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SOLUTION OF THE STEFAN PROBLEM BY INVOLVING MATERIAL SHRINKAGE

ROZWIĄZANIE ZAGADNIENIA STEFANA Z UWZGLĘDNIENIEM SKURCZU MATERIAŁU

Abstract

In this paper we describe an algorithm for solving the one-dimensional Stefan problem by involving metal shrinkage. In this algorithm we use the finite element method supplemented by the procedures allowing to define the position of moving interface and the change material size associated with shrinkage. We present also some examples illustrating the precision of the presented method.

Keywords: *solidification; Stefan problem; shrinkage*

Streszczenie

W artykule opisano algorytm rozwiązywania jednowymiarowego zagadnienia Stefana z uwzględnieniem skurczu metalu. W algorytmie tym użyto metody elementów skończonych uzupełnionej o procedury pozwalające określić położenie ruchomej granicy miedzy fazami oraz zmianę objętości materiału związaną ze skurczem. Przedstawiono również przykład przedstawiający dokładność prezentowanej metody.

Słowa kluczowe: *krzepnięcie, problem Stefana, skurcz materiału*

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1. Introduction

Difference between density of the liquid and its solid phase causes shrinkage of metal during its solidification (there exist also substances, such as water, volumes of which expand during solidification). In this process an air-gap forms between the form and the cast, which has an influence on creating an interfacial thermal resistance between the mould and the cast. This thermal resistance determines the mould heat flux and thus affects the billet's quality, such as the cracks and oscillation marks.

Solidification of pure metals is mathematically modeled by means of the Stefan problem [1–3]. This problem consists in determination of the temperature distribution in liquid and solid phases. Simultaneously, the position of the boundary between the phases should be found as well. The Stefan problem is a non-linear problem [3]. Nonlinearity is connected with the Stefan condition resulting from the heat balance on the moving interface. In simple cases it is possible to find an exact solution of the Stefan problem [4, 5], but generally to find a solution to this problem the numerical or numerically-analytical methods must be used [1, 2, 6–8].

A mathematical model for describing processes involving the simultaneous heat and mass transfer with the phase transition in foods undergoing a volume change (shrinkage or expansion) is presented in paper [9]. To approximate the solution of the problem the finite element method and the Arbitrary Lagrangian-Eulerian method were used. Natale et al. in paper [10] determined the temperature distribution in solid and liquid one-dimensional regions and the position of two free boundaries in the solidification process with either shrinkage or expansion. The results were obtained for three different boundary conditions. In all cases, the explicit solution was given by the parametric representation of a similarity type. The one-dimensional problem of pure metal solidification involving metal shrinkage was considered also in paper [11], where the perturbation method for small Stefan numbers was used to find the solution.

In this paper we intend to show an algorithm for solving the one-dimensional Stefan problem involving metal shrinkage. In this algorithm we will use the finite element method supplemented by the procedures allowing to define the position of the freezing front and the change of material size associated with material shrinkage. To determine the boundary position we use an algorithm in which, on the basis of the Stefan condition, the size of the time step is iteratively selected so that the boundary moves to the adjacent node [2]. To determine the change in size we propose a procedure based on the mass balance. We present also some examples illustrating the precision of the presented method.

2. Formulation of the problem

Let us consider a domain (ingot domain) occupied by liquid and solid phases. This domain is variable in time. Sizes of the liquid and solid phases will change, whereas the size of the ingot will change as well due to the material shrinkage involved. We consider solidification of pure metal modeled by using the Stefan problem [1, 2]. Thus, inside domain $\Omega = \{(x, t): 0 \le x \le d(t),\ 0 \le t \le t^*\}$ the heat conduction equation is given [11]:

$$c_i\rho_i \frac{\partial u(x,t)}{\partial t} = \lambda_i \frac{\partial^2 u(x,t)}{\partial x^2} + (i-1)\left(1-\frac{\rho_1}{\rho_2}\right)\frac{d\xi(t)}{dt}\frac{\partial u(x,t)}{\partial x} \tag{1}$$

$(x, t) \in D_i \times (0, t^*)$ where $i = 1$ for liquid phase, $i = 2$ for solid phase, intervals $D_1 = (0, \xi(t))$ and $D_2 = (\xi(t), d(t))$ represent the liquid and solid phases, respectively, ξ is a function describing the position of the moving boundary (the freezing front), d denotes a function describing the length of the area associated with metal shrinkage, c_i is the specific heat, λ_i is the thermal conductivity coefficient, ρ_i denotes density of the corresponding phase and $\left(1-\frac{\rho_1}{\rho_2}\right)$ is the shrinkage factor. There are also the following initial conditions given:

$$u(x, 0) = u_0, \quad \xi(0) = \xi_0, \quad d(0) = d_0 \tag{2}$$

and the boundary conditions:

$$-\lambda_1 \frac{\partial u(0,t)}{\partial x} = q(t), \qquad t \in (0, t^*) \tag{3}$$

$$-\lambda_2 \frac{\partial u(d(t),t)}{\partial x} = \alpha\left(u(d(t),t) - u_\infty\right), \qquad t \in (0, t^*) \tag{4}$$

where α is the heat transfer coefficient and u_∞ denotes the ambient temperature.

On the moving interface the condition of temperature continuity and the Stefan condition are defined as follows:

$$u(\xi(t),t)^+ = u(\xi(t),t)^- = u^* \tag{5}$$

$$\kappa \frac{d\xi(t)}{dt} = \lambda_2 \left.\frac{\partial u(x,t)}{\partial x}\right|^+_{x=\xi(t)} - \lambda_1 \left.\frac{\partial u(x,t)}{\partial x}\right|^-_{x=\xi(t)} \tag{6}$$

where u^* is the phase change temperature and κ describes the latent heat of solidification per volume unit.

In the considered problem functions u, ξ and d, describing temperature distribution, the freezing front position and the changes of area size, respectively, are unknown. The other functions (u_0, q), coefficients and constants (c_i, ρ_i, λ_i, α, κ, u^*, u_∞, ξ_0, d_0) are given.

3. Method of solution

In this section we describe the procedure for solving the problem formulated above. Supposing that the total weight of the material is equal to m_0 and is constant in time of the modeled process, we are able to write the mass balance equation $m_0 = m_1 + m_s$, where m_1 and

m_s represent the mass of the material in the liquid and the solid state, respectively. The one-dimensional problem can be used, among others, to describe the phenomena occurring inside the slab with thickness $d(t)$, height h and width l, where $d(t) << h$ and $d(t) << l$. In this case the previous equation can be written as:

$$m_0 = \xi(t)\rho_1 hl + (d(t) - \xi(t)\rho_2 hl \tag{10}$$

By transforming the above relation we can determine function d:

$$d(t) = \frac{m_0 - \xi(t)\rho_1 hl}{\rho_2 hl} + \xi(t) \tag{11}$$

The initial mass m_0 is equal to $m_0 = \xi_0\rho_1 hl + (d_0 - \xi_0)\rho_2 hl$ (equation (10) for $t = 0$), therefore:

$$d(t) = \frac{(\xi_0 - \xi(t))\rho_1}{\rho_2} + (d_0 - \xi_0) + \xi(t) \tag{13}$$

If we additionally assume that in the initial moment the whole bar is in the liquid phase, i.e. $d_0 = \xi_0$, the above equation is simplified to the form:

$$d(t) = \frac{\rho_1}{\rho_2}(d_0 - \xi(t)) + \xi(t) \tag{14}$$

To find the approximate solution of presented problem we use the finite element method [2, 12]. For moment t_k we divide interval $[0, d(t_k)]$ into n elements $0 = x^k_0 < x^k_1 < ... < x^k_{n-1} < x^k_n = d(t_k)$.

To determine the position of the interface we use an algorithm in which, on the basis of the Stefan condition, the size of the time step is iteratively selected so that the boundary moves to the adjacent node [2]. In this method we want the freezing front to move between the successive nodes starting from node x^0_n in moment $t_0 = 0$, i.e. in the k-th step the boundary should be in node x^k_{n-k}. It requires a variable size of the time step. Let us suppose that after $k - 1$ time steps (in moment t_{k-1} the boundary is in node x^{k-1}_{n-k+1}. The method assumes that after the k-th step (in moment t_k) of length Δt the boundary will be in node x^k_{n-k}. From the condition of temperature continuity it follows that in moment t_k the temperature in node x^k_{n-k} is equal to the solidification temperature u^*. In this way we obtain the heat conduction problem in intervals $[0, x^k_{n-k}]$ and $[x^k_{n-k}, d(t_k)]$ with the known boundary conditions which should be solved. We know also the temperature distribution in the previous time step. Thereby, by using the finite element method (or some other method) we can determine the temperature distribution in moment t_k and then the heat flux on the moving interface. Certainly, the determined values depend on the time step size Δt which we determine iteratively by using the Stefan condition. At the beginning of each step of calculations we assume the time step size, for instance, as equal to the final time step size from the previous stage of calculations.

Then we determine the corresponding temperature distribution in moment t_k, based on which we determine the heat fluxes on the moving interface, i.e. in node x^k_{n-k}, from the side of the liquid and solid phase. By using the Stefan condition we improve the time step size Δt and recalculate the temperature distribution in moment t_k. The process of improving the time step size is repeated until the desired accuracy ε would be reached.

We describe now the procedure of determining time step size Δt in more detail. Let us remember that elements located between the adjacent nodes have the same mass $m = m_0/n$. The length of the element for the liquid and solid phase is, respectively, equal to:

$$h_1 = \frac{m}{\rho_1} = \frac{d_0}{n}, \quad h_2 = \frac{m}{\rho_2} = \frac{d_0}{n}\frac{\rho_1}{\rho_2} \tag{17}$$

Thereby, in moment t_k the coordinates of nodes are the following:

$$x_i^k = \begin{cases} ih_l, & i \le n-k \\ (n-k)h_1 + (i-n+k)h_2, & i > n-k \end{cases} \tag{19}$$

Let us denote $u_{i,k} = u(x_i^k, t_k)$ and $u^k = [u_{0,k}, ..., u_{n,k}]^T$.

From the Stefan condition for $t = 0$ we have:

$$\kappa \frac{\xi(\Delta t) - \xi_0}{\Delta t} = \lambda_2 \left.\frac{\partial u(x,u)}{\partial x}\right|_{x=d(0)} - \lambda_1 \frac{u_{n,0} - u_{n-1,0}}{h_1} \tag{20}$$

After some transformations and by using the boundary condition we get:

$$\Delta t = \frac{-\kappa h_1}{-\alpha(u^* - u_\infty) - \lambda_1 \dfrac{u^* - u_{n-1,0}}{h_1}} \tag{21}$$

It will be the initial time step size. After determining the temperature distribution in moment t_k we make a correction of the time step size, i.e. for $k < n$ we have:

$$\Delta t = \frac{-\kappa h_1}{\lambda_2 \dfrac{u_{n-k+1,k} - u^*}{h_2} - \lambda_1 \dfrac{u^* - u_{n-k-1,k}}{h_1}} \tag{22}$$

and for $k = n$ we have:

$$\Delta t = \frac{-\kappa h_1}{\lambda_2 \dfrac{u_{n-k+1,k} - u^*}{h_2} + q(t_n)} \tag{23}$$

In the above equations we applied the boundary conditions (5) and (6) and difference quotients for the left- and right-side derivative of the temperature on the moving interface.

In order to determine the temperature in moment t_k we use the finite element method by obtaining the matrix equation [2, 12]:

$$C\dot{u} + Ku = f \tag{24}$$

where C is the heat capacity matrix and K is the heat conductivity matrix taking into account the component resulting from the convective component in equation (1). Matrices C, K and vector f are constructed on the grounds of the Galerkin method [2, 12]. Due to the movement of the boundary between the adjacent nodes, these matrices have to be recalculated for every k. If parameters \$$c$, ρ, λ, q, u_∞, α are not constant over time, the matrices and vector f have to be recalculated also for every Δt. We can discretize the above equation by using the implicit scheme:

$$\left(\frac{1}{\Delta t}C + K\right)u^k = \frac{1}{\Delta t}Cu^{k-1} + f \tag{26}$$

By solving the above system of linear equations we get the temperature distribution in moment t_k which allows us to determine the new time step size Δt.

4. Computational example

We start with a theoretical example for which an exact solution is known. In the considered example we assume: $c_1 = 1$, $c_2 = \frac{9}{5}$, $\rho_1 = 1$, $\rho_2 = \frac{10}{9}$, $\kappa = \frac{11}{10}$, $\lambda_1 = \frac{1}{2}$, $\lambda_2 = \frac{20}{9}$, $u^* = 0$, $u_\infty = -2$, $\xi_0 = d_0 = 1$, $t^* = 1$, $u_0(x) = 1 - e^{2(x-1)}$, $q(t) = e^{2(t-1)}$ and $\alpha(t) = \frac{21}{10}e^{\frac{1701}{2000}t}\left(3 - e^{\frac{1701}{2000}t}\right)^{-1}$.
An exact solution of the above problem is given by functions:

$$d(t) = 1 - \frac{t}{10}, \quad \xi(t) = 1 - t, \quad u(x,t) = \begin{cases} 1 - e^{2(x+t-1)}, & (x,t) \in D_1 \times \left(0, t^*\right) \\ 1 - e^{\frac{189}{200}(x+t-1)}, & (x,t) \in D_2 \times \left(0, t^*\right) \end{cases}$$

The calculations were performed for the grid dividing area Ω into 50, 100, 200 and 500 elements. The time step size was determined iteratively with accuracy 0.001 s. Most often three or four iterations were enough to get this accuracy. Table 1 presents the run time of the algorithm, the maximal and averaged absolute error of the time step size determination and the obtained final time.

Figure 1 displays temperature curves for the grid dividing the area into 200 elements. The dashed lines represent the approximate curves for $x_p = 0$ (dotted), $x_p = 0.5$ (dashed) and $x_p = d(t)$ (dot-dashed), whereas the solid lines represent the exact curves for these points.

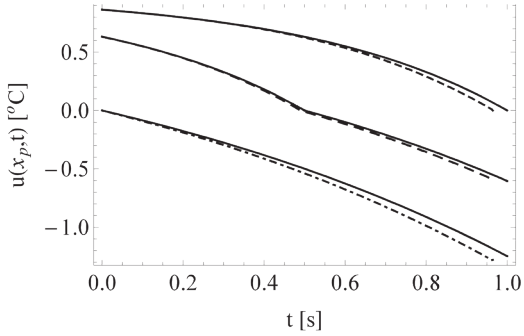

Fig. 1. Temperature curves in points $x_p = 0$ (dotted), $x_p = 0.5$ (dashed) and $x_p = d(t)$ (dot-dashed) for $n = 200$ (solid lines – exact values, dashed lines – approximate values)

Table 1

Run time and the errors of approximate solution
(Δ – absolute errors, t^* – final time)

n	Run time [s]	$\Delta_{\max}$	Δ_{avg}	T^*
50	0.345	0.0542	0.0182	0.905
100	1.764	0.0419	0.0140	0.951
200	11.170	0.0357	0.0112	0.957
500	139.406	0.0318	0.0107	0.961

Figure 2 shows the moving interface position $\xi(t)$ (left figure) and length $d(t)$ of the area (right figure). The dashed lines represent the approximate values and the solid lines represent the exact values. It can be seen that the error of time step size selection decreases with an increase of the grid density. Thus, by increasing the grid density we may get the more accurate results, although the increase in the accuracy is small with respect to the increase of the algorithm's run time.

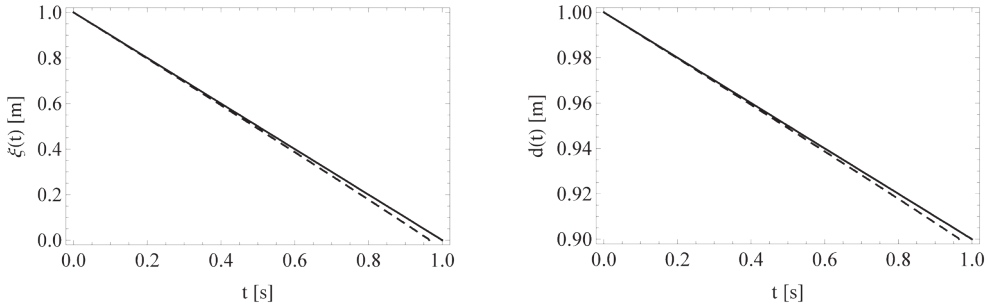

Fig. 2. Position $\xi (t)$ of the moving interface (left figure) and length $d(t)$ of the area (right figure) for $n = 200$ (solid line – exact values, dashed line – approximate values)

5. Conclusions

In this paper we have described the algorithm for solving the Stefan problem involving material shrinkage. In this algorithm we used the finite element method supplemented by the procedures allowing to define the moving interface position and the change of the material size associated with material shrinkage. To determine the boundary position we used the algorithm in which, on the basis of the Stefan condition, the time step size was iteratively determined so that the boundary moved to the adjacent node. To determine the change of size we proposed the procedure based on the mass balance.

The presented method allows to obtain more accurate results by increasing the grid density, although the increase in the accuracy is small with respect to the increase of the algorithm run time. We may also increase the accuracy by using in the finite element method the square elements instead of the linear ones or by using some other methods to solve the classical Stefan problem. In the nearest future we plan to examine both of these possibilities.

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