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Identification of phase change fronts by Bezier splines and BEM ☆

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Abstract

This paper discusses the identification of the phase change front in continuous casting. The problem is formulated and solved as a geometry inverse problem. Sensitivity analysis and boundary element method are used for the estimation of the identified values. The interface between solid and liquid phases in the process is modelled by Bezier curves.

The measured temperatures required to solve the problem are always affected by measurement errors. Extensive calculations allow us to determine the influence of measurement errors on the accuracy of the phase change front location. © 2002 Éditions scientifiques et médicales Elsevier SAS. All rights reserved.

Keywords: Inverse geometry problem; Sensitivity coefficients; BEM solution of continuous casting; Bezier splines

1. Introduction

The continuous casting of metals, alloys, semiconductor crystals, etc., is nowadays a frequently utilized technology in contemporary industry. Taking into account the quality of the casting material, an accurate determination of the location of the interface between the liquid and solid phases is very important. This location can be searched employing *direct modelling* using techniques such as the enthalpy method [1] or front tracking algorithms [2] or, as shown in this paper, by solving an *inverse geometry problem*.

The continuous casting process analyzed in this paper consists of pouring a liquid material into a mould (crystallizer) having the walls cooled by flowing water, as schematically shown in Fig. 1. Inside the mould, the liquid material solidifies and is pulled out by withdrawal rolls along x-axis. The ingot is usually additionally cooled by water sprayed over the surface outside the crystallizer.

The mathematical description of the above phenomena and the related inverse problem consists of:

- a convection–diffusion equation for the solid part of the ingot:

$$\nabla^2 T(\mathbf{r}) - \frac{1}{a} v_x \frac{\partial T}{\partial x} = 0 \tag{1}$$

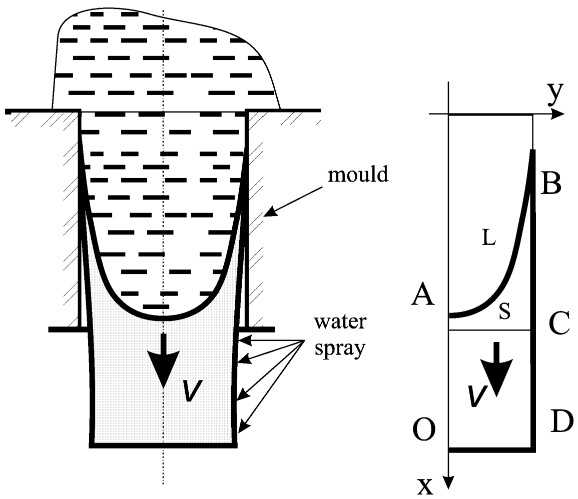

Fig. 1. Scheme of the continuous casting system and the domain under consideration.

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Nomenclature

Vectors and matrices

$\mathbf{G}, \mathbf{H}$	BEM influence matrices
$\mathbf{Q}$	vector of heat fluxes
$\mathbf{Q}_Z$	vector of normal derivative of sensitivity coefficient (respective to heat flux)
$\mathbf{r}$	space variable vector
$\mathbf{T}$	temperature vector
$\mathbf{T}_{\mathrm{cal}}$	vector of calculated temperatures
$\mathbf{T}^*$	vector of temperatures resulting from $\mathbf{Y}^*$
$\mathbf{U}$	vector of measurements
$\mathbf{V}_0, \ldots, \mathbf{V}_3$	Bezier control points
$\mathbf{V}_i^{\mathrm{I}}, \mathbf{V}_i^{\mathrm{II}}$	control point of first (I) and second (II) segment of Bezier curve
$\mathbf{W}$	covariance matrix of measurements
$\mathbf{W}_Y$	covariance matrix of prior estimates
$\mathbf{Y}$	vector of design variables
$\widetilde{\mathbf{Y}}$	vector of known prior estimates
$\mathbf{Y}^*$	vector of assumed prior estimates
$\mathbf{Z}$	matrix of sensitivity coefficients

Scalars

a	thermal diffusivity	$\mathrm{m^2 \cdot s^{-1}}$
α	convective heat transfer coefficient	$\mathrm{W \cdot m^{-2} \cdot K^{-1}}$
K_0	Bessel function of the second kind and zero order	
λ	thermal conductivity	$\mathrm{W \cdot m^{-1} \cdot K^{-1}}$
n	outward normal to the boundary	
r	distance between source and field points	m
r_x	x component of r	m
T	temperature	°C
T_m	melting temperature	°C
T_s	end temperature	°C
T_a	ambient temperature	°C
u^*, q^*	BEM fundamental solution and its heat flux analog	
v_x	x component of casting velocity	$\mathrm{m \cdot s^{-1}}$
x, y	space variables	m
Z	sensitivity coefficient	

where v_x stands for the casting velocity and a is the thermal diffusivity

- boundary conditions defining the heat transfer process along the boundaries, including the specification of the melting temperature along the phase change front

$$T(\mathbf{r}) = T_m, \qquad \mathbf{r} \epsilon \Gamma_{\mathrm{AB}} \tag{2}$$

$$T(\mathbf{r}) = T_s, \qquad \mathbf{r} \epsilon \Gamma_{\mathrm{DO}} \tag{3}$$

$$-\lambda \frac{\partial T}{\partial n} = 0, \qquad \mathbf{r} \epsilon \Gamma_{\mathrm{OA}} \tag{4}$$

$$-\lambda \frac{\partial T}{\partial n} = q(\mathbf{r}), \qquad \mathbf{r} \epsilon \Gamma_{\mathrm{BC}} \tag{5}$$

$$-\lambda \frac{\partial T}{\partial n} = \alpha\big(T(\mathbf{r}) - T_a\big), \qquad \mathbf{r} \epsilon \Gamma_{\mathrm{CD}} \tag{6}$$

where T_m stands for melting temperature, T_a is the ambient temperature, T_s is the temperature of the ingot when leaving the system and $\mathbf{r}$ is a vector of space variable. All symbols T_m, T_a, T_s represent constant temperatures.

The location of the phase change front where the temperature is equal to the melting temperature is unknown. Thus, the mathematical description is still incomplete and the problem cannot be solved. Therefore, the missing information needs to be supplemented by measurements. Usually, some temperatures, U_i, measured at selected locations are provided. If these sensors (thermocouples) are placed inside the body, the values U_i are referred to as *internal temperature responses*. If infra-red camera is used to obtain the temperatures U_i, then measurement points are located on the outer surface of the ingot.

Taking into account the kind of unknown quantity, the problem can be classified as an *inverse geometry problem*.

2. Identification of the position of the phase change front

The objective of the problem is to estimate components of vector $\mathbf{Y}$ which uniquely describes the phase change front location. In this work, two segments of Bezier splines (see Section 3) are used to approximate the interface.

The main difficulty in this kind of problem is its ill-posed nature. That is why the number of measurement sensors should be appropriate to make the problem overdetermined, or at least equal to the number of design variables. Thus, in general, inverse analysis leads to optimization procedures of the objective function Δ consisting of weighted least squares. However, in the case studied here, an additional term intended to improve stability is also introduced, i.e.,

$$\Delta = (\mathbf{T}_{\mathrm{cal}} - \mathbf{U})^{\mathrm{T}} \mathbf{W}^{-1} (\mathbf{T}_{\mathrm{cal}} - \mathbf{U}) + \big(\mathbf{Y} - \widetilde{\mathbf{Y}}\big)^{\mathrm{T}} \mathbf{W}_Y^{-1} \big(\mathbf{Y} - \widetilde{\mathbf{Y}}\big) \to \min \tag{7}$$

where vector $\mathbf{T}_{\mathrm{cal}}$ contains temperatures calculated at temperature sensor locations, $\mathbf{U}$ stands for the vector of temperature measurements and superscript T denotes transpose matrices. Symbol $\mathbf{W}$ refers to the covariance matrix of measurements. This is a diagonal matrix with values of the *maximum measurement errors* at adequate locations. Thus, the contribution of more accurately measured data is stronger than those obtained with lower accuracy. Known prior estimates are collected in vector $\widetilde{\mathbf{Y}}$, and $\mathbf{W}_Y$ stands for the covariance matrix of prior estimates. It means that on the main diagonal of matrix $\mathbf{W}_Y$ there are maximum estimated errors of identified values. It should be remembered that the coefficients of matrix $\mathbf{W}_Y$ have to be large enough to catch the minimum (these coefficients tend to infinity if prior estimates are not known). It was already found that the additional term in the objective function, containing prior estimates, plays a very important role in inverse analysis, considerably improving the stability and accuracy of the inverse procedure [3].

Identification of the position of the phase change front requires to build up of a series of direct solutions which gradually approach the correct location. This can be carried out by the following main steps:

- make the boundary problem well-posed. This means that the mathematical description of the thermal process is completed by assuming arbitrary but known values of vector $\mathbf{Y}$, called in this case as $\mathbf{Y}^*$ (as required by the direct problem)
- solve the obtained direct problem and calculate temperatures $\mathbf{T}^*$ at the sensor locations
- compare obtained temperature $\mathbf{T}^*$ and measured values $\mathbf{U}$ and modify the assumed data $\mathbf{Y}^*$.

These steps are then repeated until the updated vector $\mathbf{Y}$ minimizes the objective function (7) within a specified accuracy [3–5].

Each iteration loop involves the application of sensitivity analysis [3,6] (also known as *direct differentiation method*), utilizing the so-called sensitivity coefficients collected in matrix $\mathbf{Z}$. Sensitivity coefficients are defined as temperature derivatives with respect to the identified value, i.e.,

$$Z_{ij} = \frac{\partial T_i}{\partial Y_j} \tag{8}$$

The sensitivity coefficients are calculated by solving an appropriate direct problem obtained through differentiation of Eq. (1) and relevant boundary conditions with respect to components of vector $\mathbf{Y}$ [3,6,7]. Thus, the governing equation takes the form:

$$\nabla^2 Z(\mathbf{r}) - \frac{1}{a} v_x \frac{\partial Z}{\partial x} = 0 \tag{9}$$

with boundary conditions as in the original thermal problem, but homogeneous.

There is a number of works dealing with discussed in paper inverse problems [8–10]. Among others Zabaras et al. took advantage of deforming FEM and sensitivity coefficients to search for heat fluxes along outer surface [11] and for location of phase change interface [9,10]. In this work, the BEM [12] is applied for solving both direct thermal and sensitivity coefficient problems. The main advantage of using this method is the simplification of meshing since only the boundary has to be discretized. This is particularly important in inverse geometry problems in which the geometry of the body has to be changed in each iteration step. Furthermore, the location of the internal measurement sensors does not affect the discretization. Finally, in heat transfer analysis, BEM solutions provide direct relationship between temperatures and heat fluxes, which are both required by inverse solutions. In other words, the numerical differentiation of temperature (i.e., numerical calculations of heat fluxes) is not needed in the proposed methodology.

The BEM system of equations has boundary-only form both for the thermal and sensitivity coefficient problems

$$\mathbf{HT} = \mathbf{GQ} \tag{10}$$

$$\mathbf{HZ} = \mathbf{GQ_Z} \tag{11}$$

where $\mathbf{H}$ and $\mathbf{G}$ stand for the BEM influence matrices. Depending on the dimensionality of the problem, the fundamental solution for the convection–diffusion equation is expressed by the following formulae

$$u^* = \begin{cases} \dfrac{1}{2\pi\lambda} \exp\left(-\dfrac{v_x r_x}{2a}\right) \mathrm{K}_0\left(\dfrac{|v_x| r}{2a}\right) & \text{2-D} \\ \dfrac{1}{4\pi r\lambda} \exp\left[\dfrac{v_x (r - r_x)}{2a}\right] & \text{3-D} \end{cases} \tag{12}$$

where K_0 stands for the Bessel function of the second kind and zero order, r is the distance between source and field points, with its component along the x-axis denoted by r_x.

Through application of sensitivity analysis and some basic algebraic manipulation, minimization of the objective function leads to the following set of equations [3,13]:

$$\begin{aligned} &\left(\mathbf{Z}^{\mathrm{T}}\mathbf{W}^{-1}\mathbf{Z} + \mathbf{W}_{\mathbf{Y}}^{-1}\right)\mathbf{Y} \\ &\quad = \mathbf{Z}^{\mathrm{T}}\mathbf{W}^{-1}\left(\mathbf{U} - \mathbf{T}^*\right) + \left(\mathbf{Z}^{\mathrm{T}}\mathbf{W}^{-1}\mathbf{Z}\right)\mathbf{Y}^* + \mathbf{W}_{\mathbf{Y}}^{-1}\widetilde{\mathbf{Y}} \end{aligned} \tag{13}$$

As noticed before, the ill-posed nature of all inverse problems requires making them overdetermined by performing an appropriate number of measurements. On the other hand, it is very important to limit the number of sensors because of commonly known difficulties with data acquisition. Furthermore, each measurement introduces not only valuable information but also some noise. Application of Bezier splines permits to model the phase change front using a much smaller number of design variables and, consequently, reduce the number of sensors.

3. Application of Bezier splines

Modelling of phase change processes requires smooth curves representing phase change fronts [14]. This condition can generally fulfilled by cubic polynomials. In this paper, Bezier curves have been applied.

Such curves are made up of cubic segments. Each of these segments is based on four control points $\mathbf{V}_0$, $\mathbf{V}_1$, $\mathbf{V}_2$ and $\mathbf{V}_3$. The following formulae present the definition of Bezier cubic segments:

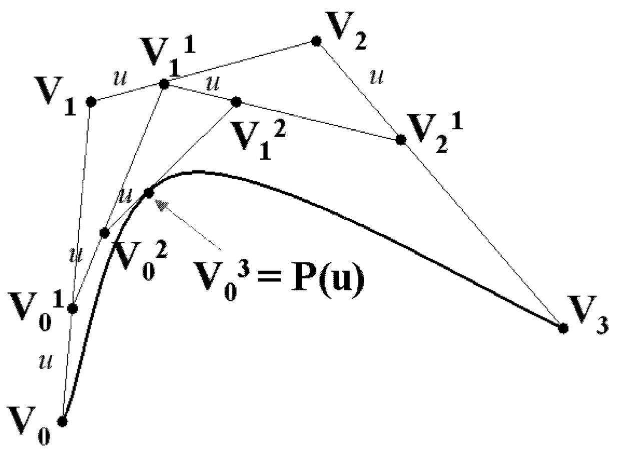

Fig. 2. One Bezier segment and its control points.

$$\mathbf{P}(u) = (1-u)^3\mathbf{V}_0 + 3(1-u)^2u\mathbf{V}_1 + 3(1-u)u^2\mathbf{V}_2 + u^3\mathbf{V}_3 \quad (14)$$

where $\mathbf{P}(u)$ stands for any point on the Bezier curve, and u varies in the range $\langle 0, 1\rangle$ (Fig. 2).

Preliminary calculations [15] have shown that two Bezier segments sufficiently approximate the phase change front. This means that the interface between solid and liquid phases is uniquely described by, at most, eight control points (i.e., sixteen coordinates in the 2-D case) which are collected in the design vector **Y**.

The proposed approach has a number of important advantages. First of all, the application of Bezier curves (cubic polynomials) ensures smoothness of the phase change front. The adequate location of control points makes the whole boundary smooth even at points which are shared by neighbouring segments. In this situation, the application of cubic boundary elements based on four nodes seems to be quite natural and straightforward.

The next very important advantage is that the application of Bezier curves permits to limit the number of identified values. In reality, some of these values (Bezier control points) are defined by additional conditions resulting from the physical nature of the problem. These conditions are listed below:

- the y-coordinate of the first and the last control point of the Bezier curve ($\mathbf{V}_0^{\mathrm{I}}$, $\mathbf{V}_3^{\mathrm{II}}$ in Fig. 3) is given because those points are located on the surface of the ingot and on the symmetry axis, respectively;
- the last control point of the first segment, $\mathbf{V}_3^{\mathrm{I}}$, and the first of the second segment, $\mathbf{V}_0^{\mathrm{II}}$, have the same position;
- two Bezier segments connect smoothly if adequate control points are collinear [16] (compare with Fig. 3)
- the equality of x-coordinates of points $\mathbf{V}_2^{\mathrm{II}}$ and $\mathbf{V}_3^{\mathrm{II}}$ ensures the existence of derivatives along the symmetry axis.

Taking into account the above conditions, the number of identified values can be limited to ten only.

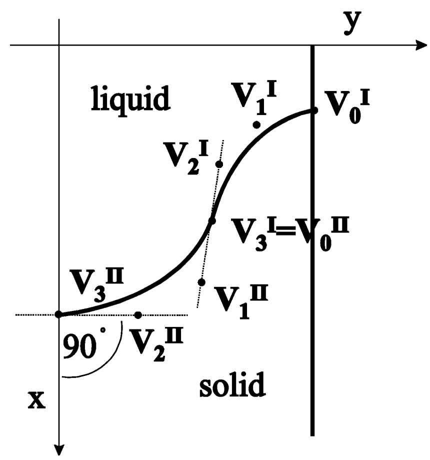

Fig. 3. Identified values in the problem with two Bezier segments.

Limiting the number of measurements is essential, mainly because of practical difficulties. Acquiring temperature measurements at points located inside the ingot requires to immerse thermocouples in the solidifying material. Of course, one thermocouple provides more than just one measurement. Knowing the casting velocity (constant value) and recording the thermocouple signal in a certain time interval, one can obtain a considerable number of measurements with a limited number of thermocouples.

The application of an infra-red camera is another method of obtaining measurements. Although temperatures are collected from the ingot surface outside the crystallizer (relatively distant from the phase change boundary), they are generally measured more accurately. However, both methods of measuring temperatures always involve measurement errors. The influence of this measurement noise on the results (interface location) is discussed in detail in the following section.

4. The influence of the number of measurements and their errors on final results

In order to demonstrate main features of the developed algorithms a case study of continuous casting of copper is solved. In the direct mathematical model, treated as a reference problem, constant thermal properties are assumed. Namely, thermal conductivity is equal to $\lambda = 370\ \mathrm{W{\cdot}m^{-1}{\cdot}K^{-1}}$, density is equal to $\varrho = 8900\ \mathrm{kg{\cdot}m^{-3}}$ and specific heat is equal to $c = 400\ \mathrm{kJ{\cdot}kg^{-1}{\cdot}K^{-1}}$. These quantities generate the thermal diffusivity equal to $a = 1.04\mathrm{E}{-4}\ \mathrm{m^2{\cdot}s^{-1}}$. Temperatures occurring in the boundary conditions are constant and equal to $T_m = 1083\,^\circ\mathrm{C}$, $T_a = T_s = 50\,^\circ\mathrm{C}$, respectively. Finally, the convective heat transfer coefficient $\alpha = 4000\ \mathrm{W{\cdot}m^{-2}{\cdot}K^{-1}}$ was assumed. All results, presented in this paper, were obtained discretizing the phase change front into 30 cubic boundary elements spanned along two Bezier segments.

4.1. Signals recorded from thermocouples

Firstly, the influence of measurement errors on the accuracy of the phase change front location was tested.

Using thermocouples is one of the most typical method connected with temperature measurements in heat transfer problems [17]. In order to obtain internal temperature responses, the set of thermocouples is immersed in solidifying material. Such an experiment was carried out by Drezet, Rappaz, Grün, Gremaud and its details concerning mentioned measurement technique are described in [17,18].

In general, manufacturers provide information on the maximum temperature errors for measurements carried out by thermocouples, for instance less than 2% [18]. In the analysis carried out here, measurement errors were assumed at five levels, to be less than 0.1%, 0.2%, 0.5%, 1% and 2%. In real conditions, the error variation can be approximated by a normal (Gaussian) distribution. In the present paper, measured temperatures were simulated by adding errors to temperatures obtained from the relevant direct solution. The errors are generated by a random generator with normal and/or uniform distribution.

Fig. 4 shows average temperature errors along the estimated phase change interface, for various levels and distributions of measurement errors.

The estimation of the phase change front location is carried out iteratively. This iterative procedure is terminated when the average temperature error stops changing or its changes do not exceed a given tolerance. In the present work, this average error consists of the difference between the temperature T at a node lying on the Bezier curve (solid-liquid boundary) and the melting temperature T_m, summed over all nodes lying on this front.

Fig. 5 presents the successive locations of the phase change interface and the relevant temperature distribution along this line for normal error distribution and two measurement errors, i.e., 0.5% (case a) and 2% (case b), respectively.

The influence of the number and location of measurement points was the next issue to investigate. This matter has significant importance, particularly when the temperature is measured inside the body using thermocouples. In this paper, three different sets of sensors, i.e., sets A, B and C (shown in Fig. 6), have been tested.

The first and second sets are obtained by immersing five thermocouples in solidifying material. In set A, the temper-

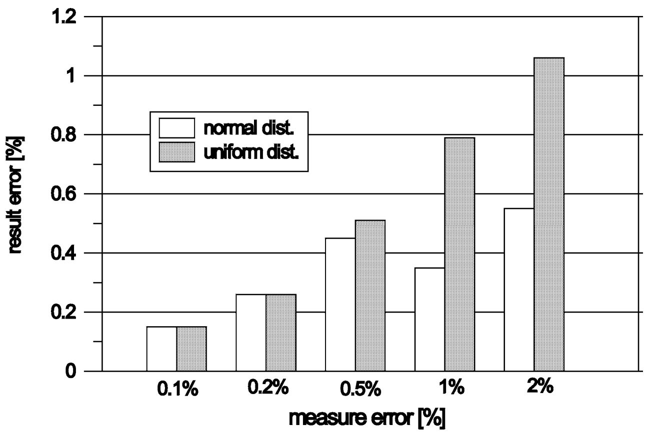

Fig. 4. Average temperature error along estimated phase change interface with various levels and distributions of error.

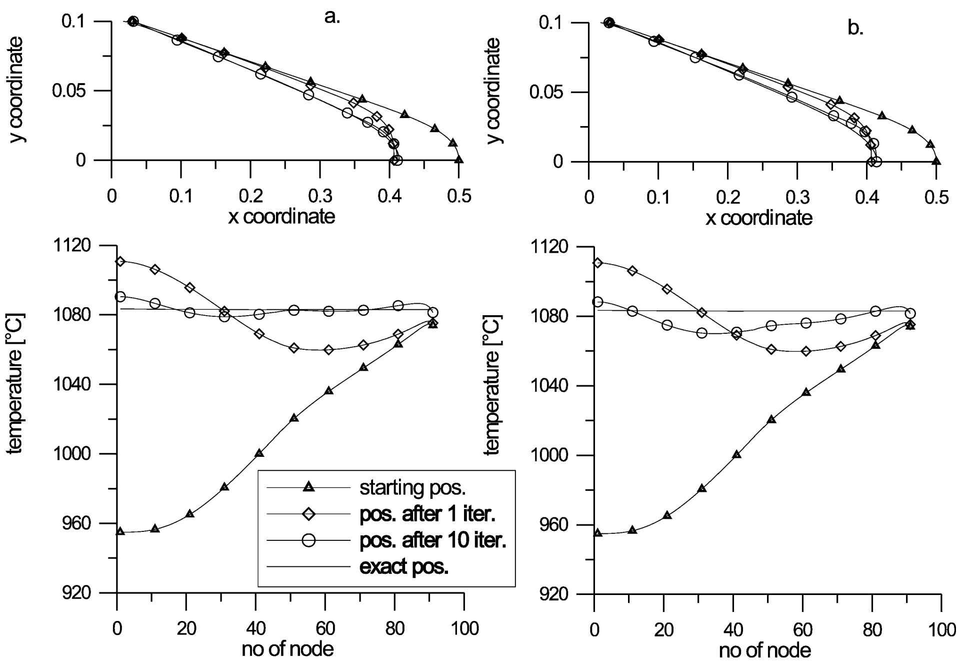

Fig. 5. Location of solid-liquid boundary and temperature distribution along this boundary. Comparison of results for measurement errors eq. 0.5% (case a) and 2% (case b).

ature is measured possibly close to the estimated boundary, while in set B sensors are located at almost equal x coordinate. The last set C consists of only two thermocouples. It was assumed that each of the thermocouples provide five measurements (in equal time intervals). This means that 25 measurements are obtained in sets A and B, and 10 in set C. For the present problem, the minimum number of measurements necessary to solve the inverse problem is equal to 10. This is because of the application of two Bezier splines to model the phase change front (the number of identified values is equal to 10).

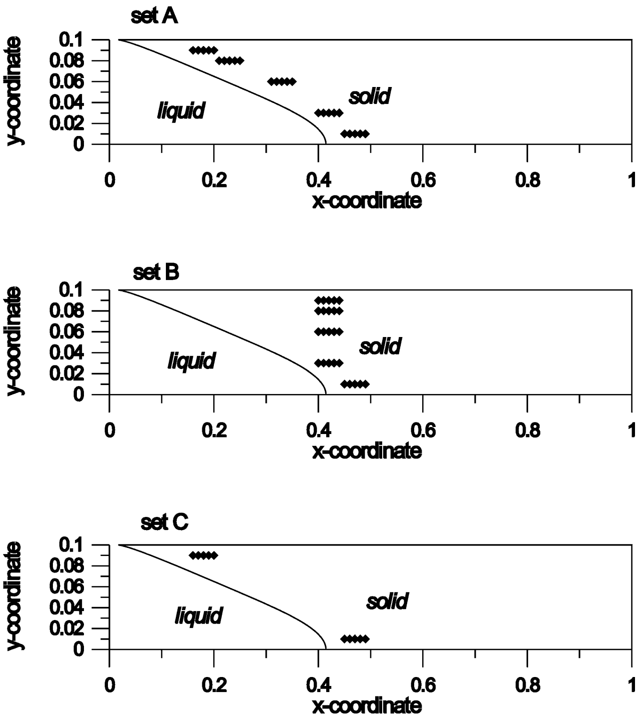

Fig. 6. Three sets of temperature sensors.

Fig. 7 shows a comparison of results obtained with 25 measurements in sets A and B. Similar comparisons for sets A and C with 10 measurements are shown in Fig. 8. In this case, each thermocouple in set A reads only two temperatures.

Results presented on Figs. 7 and 8 were obtained for measurements burden with the biggest error, i.e., 2% what is responsible for bigger average result error.

It is important to notice that proposed procedures lead to minimization of temperature differences at sensor points, which indirectly influence changes of estimated values.

The following figures show that the best results (best among tested cases) are obtained for small measurement errors (Fig. 5) and sensors placed possibly near identified values (average error is smaller for set A – Figs. 7, 8).

For the sake of legibility of figures authors gave up to show all lines in Figs. 5, 7, 8 and 10.

4.2. *Signals recorded with infra-red camera*

Infra-red camera is an alternative and relatively easy way of obtaining temperature measurements. Furthermore, these cameras measure temperatures with smaller errors (even 0.2 K). Unfortunately, the temperature has to be measured on the surface of the body outside the crystallizer. Thus, the sensor points are located at some distance from the phase change front. On the other hand, there is no strong limitation on the number of measurement points.

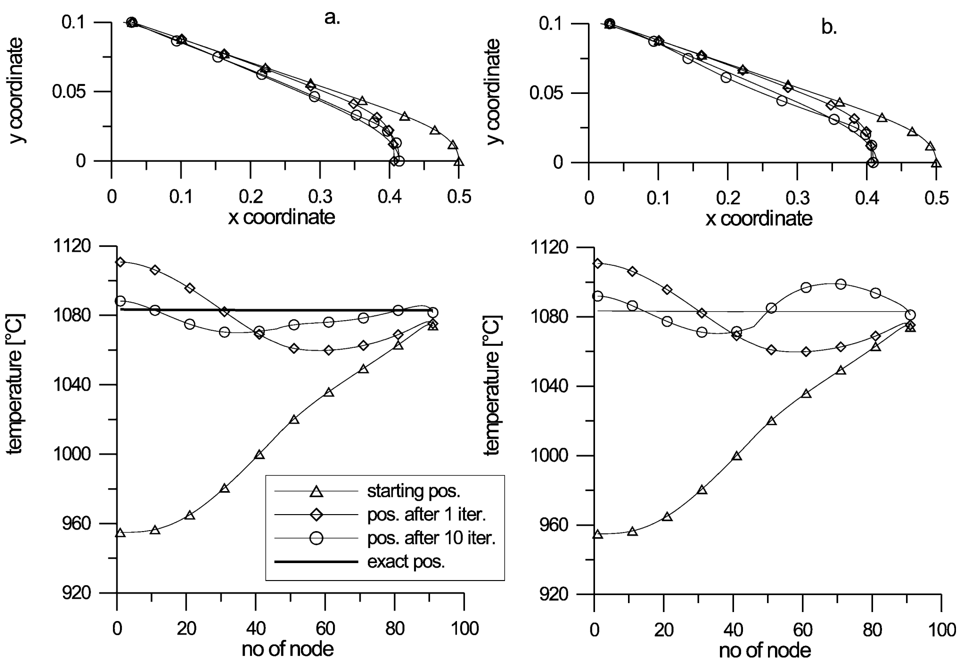

Fig. 7. Comparison of results for sets A and B (25 measurements).

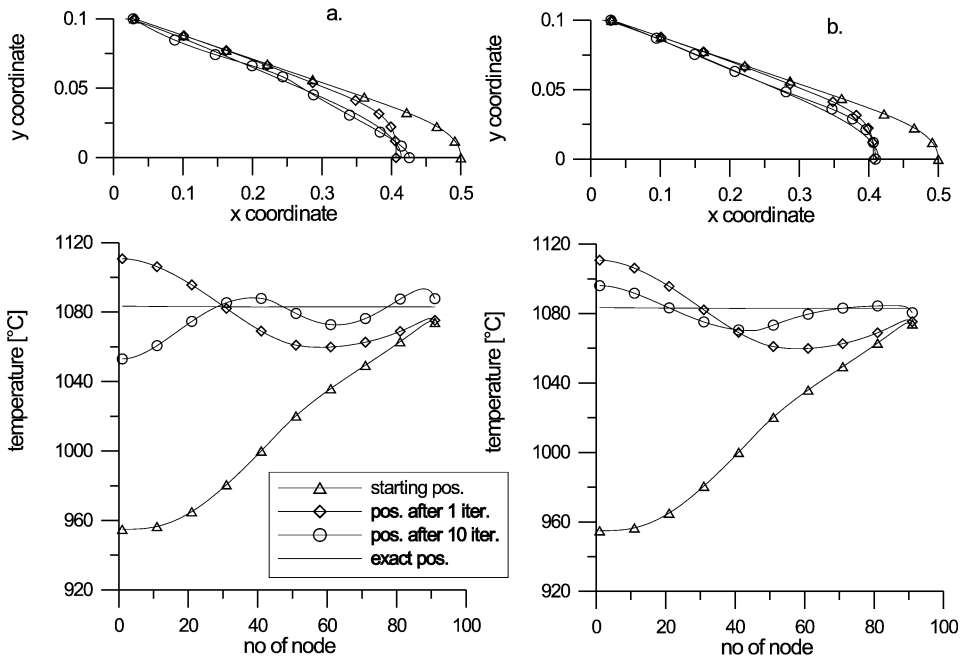

Fig. 8. Comparison of results for sets A and C (10 measurements).

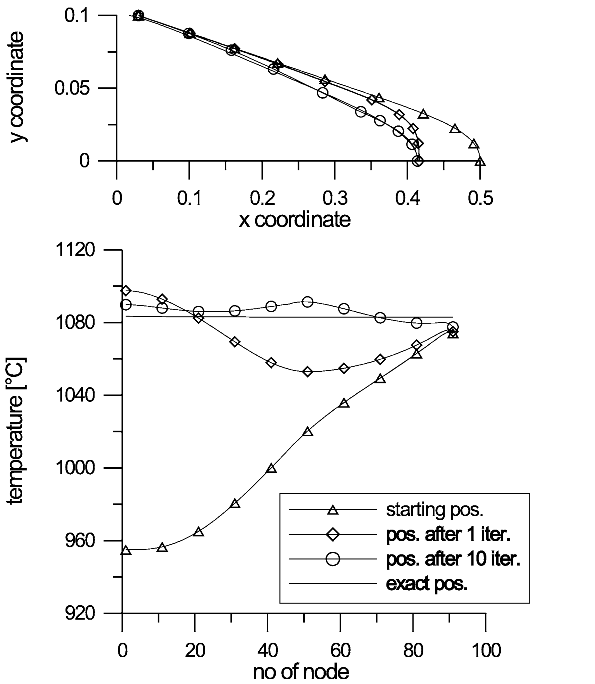

Fig. 9. Front location and temperature along the interface boundary (40 measurements, maximum error 0.2%).

Figs. 9 and 10 show results obtained by using an infra-red camera for solving inverse geometry thermal problems. The first graph shows successive phase change front locations obtained during the iteration process.

A comparison of both methods (i.e., sensors inside the body and infra-red camera) shows that results obtained for the same measurement errors are better in the case of using thermocouples. On the other hand, it is difficult to obtain

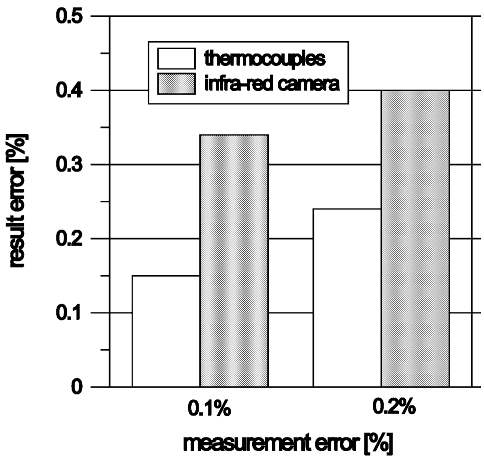

Fig. 10. Comparison of results obtained for thermocouples (25 measurements) and infra-red camera (40 measurements).

measured temperatures with such a low error level. In the case of infra-red cameras, the phase change front location is satisfactory with respect to the costs of the experiment. Furthermore, measurements can easily be repeated as many times as required.

5. Conclusions

This paper discussed the identification of the phase change front location in continuous casting. The problem is formulated as an inverse geometry problem and solved as a series of direct solutions, which gradually approached an accurate front position. The surface between solid and liquid phases is modelled by two segments of Bezier splines.

Small number of design variables (and in consequence required measurements) in geometry inverse problem is the main advantage of presented method. Application of BEM permits to build numerical mesh only along boundary of body, what is important with respect to geometry changing in iteration procedure. Furthermore the dependence of the final results on the number, location and accuracy of measurements was investigated. Temperatures were measured using thermocouples and/or infra-red cameras. The results obtained with both methods were presented and compared in this work.

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