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Determination of the boundary conditions in two-dimensional solidification of pure metals

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Analysis and modelling

ABSTRACT

Purpose: Solidification of pure metal can be modelled by a two-phase Stefan problem, in which the distribution of temperature in solid and liquid phases is described by a heat conduction equation with initial and boundary conditions. The inverse Stefan problem can be applied to solve design problems in continuous casting process.

Design/methodology/approach: In numerical calculations the alternating phase truncation method, the Tikhonov regularization and the genetic algorithm were used. The featured examples of calculations show a very good approximation of the exact solution and the stability of the procedure.

Findings: The paper presents the determination method of cooling conditions in two-dimensional solidification of pure metals. The solution of the problem consisted of selecting a heat transfer coefficient on boundary, so that the temperature in selected points of the boundary of the domain would assumed the given values.

Research limitations/implications: The method requires that it must be possible to describe the sought boundary condition by means of a finite number of parameters. It is not necessary, however, that the sought boundary condition should be linearly dependent on those parameters.

Practical implications: The presented method can be applied without any problem to solve design problems of different types, e.g. for the design of continuous casting installations (incl. the selection of the length of secondary cooling zones, the number of jets installed in individual zones, etc.).

Originality/value: The paper presents the new method of selection of the heat transfer coefficient in two-dimensional inverse Stefan problem, so that the temperature in selected points of the boundary of the domain would assumed the given values.

Keywords: Artificial Intelligence methods; Solidification; Inverse Stefan problems

1. Introduction

Solidification of pure metal can be modelled by a two-phase Stefan problem, in which the distribution of temperature in solid and liquid phases is described by a heat conduction equation with initial and boundary conditions. The position of the freezing front is described by Stefan condition and the condition of temperature continuity. The Stefan problem consists in the determination of temperature distribution within a domain and the position of the freezing front. The inverse Stefan problem consists in the determination of the initial condition, boundary conditions or thermophysical properties of a body. Lack of a portion of input information is compensated for with additional information about the effects of the initial conditions operation. In the inverse Stefan problem, it is most often assumed that the additional information is partial knowledge of the freezing front position, its velocity in a normal direction or temperature in selected points of a domain. A majority of available papers refer to the one-dimensional inverse

Stefan problem (see [1-3] and references therein), whereas studies regarding the two-dimensional inverse Stefan problem are rare [4-9].

In this paper, an algorithm will be presented that enables solving the two-dimensional inverse Stefan problem, where the additional information consists of temperature measurements in selected points of the boundary of the domain. The problem consists in the reconstruction of the function describing the heat transfer coefficient, so that the temperature in the given points of the boundary of the domain would differ as little as possible from the predefined values. Based on the given information about temperature measurement, a functional was built defining the error of an approximate solution. To find the functional's minimum, a genetic algorithm was used [10,11]. Genetic algorithms, based on mechanisms which rule the living creatures' evolution, are a very useful tool for solving the global optimization problems, including ones with a large number of variable decisions. The application of a genetic algorithm for the inverse design Stefan problem is considered in papers [12,13]. To solve a direct Stefan problem, the alternating phase truncation method was applied [14].

The inverse Stefan problem belongs to ill-posed problems, i.e. its solution is unstable due to errors of input data. This means that small errors at the beginning may cause large errors at the end. In order to avoid such behaviour, appropriate stabilizing procedures are applied. The most frequent ones are: the function specification method and the Tikhonov regularization method. In this paper, the Tikhonov regularization method has been used due to the accuracy and stability of the results obtained. To determine the regularization parameter, the discrepancy principle, proposed by Morozov, has been used [15].

2. Problem formulation

We will consider a two-dimensional problem, where additional information will be the measurements of temperature in selected points of the boundary of the domain. Let the boundary of domain $D=\Omega\times\left[0,t^*\right]$, where $\Omega=[0,b]\times[0,d]$, be divided into five parts for which an initial condition and boundary conditions are given:

$$\Gamma_0=\{(x,y,0), x\in[0,b], y\in[0,d]\},$$
$$\Gamma_1=\{(0,y,t), y\in[0,d], t\in[0,t^*]\},$$
$$\Gamma_2=\{(x,0,t), x\in[0,b], t\in[0,t^*]\},$$
$$\Gamma_3=\{(b,y,t), y\in[0,d], t\in[0,t^*]\},$$
$$\Gamma_4=\{(x,d,t), x\in[0,b], t\in[0,t^*]\}.$$

Let D_1 denotes the subset of domain D, which is occupied by a liquid phase, and let D_2 denotes the domain occupied by a solid phase. The liquid and solid phases are separated by the freezing front Γ_g.

With the known values of temperatures in selected points of the domain D_2 ($\left(x_i,y_i,t_j\right)\in D_2$):

$$T_2\left(x_i,y_i,t_j\right)=U_{ij} \tag{1}$$

$i=1,\dots,N_1$, $j=1,\dots,N_2$, where N_1 is the number of sensors and N_2 is the number of measurements from each sensor, we must determined function $\alpha(x,y,t)$ defined on boundaries Γ_3 and Γ_4, the position of the freezing front Γ_g and the distribution of temperatures T_k in domains D_k ($k=1,2$), which inside domains D_k ($k=1,2$) fulfil the heat conduction equation:

$$c_k\rho_k\frac{\partial T_k}{\partial t}(x,y,t)=\lambda_k\nabla^2 T_k(x,y,t), \tag{2}$$

on boundary Γ_0, they fulfil the initial condition ($T_0>T^*$):

$$T_1(x,y,0)=T_0, \tag{3}$$

on boundaries Γ_1 and Γ_2, they fulfil the homogeneous second kind boundary conditions:

$$-\lambda_k\frac{\partial T_k}{\partial n}(x,y,t)=0, \tag{4}$$

on boundaries Γ_3 and Γ_4, they fulfil the third kind boundary conditions:

$$-\lambda_k\frac{\partial T_k}{\partial n}(x,y,t)=\alpha(x,y,t)\left(T_k(x,y,t)-T_\infty\right), \tag{5}$$

whereas on the freezing front Γ_g, they fulfil the temperature continuity condition and the Stefan condition:

$$T_1(x,y,t)\big|_{\Gamma_g}=T_2(x,y,t)\big|_{\Gamma_g}=T^*, \tag{6}$$

$$-\lambda_1\frac{\partial T_1(x,y,t)}{\partial n}\bigg|_{\Gamma_g}+\lambda_2\frac{\partial T_2(x,y,t)}{\partial n}\bigg|_{\Gamma_g}=L\rho_2\mathbf{v}_n, \tag{7}$$

where c_k, ρ_k and λ_k are the specific heat, the mass density and the thermal conductivity in the liquid phase ($k=1$) and solid phase ($k=2$), respectively, α is the heat transfer coefficient, T_0 is the initial temperature, T_∞ is the ambient temperature, T^* is the temperature of solidification, L is the latent heat of fusion, $\mathbf{v}_n$ is the freezing front velocity vector in a normal direction, and t, x and y refer to time and spatial locations, respectively.

Function $\alpha(x,y,t)$, describing the heat transfer coefficient, will be sought in the form of a function dependent (in a linear or non-linear way) on n parameters:

$$\alpha(x,y,t)=\alpha(x,y,t;\alpha_1,\alpha_2,\dots,\alpha_n). \tag{8}$$

Let V_α denotes a set of all functions in the form of (8), where $\alpha_i\in\left[\alpha_i^l,\alpha_i^u\right]$ for $i=1,2,\dots,n$.

For the determined function $\alpha(x,y,t)\in V_\alpha$, the problem (2)-(7) becomes a direct Stefan problem, the solution of which allows to find the courses of temperatures $T_{ij}=T_2\left(x_i,y_i,t_j\right)$ corresponding to function $\alpha(x,y,t)$. By taking advantage of the calculated temperatures T_{ij} and the given temperatures U_{ij}, we can build a functional which will determine the error of the approximate solution:

$$J(\alpha)=\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\left(T_{ij}-U_{ij}\right)^2+\gamma\int_S \omega(r)(\alpha(r))^2\,dr, \tag{9}$$

where γ is the regularization parameter, $\omega(r)$ is a weight function, $S=\Gamma_3\cup\Gamma_4$, and r ia a point of surface S.

To determine the regularization parameter, the discrepancy principle proposed by Morozov was used [12,15], according to which the regularization parameter is determined from the equality:

$$\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\left(T_{ij}-U_{ij}\right)^2=\delta, \tag{10}$$

where δ is error estimation of the input data. In practice, for a selected set of values γ_j, $j=1,\ldots,n$, of the regularization parameter, there is element minimizing the Tikhonov functional (9). Next, such value is selected as the sought regularization parameter, for which equation (10) is satisfied with the required accuracy.

3. Algorithm and calculations

To minimize the Tikhonov functional (9), genetic algorithms were applied [10,11]. In the used algorithm, the vector of decision variables was encoded in the form of a chromosome being a vector of real numbers (real number representation). In the algorithm a tournament selection was applied. The selection is carried out so that two chromosomes are drawn and the one with better fitness, goes to a new generation. There are as many draws as individuals that the new generation is supposed to include. As the crossover operator, arithmetical crossover was applied, where as a result of crossing of two chromosomes, their linear combinations are obtained. In the calculations, a nonuniform mutation operator was used as well. An elitist model was also applied in the algorithm, where the best individual of the previous population is saved and, if all individuals in the current population are worse, the worst of them is replaced with the saved best individual from the previous population. The following genetic algorithm parameters were used for the calculations: population size is equal to 70, number of generations is equal to 1000, crossover probability is equal to 0.7, mutation probability is equal to 0.1.

In the alternating phase truncation method [14] the finite differences method was used. The calculations having been made on a grid of discretization intervals equal $\Delta t=0.1$ and $\Delta x=b/500$ ($b=0.1$ [m]). A (reasonable) change of the grid density did not significantly affect the results obtained.

Function α describing the heat transfer coefficient was sought in the form:

$$\alpha(r)=\begin{cases}\alpha_1 & r\in\Gamma_4\cap[0,t_1]\\ \alpha_3 & r\in\Gamma_4\cap(t_1,t_2]\\ \alpha_5 & r\in\Gamma_4\cap(t_2,t^*]\\ \alpha_2 & r\in\Gamma_3\cap[0,t_1]\\ \alpha_4 & r\in\Gamma_3\cap(t_1,t_2]\\ \alpha_6 & r\in\Gamma_3\cap(t_2,t^*]\end{cases}$$

where $t_1=38$ [s], $t_2=93$ [s], $t^*=600$ [s]. The exact values of the coefficients α_i are:

$\alpha_1=1200$, $\alpha_3=800$, $\alpha_5=250$,

$\alpha_2=800$, $\alpha_4=500$, $\alpha_6=250$.

It was assumed that the temperature measurements were made on the domain boundary (e.g. using a thermovision camera, $N_1=1$). The reading of the temperature was conducted every 1 [s] or 2 [s]. This corresponded to a situation where the measured temperature values were 500 or 250, respectively. Calculations were carried out for exact values of the input data and for values disturbed with a random error of normal distribution and magnitude of 1% and 2%. In each case, calculations were carried out for five different initial settings of a pseudorandom numbers generator.

The results of the reconstruction of the heat transfer coefficient at various zones for a different number of control points and different perturbation are compiled in Tables 1 and 2. The tables also show the mean values (for five runs of the genetic algorithm) of the reconstructed parameters, the relative percentage error, with which those values were reconstructed, the standard deviation value and the standard deviation in the percentage of mean value. As can be seen from the results presented, in the case of accurate input data, the parameters sought are reconstructed with minimum errors (not exceeding 0.028%), resulting from the adopted criterion of the optimization procedure completion (maximum number of generations). In the case of the input data given with perturbation, the parameters sought are reconstructed with errors much smaller that the error value at input. In case of perturbation equal to 1% maximal relative percentage error not exceeding 0.39%, and in case of perturbation equal to 2% not exceeding 0.55%. Also the scatter of the obtained values (determined by standard deviation) is insignificant (not higher than 0.08%). The errors of the temperature distributions which were reconstructed are significantly lower than the input data error. In all calculations the location of the freezing front was reconstructed with very good exactness.

4. Conclusions

An algorithm that enables solving the three-phase inverse Stefan problem is presented. The problem consists in the reconstruction of the function describing the heat transfer coefficient on the boundary, so that the temperature in the given points of the domain would differ as little as possible from the predefined values. In calculations the generalized alternating phase truncation method, the genetic algorithm and the Tikhonov regularization were used.

Table 1.
Calculation results for temperature control conducted every second (α - reconstructed parameters of function describing the heat transfer coefficient, e - relative percentage error, σ - standard deviation, σ^p - standard deviation in the percentage of mean value)

α	e [%]	σ	σ^p [%]
	0%		
1199.97	0.0025	0.2614	0.0218
799.82	0.0223	0.4397	0.0550
250.00	0.0007	0.1962	0.0785
800.02	0.0020	0.1531	0.0191
500.14	0.0278	0.3507	0.0701
249.99	0.0038	0.1814	0.0726
	1%		
1200.13	0.0112	0.1348	0.0112
800.49	0.0607	0.3263	0.0408
250.02	0.0073	0.1781	0.0712
801.44	0.1796	0.0878	0.0110
499.96	0.0084	0.2169	0.0434
249.85	0.0616	0.1771	0.0709
	2%		
1197.74	0.1885	0.1100	0.0092
801.73	0.2166	0.2618	0.0327
250.22	0.0867	0.0735	0.0294
802.80	0.3505	0.1045	0.0130
498.90	0.2190	0.2413	0.0484
249.94	0.0255	0.0715	0.0286

Table 2.
Calculation results for temperature control every two seconds (notations the same as in Table 1)

α	e [%]	σ	σ^p [%]
	0%		
1200.02	0.0019	0.2273	0.0189
799.87	0.0157	0.3288	0.0411
249.96	0.0157	0.1604	0.0642
799.99	0.0015	0.2062	0.0258
500.08	0.0159	0.2863	0.0573
250.06	0.0228	0.1761	0.0704
	1%		
1201.79	0.1492	0.1019	0.0085
802.10	0.2623	0.3095	0.0386
249.66	0.1350	0.1196	0.0479
799.83	0.0210	0.0848	0.0106
498.09	0.3828	0.2321	0.0466
250.41	0.1620	0.1263	0.0504
	2%		
1197.87	0.1774	0.1401	0.0117
803.11	0.3882	0.0663	0.0083
249.79	0.0845	0.1665	0.0666
801.03	0.1288	0.0928	0.0116
497.28	0.5443	0.1152	0.0232
250.40	0.1606	0.1548	0.0618

The featured examples of calculations show a very good approximation of the exact solution and stability of the algorithm in terms of the number of control points and the input data errors. Another important thing is a small scatter of the results obtained during calculations for different initial settings of the pseudorandom numbers' generator.

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