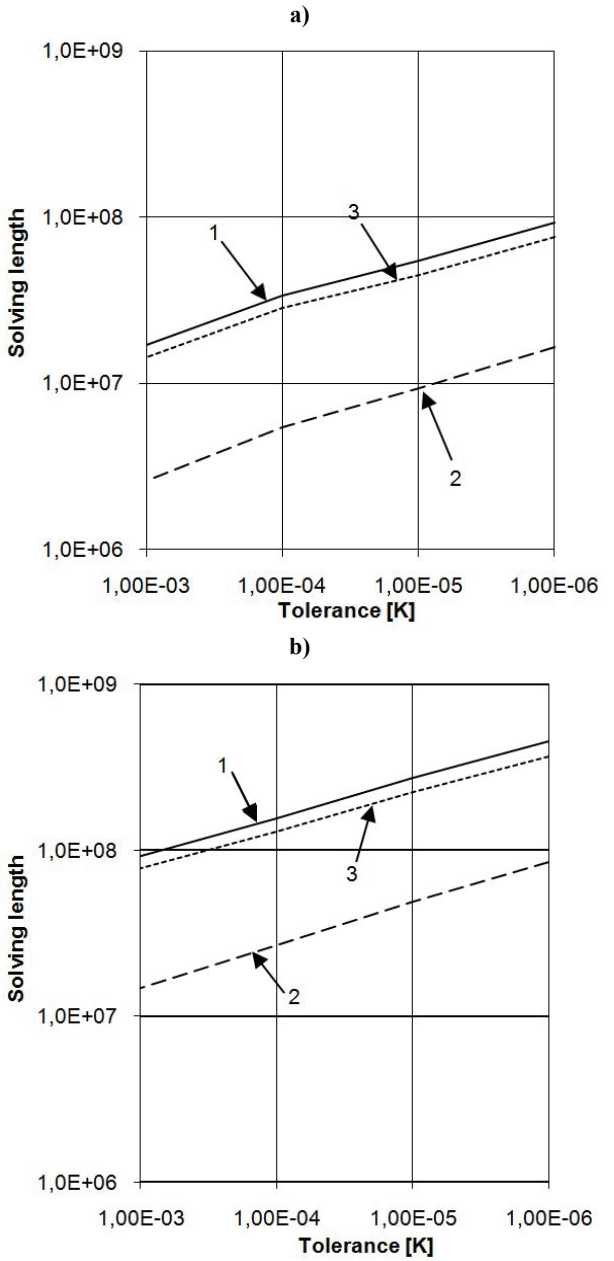

Fig. 3. Comparison of the solving length of the GS (1) and GSRIN (2) solution and difference between these values (3) as a function of the tolerance. Simulation time: a) 1800 s, b) 3600 s.

It was not advisable do decrease the tolerance of the numerical calculation of the temperature field in the solidification modeling by CAFD method, because it was invoked the solving length prolongation and may results in the error increasing.

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REDUKCJA CZASU OBLICZEŃ W MODELOWANIU KSZTAŁTOWANIA SIĘ MIKROSTRUKTURY PODCZAS KRYSTALIZACJI METODĄ CAFD

Streszczenie

Metoda CAFD (od ang. Cellular Automaton + Finit Difference, połączenie metod automatu komórkowego i różnic skończonych) jest jedną z dobrze znanych metod modelowania zmian mikrostruktury stopów podczas krystalizacji. W modelowaniu mikrostruktury za pomocą CAFD kształt rosnących ziaren i końcowa struktura są wynikami modelowania, a nie zakładane z góry.

Proces krystalizacji metali i stopów jest typowym przykładem systemów, w modelowaniu których należy uwzględniać różne zjawiska fizyczne, dla opisu których potrzebna jest zróżnicowana skala wymiarowa i czasowa. Cecha ta musi być uwzględniona w modelowaniu procesów tworzenia się mikrostruktury, a mianowicie podczas rozwiązywania zagadnień przenoszenia ciepła, dyfuzji składników w ciekłej i stałej fazach, termodynamiki nierównowagowych przemian fazowych w warunkach niejednorodności składu chemicznego rosnących ziaren i zanikającej fazy macierzystej, kinetyki zarodkowania i wzrostu ziaren.

Kompletne rozwiązania numeryczne, uwzględniające opisane wyżej zjawiska są bardzo czasochłonne. W niniejszej pracy przeanalizowano możliwość przyspieszenia poszukiwania rozwiązania numerycznego dla schematu niejawnego obliczenia pola temperatury za pomocą zróżnicowanej ilości iteracji równań modelowych. Wyniki modelowania numerycznego w celu sprawdzenia poprawności metody skonfrontowano z rozwiązaniem analitycznym zadania Schwarza.

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