METALLURGY AND FOUNDRY ENGINEERING – Vol. 37, 2011, No. 1

Andriy Burbelko* , Jacek Początek**

REDUCTION OF THE CALCULATION TIME IN THE MODELING OF THE MICROSTRUCTURE FORMATION BY CAFD METHOD

1. INTRODUCTION

Numerical methods based on the CAFD method [1] (Cellular Automaton + Finite Differences) have a wide application in the simulation of the following physical phenomena: heat transfer, components diffusion in the solid and liquid, nonequilibrium thermodynamic of the phase transformation under the condition of inhomogeneous chemical composition of growing and vanishing substances, grain nucleation and growth. This method can predict the temperature and concentration fields [2].

In the CAFD models parabolic nonlinear differential equations are solved numerically by finite differences method. The order of magnitude of lattice cell size used for the microstructure modeling is equal to one micron. That is why the CAFD models are time consuming.

The „bottleneck" of the modeling is the temperature calculation because for the real properties of metals and alloys the time step in the temperature simulation is a few order of magnitude shorter than in the diffusion fields solution [3]. The main aim of this paper is the verification of the ability to accelerate the numerical Gauss-Seidel (GS) solution for the implicit scheme of temperature field calculation by means of the reduced number of the successive approximation in the iterative solution of the set of model difference equations.

2. TEMPERATURE FIELD CALCULATION

From the mathematical point of view, the heat flow in the adjoining sub-domains of different substances with a common moving interface *B* between them may be described by the non-linear differential equation:

* Ph.D., D.Sc. ** M.Sc.: Faculty of Foundry Engineering, AGH University of Science and Technology, Kraków, Poland; e-mail: abur@agh.edu.pl

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

with a zero source function $Q = 0$ and moving boundary condition on B

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

where:

T – temperature,
τ – time,
c – volumetric heat capacity,
λ – heat conductivity,
$\mathbf{u}$ – vector of the interface migration velocity,
L – enthalpy of the phase transformation at the interface.

In the numerical solution the linear equation was substituted by the non-linear with the following source function:

$$Q = L\frac{df_s}{d\tau} \tag{3}$$

where f_s – volume fraction of the new phase.

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

In the numerical solution thermal conductivity equation (1) is substituted by the set of difference equations (one equation for one lattice node i)

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

where:

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

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

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

T'_i – temperature of the node i in the previous time step,
Δf_i – change of the new phase volume fraction during the last time step $\Delta\tau$,
$\lambda_{i,j}$ – mean value of the heat conductivity between two adjacent cells i and j.

Calculations of the temperature and concentration fields are the important parts of the CAFD simulation. Matrix D for the coefficients of the set of equations (4) has a diagonal structure. According to [4, 5] the Gauss-Seidel (GS) solution method is the most effective for the iterative solution of sets of equations with a diagonal matrix. This method consists of the iterative solution of set (4) and sequential substitution of unknown variables by results of the previous step:

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

where indices k and $k+1$ means previous and present steps of the iterative process.

The iterative process will compete when

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

where ε is a predetermined tolerance value.

The ability of the acceleration of the numerical solution in the non-uniform temperature field modeling was analyzed by the GS method with reduced iteration number (GSRIN). In the proposed algorithm further sequential substitutions of the unknown variables T_i were excluded from the iteration loops from the step when the following condition will be fulfilled:

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

This implies that GS method described by the set of equation (7) was substituted by following:

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

The precision of the proposed algorithm was verified by confrontation of the obtained results of the calculation with the known analytical solution of the Schwarz task [6].

3. SCHWARZ ANALYTICAL SOLUTION

Analytical solution for the heat transfer in the two adjacent half-spaces (one occupied by a superheated metal and next one by a mold material) was presented in [6]. This solution was obtained for the uniform initial conditions and gives the temperature distribution in the

both half-spaces and the position of the solidifi-cation front. The solution may be used for the temperature calculation in the one-dimensional system „casting – mold" when the convection phenomenon may be neglected. It was assumed that the solidification temperature T_S is constant.

Heat resistance in the contact between metal and mold was neglected. For the temperature distribution as in the half-space of metal, as in the half-space of mold following general solution was obtained:

$$T_i(x,\tau) = A_i + B_i \operatorname{erf}\left(\frac{x}{2\sqrt{a_i\tau}}\right) \tag{12}$$

Specific solutions for the liquid metal (i = 1), for solid metal (i = 2) and for mold (i = 3) are:

$$T_1(x,\tau) = T_L + (T_S - T_L)\left[1 - \operatorname{erf}\left(\frac{x}{2\sqrt{a_1\tau}}\right)\right]\left[1 - \operatorname{erf}\left(\beta\sqrt{\frac{a_2}{a_1}}\right)\right]^{-1} \tag{13}$$

$$T_2(x,\tau) = T_C + (T_S - T_C)\operatorname{erf}\left(\frac{x}{2\sqrt{a_2\tau}}\right)(\operatorname{erf}\beta)^{-1} \tag{14}$$

$$T_3(x,\tau) = T_C + (T_M - T_C)\operatorname{erf}\left(\frac{x}{2\sqrt{a_3\tau}}\right) \tag{15}$$

where T_L and T_M – initial values of the temperature in the half-spaces of metal and mold (respectively), $a = \lambda/c$ – thermal diffusivity, x – distance from the contact, τ – time, erf() – Gauss error function.

Temperature T_C in the contact between metal and mold is the constant calculated from the relation:

$$T_C = \left(T_S + T_M \frac{b_3}{b_1}\operatorname{erf}\beta\right)\left(\frac{b_3}{b_1}\operatorname{erf}\beta + 1\right)^{-1} \tag{16}$$

where solidification constant β is the solution of the following equation:

$$\frac{b_3(T_S - T_M)}{\frac{b_3}{b_1}\operatorname{erf}\beta + 1}\exp\left(-\beta^2\right) - \frac{b_1(T_L - T_S)}{1 - \operatorname{erf}\beta}\exp\left(-\beta^2\right) = \sqrt{\pi a_1}\rho_1 L_1\beta \tag{17}$$

where $b = \sqrt{\lambda c}$ is a heat accumulation constant.

4. SIMULATION RESULTS

Numerical solution was obtained on the one-dimensional lattice with 2000 nodes and spatial step equal to 1 mm. Properties of the materials and initial conditions are presented in the Table 1.

Table 1. Materials properties and initial conditions

Name	Symbol	Value for		Units
		metal	mold	
Volumetric heat capacity	c	6 026 400	762 840	J/(m^3·K)
Heat conductivity	λ	18	1.0	W/(m·K)
Initial temperature	$T_{L/M}$	1 205	20	^{o}C
Enthalpy of the phase transformation	L_1	267 955	–	J/kg
Solidification temperature	T_S	1 200	–	^{o}C
Solidification constant	β	0.2065		–

For the evaluation of the solution precision the mean square error was used:

$$\delta = \sqrt{\frac{\sum_{i=1}^{n} \left(T_{Sch,i} - T_{N,i}\right)^2}{n}} \tag{18}$$

where:

T_{Sch} – results obtained from the analytical Schwarz solution,
T_N – results of numerical solutions,
n – number of nodes in the lattice.

Temperature distribution according to Schwarz's solution is presented in Figure 1a for $L_1 = 0$ after the time 5400 s. Divergences between numerical solutions and analytical ones are shown in Figures 1b–d for different tolerance of the numerical solutions ε (10^{-6}, 10^{-5} and 10^{-4} K). The behavior of numerical solutions by using GS and GSRIN methods are similar: the smaller tolerance value, the smaller difference between numerical and analytical solutions take place.

Values of the mean square error for modeling time 5400 s as a function of tolerance are shown in Figure 2a. As indicated in this picture, for the smaller tolerance the results of the numerical modeling are closer to the analytical solution.

For the estimation of hardware loading during the numerical solution the total number of the iterative scheme (8) used for every node was counted for the GS and GSRIN algorithms. Results were presented in Figure 2b. As illustrated, the smaller tolerance of the iteration, the more operation were necessary for the temperature distribution determination for both schemes, but for the GS method the hardware loading is almost three times greater than for the GSRIN.

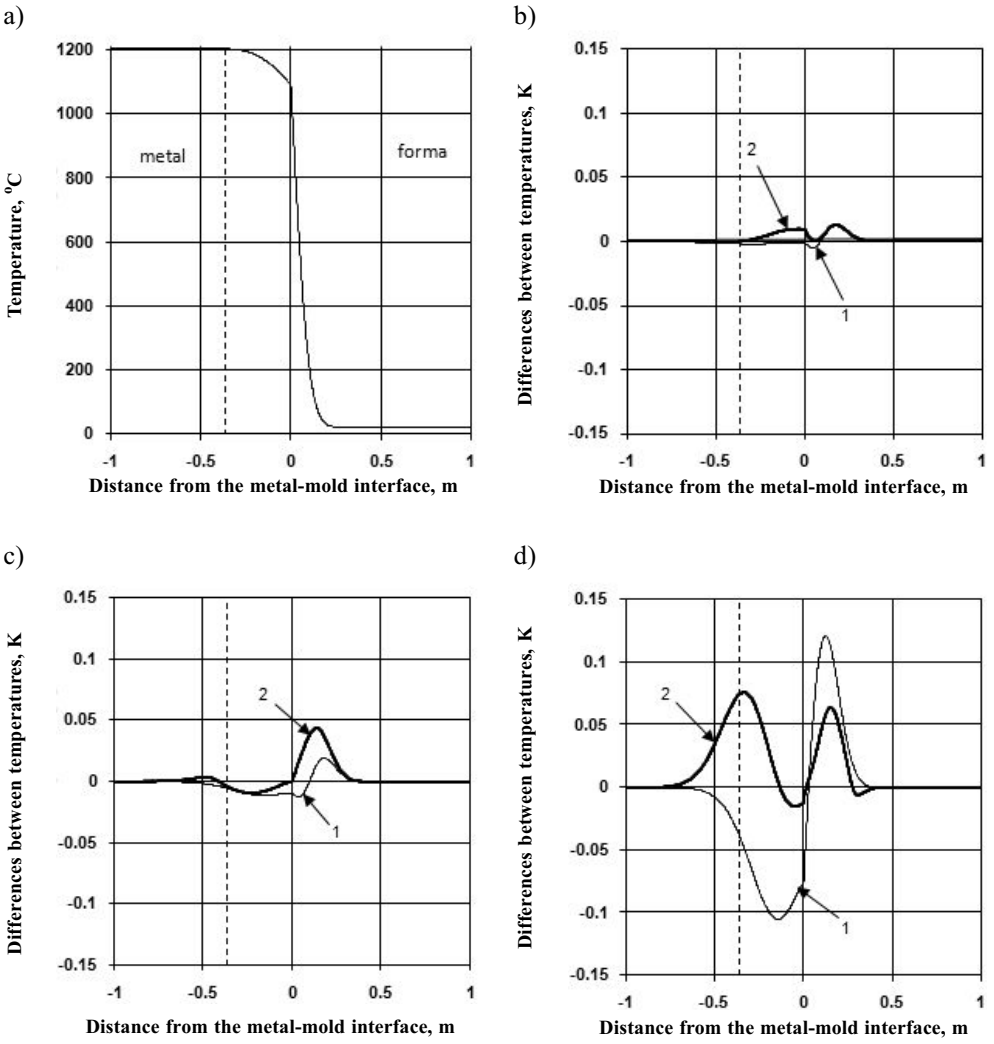

Fig. 1. *Analytical Schwarz solution (a) and differences between exact and numerical solutions as function of distance from the sub-domain contact position for the GS (1) and GSRIN (2) methods for* $L_1 = 0$*; dashed line – solidification front position. Tolerance value* ε*: b)* $1e^{-6}$ *K; c)* $1e^{-5}$ *K; d)* $1e^{-4}$ *K. Simulation time* $\tau = 5400$ *s*

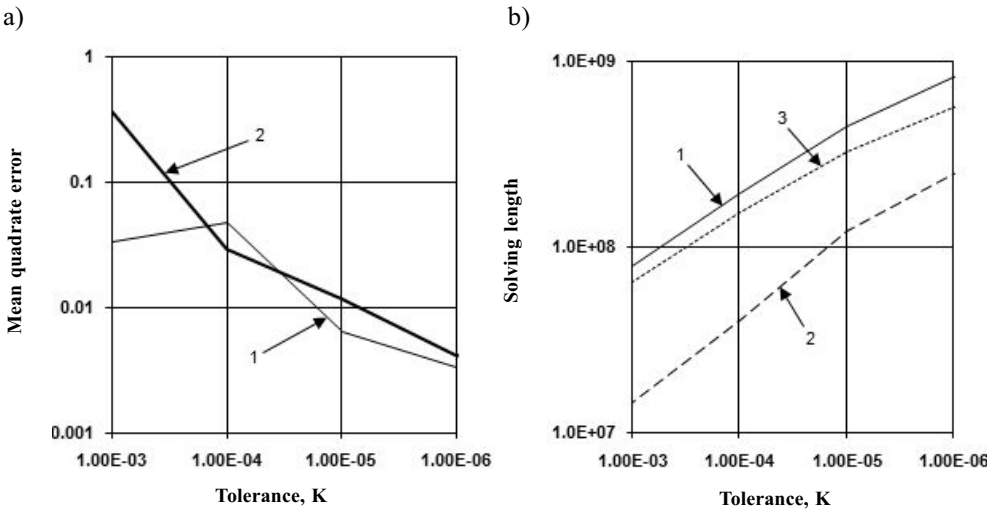

Fig. 2. *Mean square error of the temperature distribution (a) and number of operation (b) for the different numerical solution tolerance: 1 – for the GS scheme; 2 – for the proposed GSRIN scheme; 3 – saving of GSRIN solution against GS. Simulation time* τ *= 5400 s*

Temperature distribution according to Schwarz solution for non-zero heat source at solid-liquid interface (L_1 according to Tab. 1) is presented in Figure 3a after the time 5400 s. As viewed in these figures, the solid layer width is smaller in this case than in the previous solution. Divergences between numerical solutions and analytical ones are shown in Figure 3b–d for the same tolerance values of the numerical solutions ε. Numerical simulation results for both algorithms (GS and GSRIN) also in this case are similar.

Values of the mean square error for modeling time 5400 s as a function of tolerance are shown in Figure 4a. For the tolerance 10^{-4} K, as indicated in these figures, both methods gave similar results. Unfortunately, smaller ε does not improves calculation accuracy. The probable reason of this behavior of numerical solution is connected with the discrete character of the solidification front position quantification in the CAFD models. Points where temperature value is equal to *Ts* are placed always in the lattice nodes. Position of the solid-liquid interface was estimated with the tolerance equal to half spatial step of the lattice and was changed step-wise. In the analytical solution the interface position changes continuously.

For the comparison of both algorithms' efficiency in this case the total number of operation was counted (as previously). These results are shown in Figure 4b. As it is indicated in this figure, the smaller tolerance value the more operation number is necessary for the task with a non-zero source function. In this case the proposed GSRIN algorithm is more time-saving than known GS.

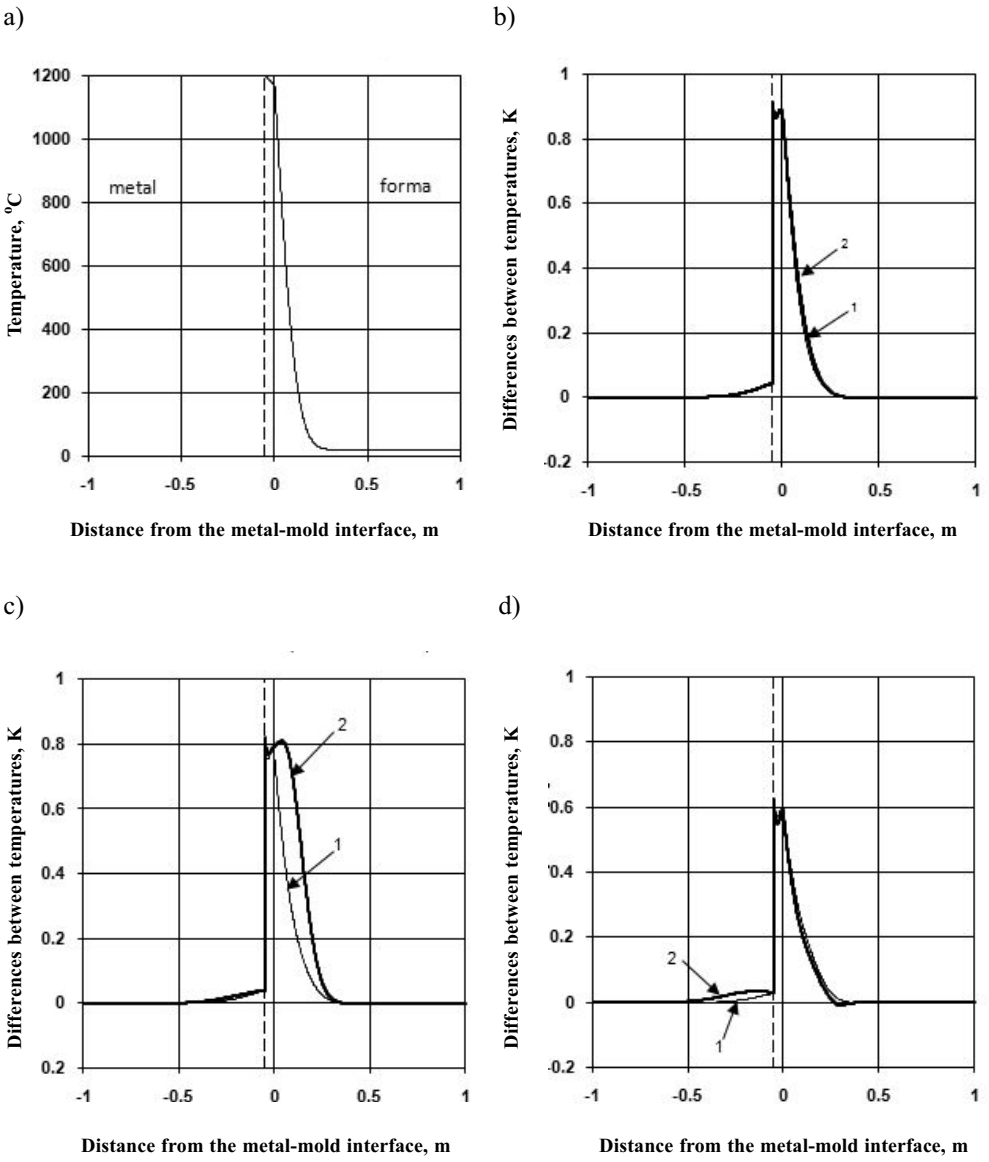

Fig. 3. *Analytical Schwarz solution (a) and differences between exact and numerical solutions as function of distance from the sub-domain contact position for the GS (1) and GSRIN (2) methods for the non-zero heat source function; dashed line – solidification front position. Tolerance value ε: b) 10^{-6} K; c) 10^{-5} K; d) 10^{-4} K. Simulation time τ = 5400 s*

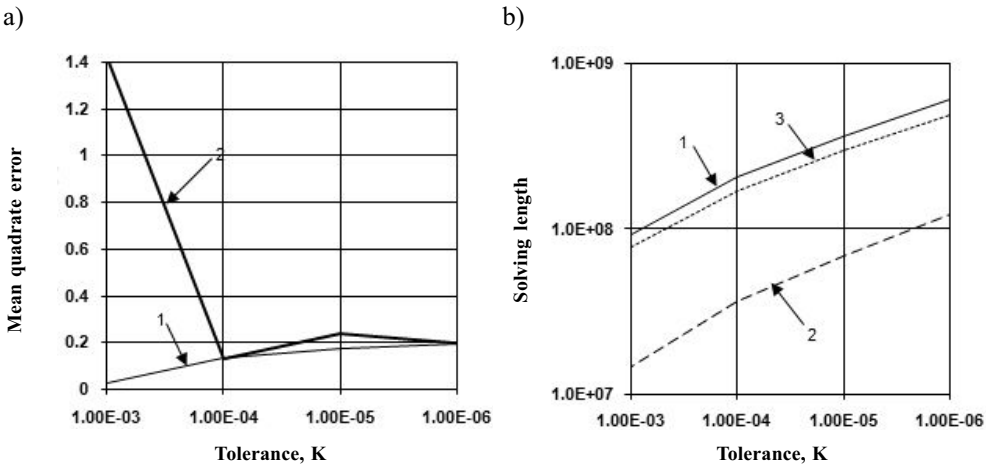

Fig. 4. *Mean square error of the temperature distribution (a) and number of operation (b) for the different numerical solution tolerance: 1 – for the GS scheme; 2 – for the proposed GSRIN scheme; 3 – saving of GSRIN solution against GS. Simulation time* $\tau = 5400$ *s*

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 the temperature value estimation in the different lattice nodes.

The results of the GSRIN solution are close to the results obtained by classical GS scheme.

The precision of the temperature distribution estimation in the solidification simulations by CAFD models is limited. Higher tolerance (smaller ε value) of the implicit iterative numerical solution does not give the best results and the smaller mean square difference between numerical solution results and exact analytical. The possible reason of this solution behavior is the discrete character of changes of the solidification front position. That is why the so high tolerance (small ε) fraught with risks of a too long duration of solution and error growth.

This study was performed under AGH-UST Project No. 10.10.170.297

REFERENCES

[1] *Brown S.G.R.*: Simulation of diffusional composite growth using the cellular automaton finite difference (CAFD) method, J. Mater. SCI., 33 (1998), 4769–4773

[2] *Zhu M.F., Hong C.P., Stefanescu D.M., Chang Y.*: Computational modeling of microstructure evolution in solidification of aluminum alloys, Metall. Mater. Trans. B, 38 (2007) 4, 517–524

[3] *Gurgul D., Burbelko A.A., Fraś E., Guzik E.*: Multiphysics and multiscale modelling of ductile cast iron solidification, Archives of Foundry Engineering, 10 (2010), 35–40

[4] *Taler J., Duda P.*: Rozwiązywanie prostych i odwrotnych zagadnień przewodzenia ciepła, WNT, Warszawa 2003

[5] *Chapra S.C., Canale R.P.*: Numerical methods for Engineers, Fifth Edition, McGras-Hill, 2006

[6] *Schwarz C.*: Die Rechnerische Behandlung der Abkühlung- und Erstarrungsvorgange bei Flüssigem Metall, Arch. für Eisenhüttenwesen, (1931) 3, 39–148

Received
January 2011