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An inverse solution for the steady temperature field within a solidified layer

GRAHAM E. BELL
Department of Applied Mathematics, University of St. Andrews, St. Andrews, Fife, Scotland

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Abstract—A stream of warm liquid solidifies on a cold plate of finite width. The steady temperature distribution within the solidified layer is obtained numerically using an inverse formulation technique. The computational difficulties posed by the problem are discussed and the success of the inverse formulation in overcoming these difficulties is demonstrated. The potential dangers involved are also identified.

INTRODUCTION

IN THE last decade or so, there has been considerable interest in the design and performance of computational techniques for both free and moving boundary problems. However, in realistic models of industrial processes, the location of an uknown boundary curve is often just one of a number of awkward features that have to be catered for in a computer simulation. In a recent paper by Bell and Wood [1] a test problem is posed in which the accurate prediction of the position of a moving boundary is bedevilled by the existence of a boundary singularity. They discuss the application of the enthalpy method to their test problem and demonstrate the computational difficulties that are encountered. Physically, the problem they consider is artificial and was constructed in order to gain some indication of the performance of a simple numerical approach. As might be expected, they conclude that standard finite-difference techniques designed for moving boundary problems are unlikely to perform well on such problems without excessive computational effort.

Siegel [2] has investigated the extent of solidification of a warm liquid flowing longitudinally over a cold plate of finite width. The mathematical model of the process contains the same awkward features as the artificial problem considered by Bell and Wood [1]. Siegel obtained by a series of conformal transformations an analytical expression for the location of the solid–liquid interface in its equilibrium position. His very complicated mathematical analysis is not easily generalized to other problems, although he has been successful in applying his approach to some other situations [3, 4]. In this paper, interest is confined to the numerical solution of the problem discussed by Siegel [2]. From the computational point of view, the difficulties posed are essentially the same as those encountered by Bell and Wood. It is necessary to locate the position of a non-trivial boundary curve when an adjacent, fixed boundary contains a boundary singularity. A boundary singularity will seriously impair the accuracy of a numerical technique unless it is specifically catered for within the numerical scheme. The computational cost of modifying standard finite-difference, or finite-element, methods in order to obtain a reasonably accurate solution on even a mainframe machine is high.

It is the purpose of this paper to discuss an alternative approach to the numerical solution of free boundary problems which is considerably less sensitive to the presence of boundary singularities. The approach to be discussed is essentially the same as the inverse formulation proposed by Jeppson [5] who was concerned with modelling the steady flow of a liquid through a porous dam. In order to simplify the complex geometry of a three-dimensional flow problem, he transformed the equations so that the space coordinates became the dependent variables. The independent variables were chosen to be the velocity potential and two appropriately defined stream functions.

In the problem to be considered in the next section a flow function is defined to augment the temperature at each point in the solidified layer. The problem is then reformulated with these two quantities taken as the independent variables. The transformed region becomes a unit square and the unknown coordinates of intersection of flow lines and isotherms are determined numerically using standard finite-difference approximations. The potential for this form of approach to the solution of melting and freezing problems has already been demonstrated [6]. However, certain aspects of the technique have only recently been observed and these are investigated in detail here.

Inverse formulation is really just a special case of the more general technique of automatic grid generation. Winslow [7] describes how non-uniform difference grids can be defined in terms of the solution of potential problems. Godunov and Prokopov [8] implement Winslow's grid generation procedure to solve a moving boundary problem in gas dynamics. Thompson *et al.* [9] have generalized Winslow's work to allow some control over the positioning of grid points around the boundary. More recently, Rieger *et al.* [10] have successfully applied body fitted coordinates to a moving boundary problem.

However, automatic grid generators are, quite

NOMENCLATURE

a	half-width of plate
f	total flow through region R
h	size of finite-difference grid
H	convective heat transfer coefficient at solid–liquid boundary
K	conductivity of the frozen liquid
Q	rate of removal of heat per unit length of the plate, $2Kf(T_F - T_0)$
R	solidified region in first quadrant expressed in dimensionless coordinates (x, y)
T	temperature within frozen layer
T_F	freezing temperature of liquid
T_L	bulk temperature of flowing liquid
T_0	temperature of plate
u	dimensionless temperature, $1-(T-T_0)/(T_F-T_0)$
v	dimensionless flow function
x_0	free boundary intercept with x-axis
y_0	free boundary intercept with y-axis.

Greek symbols

α	solidification parameter, $aH(T_L - T_F)/K(T_F - T_0)$
η	variable in direction of outward drawn normal to specified curve
ϕ	location of free boundary.

naturally, independent of the physical quantities under investigation in any given problem. The advantage of combining the process of solution with that of grid generation is clearly realized by Thompson and his colleagues, although it is not pursued. The method of inverse formulation [5] is a particular example of this combined process.

The solution of free and moving boundary problems by the interchange of independent and dependent variables is by no means a new idea. Crank and his co-workers [11–13] have experimented with a number of different schemes. They all involve just partial transformations in the sense that one dependent variable changes role with one of the space coordinates. Boadway [14] adopted the same strategy for Laplace's equation and he systematically derives general relationships for such transformations.

PROBLEM SPECIFICATION AND METHOD OF SOLUTION

Consider the problem investigated by Siegel [2] of a warm liquid, at a constant bulk temperature T_L, flowing over a cold plate of width $2a$ maintained at a constant temperature T_0. The edges of the plate are insulated. The liquid solidifies at some intermediate temperature T_F and a frozen layer forms on the plate. It is assumed that heat is supplied to the frozen layer by convection within the liquid and that the convective heat transfer coefficient, H, at the solid–liquid interface is constant. A steady-state is reached when the heat supplied by convection at the interface is conducted through the frozen layer and removed by the cooling plate. Interest is confined to the steady-state temperature field within the solidified layer and the position of the interface (free boundary) has to be determined as part of the solution. The problem is depicted in Fig. 1 where the liquid is flowing in the Z-direction. Assuming the length of the cooling plate is infinite (or large in comparison to the width $2a$), the configuration may be considered two-dimensional.

In terms of non-dimensional variables, and using subscripts to denote differentiation, the process may be described by

$$\nabla^2 u = 0, \quad (x, y) \text{ in } R \tag{1}$$

$$u = 1, \quad y = 0, \quad 0 \leqslant x \leqslant 1 \tag{2}$$

$$u = 0, \quad \phi(x, y) = 0 \tag{3}$$

$$u_x = 0, \quad x = 0, \quad 0 < y < y_0 \tag{4}$$

$$u_y = 0, \quad y = 0, \quad 1 < x < x_0 \tag{5}$$

and

$$u_\eta = -\alpha, \quad \phi(x, y) = 0 \tag{6}$$

where, for convenience of presentation, the non-dimensional temperature

$$u = 1-(T-T_0)/(T_F-T_0)$$

$$x = X/a, \quad y = Y/a$$

and

$$\alpha = aH(T_L - T_F)/K(T_F - T_0).$$

The unknown free boundary is denoted by $\phi(x, y) = 0$, and x_0 and y_0 denote its intersection with the x and y axes, respectively. The extent of solidification is determined by the parameter α. As the value of α is decreased, the size of the solidified layer will increase.

It should be noted that $x = 0$ ($X = 0$ in Fig. 1), is a

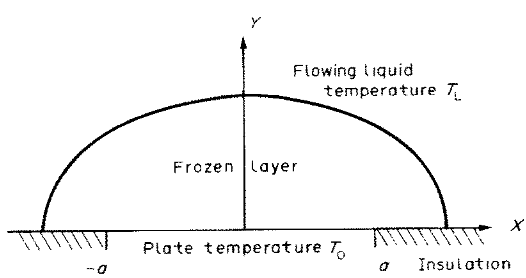

FIG. 1. Problem configuration.

line of symmetry and in the following analysis the right-hand quadrant is considered. The region occupied by the solidified layer in this quadrant is denoted by R. Throughout the remainder of this paper all magnitudes will be expressed in terms of the non-dimensional quantities defined earlier.

From a computational point of view the problem specified in equations (1)–(6) presents formidable difficulties if an accurate solution is to be obtained. The determination of the location of the free boundary has to be an integral part of the solution process which is hindered by the existence of a boundary singularity at (1, 0). The form of the singularity is identical to that discussed originally by Motz [15]. In the neighbourhood of (1, 0) the temperature gradient is large. The accuracy of numerical techniques that involve the approximation of the flux by a formula based on a polynomial is significantly impaired. The computational difficulties encountered when using standard techniques are illustrated in ref. [1].

During the last 20 years considerable interest has been focused on ways of overcoming the disruptive effect of boundary singularities in fixed boundary value problems. However, similar free boundary problems have received little attention by comparison. Here the difficulties are successfully circumvented by transformation.

Consider the introduction of a flow function

$$v(x,y) = -\frac{1}{f}\int_C u_\eta \, dc$$

where C is any curve lying wholly within R which joins a point P in R to any point lying on the boundary $x = 0$ $(0 < y < y_0)$ and f is a constant to be determined. The derivative in the integrand is in the direction of the outward drawn normal to the curve C. By insisting that $v = 1$ when P lies on the line $y = 0$, $1 < x < x_0$, the constant f represents the quantity of heat per unit length of the plate being removed from the liquid in unit time. As only steady temperatures are being considered, it may easily be deduced that

$$fv_x = -u_y, \quad fv_y = u_x \tag{7}$$

and

$$\nabla^2 v = 0.$$

Hence, a conjugate problem may be defined in terms of $v(x, y)$. The level curves of v (flow lines) are orthogonal to those of u (isotherms) and consequently

$$u_x v_x + u_y v_y = 0. \tag{8}$$

The advantage of not defining a flow function in terms of the usual Cauchy–Riemann equations will become apparent shortly.

Transforming $u(x, y)$ and $v(x, y)$ so that (x, y) are the dependent variables and (u, v) are the independent variables produces the relationships

$$Ju_x = y_v, \quad Jv_x = -y_u, \quad Ju_y = -x_v \tag{9}$$

and

$$Jv_y = x_u$$

where J is the Jacobian

$$x_u y_v - y_u x_v.$$

From equations (7) and (9) it is easily shown that, within the unit square $0 < u, v < 1$

$$f^2 x_{uu} + x_{vv} = 0 \tag{10}$$

and

$$f^2 y_{uu} + y_{vv} = 0. \tag{11}$$

In addition, equations (2)–(6) yield the following boundary conditions on the sides of the unit square:

$$\text{on } u = 0, \quad y_u^2 + x_u^2 = 1/\alpha^2, \tag{12a}$$

$$y_v^2 + x_v^2 = f^2/\alpha^2; \tag{12b}$$

$$\text{on } u = 1, \quad y = 0, \quad x_u = 0; \tag{13a, b}$$

$$\text{on } v = 0, \quad y_v = 0, \quad x = 0; \tag{14a, b}$$

$$\text{on } v = 1, \quad y = 0, \quad x_v = 0. \tag{15a, b}$$

Also, it should be noted that at the point (1, 1) in the (u, v) space $x = 1$.

In terms of (u, v) it is necessary to solve numerically a pair of simple partial differential equations [equations (10) and (11)] subject to the appropriate boundary conditions [taken from equations (12) to (15)] on a unit square. Standard finite-difference approximations may be applied with ease. The value of f has to be determined as part of the solution process but this does not present difficulties.

If $v(x, y)$ had been defined as the harmonic conjugate of $u(x, y)$, as is more usual, the transformed region would have been a rectangle of unknown length f. The transformed problem would still be a free boundary problem, albeit an easier one. The flow function defined earlier removes the need for a further transformation prior to computation.

The design of a suitable computational scheme to find the solution for x, y and f in terms of (u, v) is straightforward. For the sake of brevity only an outline of the computational details is given.

COMPUTATIONAL PROCEDURE

General outline

A square finite-difference grid of size h is superimposed on the unit square such that $mh = 1$, where m is an integer. All equations are approximated using second-order difference replacements and the resulting system of algebraic equations is solved iteratively, using the Gauss–Seidel iteration. Each iterative cycle contains three stages. Firstly, the values of y are updated from the difference approximation of equation (11) subject to the conditions imposed by approximating the boundary conditions, of which more will be said shortly. The second stage is to update the values of x, from the difference replacement of equation (10), in a similar manner. The final stage is to update the value of f. There are numerous possibilities for the evaluation of f. As the value of f represents the total flow through the region R, it may be determined in the usual way on some suitably chosen curve. Here, the curve is taken to be the isotherm $u = 0.5$. One expression for the transformed integral is

$$f = -\int_{u=1/2} u_\eta \, dc = -\int_0^{0.5} (x_v/y_u)\, dv + \int_{0.5}^{1} (y_v/x_u)\, dv. \quad (16)$$

It is convenient to choose this particular form for f in order to avoid an integrand which becomes indeterminant at either $v = 0$ or 1.

The expressions in the above formula for f are approximated in such a way as to ensure $O(h^2)$ accuracy.

Boundary conditions

The conditions on three sides of the square, equations (13)–(15), are easily approximated and incorporated into the computational scheme. The conditions arising from the free boundary, equations (12a) and (12b), are not so readily accomodated.

Firstly, equation (12b) is unusual in that it relates derivatives along the line $u = 0$ rather than across it. In terms of the computational scheme this equation offers little help. However, equations (12a) and (12b) are related by virtue of equations (7). The transformed versions of those two relationships are

$$y_u = -x_v/f \quad \text{and} \quad x_u = y_v/f \qquad (17a, b)$$

and these will be used in conjunction with equation (12a).

Equation (12a) also presents problems which were not apparent in the initial graphical results presented in ref. [6] in Seattle. If, for example, equation (12a) is used to provide a boundary condition for y in the first stage of the iterative cycle then it is necessary to approximate the nonlinear equation

$$y_u = -\{1/\alpha^2 - x_u^2\}^{1/2}. \qquad (18)$$

A convenient approximation of equation (18) is

$$(\mu\delta)_u y(0, v) = -\left\{\frac{h^2}{\alpha^2} - [(\mu\delta)_u x(0, v)]^2\right\}^{1/2}$$

and it is compatible with the overall scheme provided that the discretization errors involved remain small in comparison to the RHS of equation (18). Unfortunately, this is not the case. As $v \to 1$ along $u = 0$

$$x_u \to -1/\alpha$$

and

$$y_u \to 0.$$

Superficially it would appear that a slight loss of accuracy will occur in values at points close to (0, 1) in the (u, v) space. Sadly the consequences are more serious. A loss of accuracy in the computed y values will be transmitted, via the boundary condition (17b), to the new x values at Stage 2 of the iterative cycle. On returning to Stage 1 of the process the updated y values are impaired further and so on in each stage of the computational procedure.

It is not too difficult to anticipate the outcome. The discretisation error in the computed solution, in the locality of (0, 1), will be of $O(1)$. On reflection, it is somewhat surprising that this localized lack of convergence is not evident in the initial results presented in ref. [6]. However, when the solutions are recomputed on a sequence of increasingly finer grids the lack of convergence is revealed.

Clearly, the nonlinear condition on the free boundary has to be implemented with care. In the procedure adopted here, and verified computationally in the next section, equation (18) is approximated as indicated but is only applied at points on $u = 0$ for which $0 \leqslant v \leqslant \frac{1}{2}$. On the remainder of the boundary line equation (17a) is suitably approximated.

At Stage 2 of the iterative cycle, when new x values are computed, condition (12a) is rewritten as

$$x_u = -\left\{\frac{1}{\alpha^2} - y_u^2\right\}^{1/2}$$

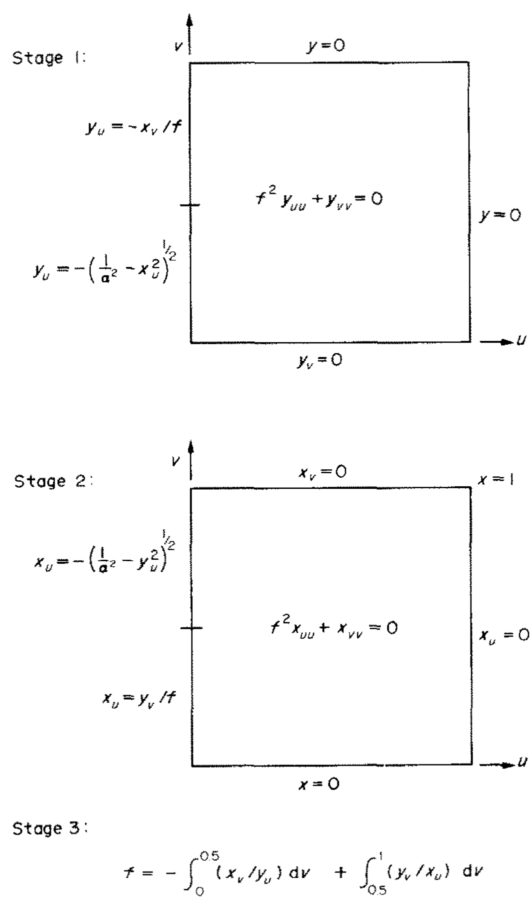

FIG. 2. Problem specification.

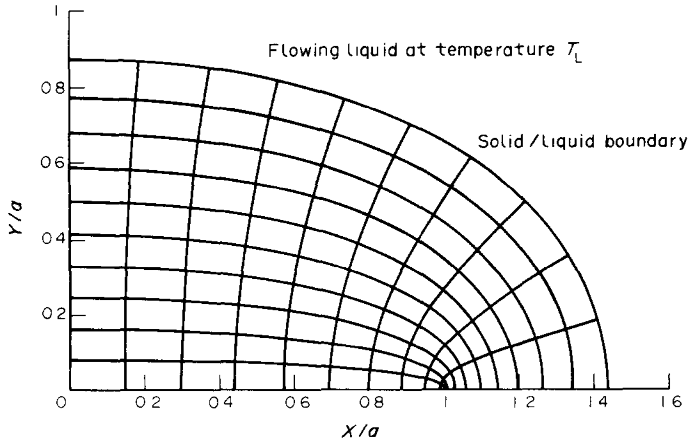

FIG. 3. Isotherms and flow lines (h = 0.025). (Only every fourth line shown.)

and again the derivatives are approximated as indicated earlier. The resulting nonlinear difference approximation is only applied at points on $u = 0$ where $\frac{1}{2} \leqslant v \leqslant 1$. This boundary condition is not applied on the other half of the boundary line as convergence problems may also be anticipated as $v \to 0$ (i.e. when $x_u \to 0$). An approximation of equation (17b) is used on this remaining part of the boundary line $u = 0$.

Finally, to clarify the overall computational procedure a complete problem specification is displayed in Fig. 2. All derivatives are approximated to $O(h^2)$ accuracy with the hope that the computed solution will display a similar trend.

NUMERICAL RESULTS

Numerical results have been obtained on a succession of increasingly finer finite-difference grids. The grid spacings used were $h = 0.1, 0.05$ and 0.025. In all the calculations the solidification parameter, α, was taken to be unity. The effect upon the shape of the solidified region of the value of α is illustrated by Siegel [2].

Siegel's analysis provides the precise location of the free surface and an expression for the total flow of heat through the solidified layer. These will be used to assess the validity of the numerical procedure discussed here. In addition, it is possible to extend Siegel's analysis to obtain expressions for the temperature, u, or the flow function, v, on each of the four boundary segments. Values obtained in this way will be referred to as the 'exact' solution even though it was necessary to evaluate the mathematical expressions numerically.

The inverse formulation solution provides the (x, y) coordinates of the intersection of flow lines and isotherms. Figure 3 presents, in graphical form, the numerical solution obtained on the finest of the three grids used. Only every fourth isotherm and flow line is depicted. The lines joining the solution points are drawn by a standard graphics routine.

In Fig. 4 the exact solution is used to assess the accuracy and convergence properties of the numerical procedure. The values quoted represent the distance between the exact location of an intersection and the computed location for points on the four boundary segments. As may be observed, the anticipated lack of convergence on the free boundary has been successfully overcome. However, the global rate of convergence would appear to be at best $O(h)$. The singularity at the edge of the cooling plate still has an effect and, although

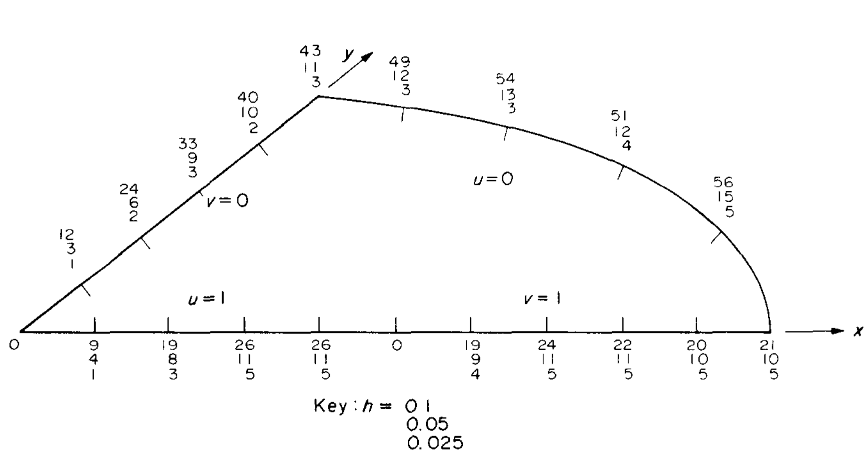

FIG. 4. Error × 10^4 at points around the boundary for successively finer grids.

Table 1. Estimates of the rate of removal of heat

h	f
0.1	1.8469
0.05	1.8590
0.025	1.8625
Exact	1.8639

the accuracy of the solution is not seriously impaired, the rate of convergence suffers. This imperfection must be put into perspective. A standard numerical technique, as in ref. [1], could not have achieved this degree of precision. It must be remembered that the singularity has not been treated. Its disruptive influence has merely been reduced by a particular form of coordinate transformation. The uniform grid used here may be interpreted as corresponding to a non-uniform mesh over the original region R in which the finest gradations occur in the locality of the singular point.

An examination of the estimates of f obtained by the inverse formulation technique provides further validification of the numerical procedure. These are given in Table 1. The rate of removal of heat from the liquid per unit length of the plate is given by

$$Q = 2Kf(T_F - T_0)\ (\mathrm{W\ m^{-1}}).$$

Even on the coarsest of the three grids the error in the predicated rate of removal of heat from the flowing liquid is less than 1%.

CONCLUDING REMARKS

Automatic grid generating codes and body-fitted coordinate systems are now fairly common in the solution of field equations. The application of these routines to free and moving boundary problems is a more recent development. In contrast to the amount of effort expended in the design of such routines, little attention appears to have been given to the accuracy and, indeed, the validity of the results obtained. This is especially true for problems which contain awkward features such as sharp corners or discontinuous boundary data.

The results presented here inspire confidence in the inverse formulation approach to such problems. An added advantage is that the processes of grid generation and problem solution are combined. At present it appears that inverse formulation is the best way of tackling free boundary problems in regions typified by Fig. 1. However, the dangers involved are evident. Nonlinearities in the transformed equations must be approximated with care. Also, the effect of a singularity is not entirely removed by the transformation.

The pleasing feature of the technique discussed in this paper is that an otherwise difficult computational problem has been reduced to manageable proportions. The experience gained is invaluable in the search for robust computational techniques suitable for the accurate solution of corresponding transient heat transfer problems.

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UNE SOLUTION INVERSE POUR LE CHAMP DE TEMPERATURE DANS UNE COUCHE SOLIDIFIEE

Résumé—Un écoulement de liquide chaud se solidifie sur une plaque froide de longueur finie. La distribution stationnaire de température dans la couche solidifiée est obtenue numériquement en utilisant une technique de formulation inverse. Les difficultés de calcul posées par le problème sont discutées et on démontre le succès de la formulation inverse en surmontant ces difficultés. Les dangers potentiels sont aussi identifiés.

INVERSE LÖSUNG FÜR DAS STATIONÄRE TEMPERATURFELD IN EINER VERFESTIGTEN SCHICHT

Zusammenfassung—Ein warmer Flüssigkeitstrom verfestigt sich an einer kalten Platte von endlicher Breite. Mit Hilfe einer inversen Darstellungstechnik ergibt sich auf numerische Weise die stationäre Temperaturverteilung in der verfestigten Schicht. Die rechentechnischen Schwierigkeiten, die bei dem Problem zutage treten, werden erörtert. Der Erfolg der inversen Darstellung bei der Überwindung dieser Schwierigkeiten wird veranschaulicht, wobei auch mögliche Gefahren aufgezeigt werden.

ОБРАТНОЕ РЕШЕНИЕ ДЛЯ ЗАДАЧИ СТАЦИОНАРНОЙ ТЕПЛОПРОВОДНОСТИ ВНУТРИ СЛОЯ ЗАТВЕРДЕВАЮЩЕЙ ЖИДКОСТИ

Аннотация—Струя остывающей жидкости затвердевает на охлажденной пластине конечной толщины. Для этого случая методом обратной задачи получено стационарное распределение температур внутри затвердевшего слоя. Обсуждаются возникающие при решении трудности и показаны преимущества используемой постановки в их разрешении.