Int. J. Heat Mass Transfer. Vol. 24, No. 8, pp. 1335–1343, 1981.
Printed in Great Britain

0017-9310/81/081335-09 $02.00/0

NUMERICAL SOLUTION OF MOVING BOUNDARY PROBLEMS BY BOUNDARY IMMOBILIZATION AND A CONTROL-VOLUME-BASED FINITE-DIFFERENCE SCHEME

C. F. HSU, E. M. SPARROW and S. V. PATANKAR
Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN 55455, U.S.A.

(*Received* 28 *November* 1980 *and in revised form* 2 *February* 1981)

Abstract—A methodology is set forth for the numerical solution of transient two-dimensional diffusion-type problems (e.g. heat conduction) in which one of the boundaries of the solution domain moves with time. The moving boundary is immobilized by a coordinate transformation, but the transformed coordinates are, in general, not orthogonal. Furthermore, with respect to a given control volume in the new coordinate system, mass appears to pass through the control surface which bounds the volume, and this mass movement brings about a convection-like transport of energy. The energy equation for a moving, nonorthogonal control volume is derived in general and then specialized to the transformed coordinate system associated with the immobilization of the moving boundary. A fully implicit scheme is used to discretize the control volume energy equation. The spatial derivatives are discretized by either of two schemes depending on the size of the pseudo-convection relative to the diffusion. The energy balance at the moving boundary of the solution domain is also transformed and discretized. A numerical procedure is then developed for solving the discretized energy equations. The use of the control volume formulation and the solution methodology will be illustrated for a specific physical situation in a companion paper that follows this paper in the journal.

NOMENCLATURE

f, arbitrary function;
H, axial extent of solution domain;
h_{NC}, natural convection heat transfer coefficient;
$\hat{\mathbf{i}}_r$, unit vector in r-direction;
$\hat{\mathbf{i}}_z$, unit vector in z-direction;
k, thermal conductivity;
$\mathbf{n}$, unit vector along normal;
T, temperature;
T^*, fusion temperature;
T_∞, temperature of liquid melt;
R, dimensionless radial coordinate, r/r_w;
r, radial coordinate;
r_w, radial coordinate at inner boundary of solution domain;
r_δ, radial coordinate at the moving boundary;
S, control surface;
Ste, Stefan number;
t, time;
$\mathbf{u}_b$, velocity of control volume boundary;
$\mathbf{u}_\delta$, velocity of moving boundary;
V, control volume;
z, axial coordinate;

Greek symbols

α, thermal diffusivity;
β, function, $\eta(\partial\Delta/\partial\xi)$;
Γ, function, equation (25);
Δ, dimensionless thickness, δ/r_w;
δ, radial thickness of solution domain;
η, transformed coordinate, $(r - r_w)/\delta$;
θ, dimensionless temperature;
Λ, function, equation (25);
λ, latent heat of fusion;
ξ, transformed coordinate, z/r_w;
ρ, density;
τ, dimensionless time, $(\alpha t/r_w^2)Ste$;
χ, function, $(1 + \beta^2)$;
ψ, function, equation (25);
Ω, function, equation (24).

Subscripts

P, N, S, E, W locations of grid points, Fig. 2.

Superscript

τ, at time τ;
no superscript denotes time $(\tau + \delta\tau)$.

INTRODUCTION

DURING the freezing of a liquid on a cooled surface, a solidified layer is formed which increases in thickness as time passes. Thus, the heat conduction across the solid from the liquid–solid interface to the cooled surface takes place in a domain whose size and shape change with time. In addition to heat conduction during freezing, there are other relevant technical problems where diffusion processes take place in regions which have one or more moving boundaries. Only a limited number of moving boundary problems admit an analytical solution. These include, in the main, the classical one-dimensional Stefan and Neumann problems and their variants [1,2]. Numerical techniques are generally required for the solution of two-dimensional moving boundary problems as well as for many one-dimensional problems.

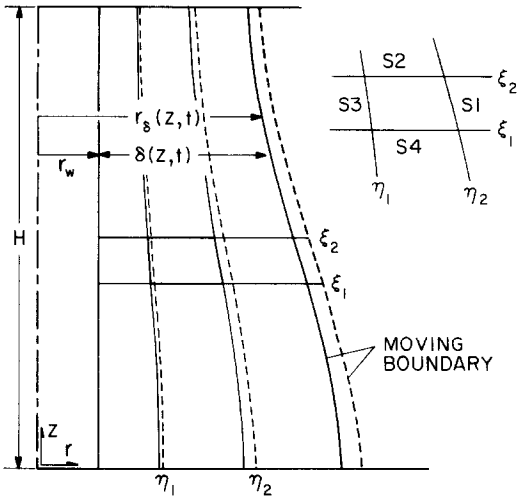

FIG. 1. Schematic diagram of a representative two-dimensional moving boundary problem showing the transformed coordinates ξ and η.

The focus of this paper is the development of a methodology for the numerical solution of two-dimensional diffusion-type moving boundary problems (i.e. problems where the moving boundary does not lie along a coordinate line). The basis of the method is a coordinate transformation which causes the moving boundary to be stationary in the transformed coordinate system. In general, the transformed coordinate system will not be an orthogonal one. As a consequence, the derivation of a finite-difference representation of the conservation equations involves features that are not found in conventional diffusion problems where orthogonal coordinate systems are the rule.

The use of a coordinate transformation to immobilize a moving boundary in two-dimensional diffusion problems has already been described in papers by Saitoh [3] and by Duda *et al.* [4]. Their approach was to apply the immobilizing coordinate transformation to the differential equation of energy conservation, which results in a relatively more complex differential equation that reflects the nonorthogonal nature of the coordinates (e.g. there are mixed derivatives involving both space coordinates). Then, each term of the transformed differential equation is individually discretized by employing established techniques for approximating derivatives by differences.

The present approach differs in a fundamental way from that of [3] and [4]; indeed, the only common ground is the use of a coordinate transformation to immobilize a moving boundary. Here, use is made of the control volume formulation to obtain the difference equations. There are two features of the control volume approach which appear especially attractive. One of these is that it facilitates physical interpretation of the terms which result from the coordinate transformation. Thus, for example, a convection-like transport of energy can be identified which results from the movement of mass across coordinate lines in the transformed domain. The second attractive feature of the control volume approach is that it ensures global energy conservation.

It is to be expected that the formulation of a control volume approach in a nonorthogonal coordinate system will involve more analysis than is required when control volumes are used in conventional orthogonal coordinates. The first step is to derive the energy conservation principle for a control volume bounded by coordinate lines in the nonorthogonal transformed coordinate system. Then, this conservation principle, which is in integral form, is discretized to yield the governing algebraic equations of the problem. The discretization takes different forms depending on the importance of the aforementioned pseudo-convective transport of energy relative to the diffusive transport. For most moving boundary problems, the pseudo-convection is small compared with the diffusion, and a relatively simple discretization scheme can be used. For those cases where convection is a significant contributor, a more elaborate discretization is needed. Both of these discretizations are discussed in the paper. Indeed, the opportunity to readily distinguish the two types of discretizations is a dividend provided by the control volume formulation. The analysis also takes account of the energy balance at the moving boundary. That energy balance includes terms which reflect the physical processes which are responsible for the movement of the boundary.

When this work was first undertaken, the primary motivation was to solve a specific physical problem. However, as the work progressed, it became evident that the solution methodology was of interest in its own right. It also became apparent that the description of the method would require a paper-length presentation, such that the inclusion of results for a specific problem would give rise to an inordinately long paper in which the numerical results, languishing near the end, might well lose their impact. Therefore, a two-paper sequence has been prepared. The present paper describes the methodology, while the following paper (pp. 1345–1357) illustrates the application of the methodology in terms of a specific physical problem.

The control volume formulation presented here leans heavily on the work of Hossfeld [5]. Hossfeld solved the problem of natural convection in the liquid melt adjacent to a heated tube situated in a solid phase-change medium. Although this paper deals with problems different from that of Hossfeld, his control volume approach continues to be applicable. It has been adapted and recast in a form that is appropriate for the present class of problems.

THE CONTROL VOLUME FORMULATION

Description of the problem

In the development which follows, attention will be focused on axisymmetric problems, with the formulation for plane problems falling out as a special case. A schematic view of the situation to be studied is

shown in Fig. 1. As seen there, the solution domain has a stationary inner boundary whose radius is $r = r_w$ (e.g. the wall of a tube). The outer boundary moves with time and is curved; its radial coordinate will be denoted by $r_\delta(z, t)$ while the instantaneous thickness of the layer at z is $\delta(z, t)$. The lower and upper boundaries, respectively at $z = 0$ and $z = H$, are fixed.

For concreteness, the solution methodology will be phrased in terms of transient heat conduction, although it is equally applicable to other analogous transient diffusion-dominated problems. If a specific problem were to be considered, then the thermal conditions at the boundaries of the solution domain would have to be given. However, the specific nature of the thermal boundary conditions at the nonmoving boundaries $r = r_w, z = 0$ and $z = H$ does not affect the unique features of the solution methodology (i.e. those related to the presence of a curved moving boundary). Indeed, although the methodology takes cognizance of the curved moving boundary, it can be developed without consideration of the mechanism which causes the boundary to move.

In light of the foregoing, neither the boundary conditions at the fixed boundaries nor at the moving boundary will be considered during the main part of the formulation of the solution methodology. Once that development has been completed, some consideration will be given to a representative thermal condition at the moving boundary. The role of the thermal conditions at all the boundaries will be illustrated in the solution to the specific problem that is described in the companion paper.

The moving control volume

The first step in the analysis is to introduce a transformation of coordinates which immobilizes the moving boundary

$$\eta = (r - r_w)/\delta, \quad \xi = z/r_w \tag{1}$$

so that $\eta = 1$ at all points on the moving boundary at all times. In terms of the new coordinates, the solution domain is defined by $0 \le \xi \le H/r_w, 0 \le \eta \le 1$. Lines of $\xi =$ constant and $\eta =$ constant are illustrated in Fig. 1. It is evident that a control volume contained between lines $\eta = \eta_1, \eta = \eta_2$ and $\xi = \xi_1, \xi = \xi_2$ is a curvilinear element with nonorthogonal sides.

It is relevant to examine the behavior of the aforementioned control volume as the moving boundary advances. If the moving boundary were to advance from a position represented by the solid line in Fig. 1 to a position represented by the dashed line, the lines $\eta = \eta_1$ and $\eta = \eta_2$ would also advance, as indicated by the corresponding dashed lines (the $\xi = \xi_1$ and $\xi = \xi_2$ lines remain stationary). Thus, as the boundary moves rightward, the control volume also moves rightward. This motion is responsible for a convection-like transfer of energy across the $\eta =$ constant faces of the control volume.

Energy conservation for the control volume

To derive the energy conservation equation for the moving control volume, use is made of a generalization of the Leibniz rule for differentiation of an integral

$$\mathrm{d}/\mathrm{d}t\left[\int_V f\,\mathrm{d}V\right] = \int_V (\partial f/\partial t)\,\mathrm{d}V + \int_S f\mathbf{u}_b \cdot \mathbf{n}\,\mathrm{d}S \tag{2}$$

in which V and S denote the volume and surface of the control volume, respectively, $\mathbf{n}$ is the local unit vector normal to the surface, and $\mathbf{u}_b$ is the velocity of the boundary. The quantity f is any function of position and time, which will be associated here with a dimensionless temperature θ (suitably defined for each specific problem) and substituted into equation (2).

The derivative $\partial\theta/\partial t$ which appears in equation (2) after the substitution $f = \theta$ can be eliminated by employing the energy equation

$$\partial\theta/\partial t = \alpha\nabla^2\theta. \tag{3}$$

It may also be noted that

$$\int_V \nabla^2\theta\,\mathrm{d}V = \int_S \nabla\theta \cdot \mathbf{n}\,\mathrm{d}S \tag{4}$$

so that equation (2) becomes

$$\mathrm{d}/\mathrm{d}t\left[\int_V \theta\,\mathrm{d}V\right] = \int_S (\alpha\nabla\theta + \theta\mathbf{u}_b)\cdot\mathbf{n}\,\mathrm{d}S \tag{5}$$

which expresses energy conservation for the moving control volume.

To facilitate evaluation of the surface integral that appears on the right-hand side of equation (5), reference may be made to the enlarged version of the control volume that is shown at the upper right of Fig. 1. As suggested there, the surface integral may be subdivided into a sum of four surface integrals, respectively over the segments $S1$, $S2$, $S3$ and $S4$. It may also be noted that since the control volume moves radially outward with time, $\mathbf{u}_b = 0$ on $S2$ and $S4$.

For the evaluation of the surface integrals, expressions are needed for the element of surface $\mathrm{d}S$, the unit vector $\mathbf{n}$, the boundary velocity $\mathbf{u}_b$, and the gradient operator ∇. To derive these expressions, it is first necessary to consider a formal coordinate transformation from (r, z, t) to (η, ξ, τ). Among these, η and ξ have already been defined by equation (1), while τ is a dimensionless time given by

$$\tau = (\alpha t/r_w^2)Ste \tag{6}$$

where Ste, the Stefan number, is a constant parameter to be assigned for each solution. The presence of Ste in the dimensionless time τ is entirely arbitrary, and it may be omitted (i.e. set equal to one). However, for certain thermal conditions at the moving boundary of the domain ($r = r_\delta, \eta = 1$), the definition (6) eliminates Ste from the boundary condition, thereby justifying the form of the definition.

The transformation equations are

$$(\partial/\partial r)_{z,t} = (1/r_w\Delta)(\partial/\partial\eta)_{\xi,\tau} \tag{7}$$

$$(\partial/\partial z)_{r,t} = -(\beta/r_w\Delta)(\partial/\partial\eta)_{\xi,\tau} + (1/r_w)(\partial/\partial\xi)_{\eta,\tau} \tag{8}$$

$$(\partial/\partial t)_{r,z} = (\alpha Ste/r_w^2) \times [-(\eta/\Delta)(\partial\Delta/\partial\tau)(\partial/\partial\eta)_{\xi,\tau} + (\partial/\partial\tau)_{\xi,\eta}] \quad (9)$$

in which

$$\Delta = \delta/r_w, \quad \beta = \eta(\partial\Delta/\partial\xi). \quad (10)$$

The evaluation of the right-hand side of equation (5) over $S1$ will now be performed. The surface element dS may be written as

$$dS = 2\pi r(dr^2 + dz^2)^{1/2} = 2\pi r\, dz[1 + (dr/dz)^2]^{1/2} \quad (11)$$

$$dS = 2\pi r_w^2 R\chi^{1/2}\, d\xi \quad (12)$$

with

$$\chi = 1 + \beta^2, \quad R = r/r_w = 1 + \eta\Delta. \quad (13)$$

The unit vector $\mathbf{n}$ that is normal to $S1$ is obtained by noting that the gradient of η is normal to a line of constant η, so that

$$\mathbf{n} = \nabla\eta/|\nabla\eta|. \quad (14)$$

The gradient operator ∇ in axisymmetric cylindrical coordinates is

$$\nabla = \hat{\mathbf{i}}_r(\partial/\partial r) + \hat{\mathbf{i}}_z(\partial/\partial z). \quad (15)$$

By making use of equations (7) and (8), ∇ takes the form

$$\nabla = \hat{\mathbf{i}}_r(1/r_w\Delta)(\partial/\partial\eta) + \hat{\mathbf{i}}_z[-(\beta/r_w\Delta)(\partial/\partial\eta) + (1/r_w)(\partial/\partial\xi)]. \quad (16)$$

When equation (16) is employed in conjunction with (14), there is obtained

$$\mathbf{n} = (\hat{\mathbf{i}}_r - \beta\hat{\mathbf{i}}_z)/\chi^{1/2}. \quad (17)$$

Also, since $S1$ moves radially outward with time

$$\mathbf{u}_b = \hat{\mathbf{i}}_r(\partial r/\partial t)_{\xi,\eta} = \hat{\mathbf{i}}_r\eta(\alpha Ste/r_w)(\partial\Delta/\partial\tau). \quad (18)$$

Equations (11) and (16)–(18) contain all the ingredients needed to evaluate the right-hand side of equation (5) over $S1$. The result is

$$2\pi r_w\alpha\int_{\xi_1}^{\xi_2}[(\chi/\Delta)(\partial\theta/\partial\eta) - \beta(\partial\theta/\partial\xi) + \eta\theta Ste(\partial\Delta/\partial\tau)]R\, d\xi. \quad (19)$$

The evaluation of the integral over S^3 follows steps identical to those for S^1 and, therefore, there is no need to display the derivation for the $S3$ boundary.

The evaluation of the right-hand side of equation (5) over surfaces $S2$ and $S4$ is simpler than the just-completed evaluation for surfaces $S1$ and $S3$. This is because for $S2$ and $S4$, the normal to the surface is parallel to the z (or ξ) axis, and $\mathbf{u}_b = 0$. Thus, for example, for $S2$

$$\mathbf{n} = \hat{\mathbf{i}}_z, \quad \nabla\theta\cdot\mathbf{n} = -(\beta/r_w\Delta) \times (\partial\theta/\partial\eta) + (1/r_w)(\partial\theta/\partial\xi). \quad (20)$$

Furthermore,

$$dS = 2\pi r\, dr = 2\pi r_w^2 R\Delta\, d\eta. \quad (21)$$

With equations (20) and (21), the right-hand side of equation (5), when evaluated for surface $S2$, becomes

$$2\pi r_w\alpha\int_{\eta_1}^{\eta_2}[(\partial\theta/\partial\xi) - (\beta/\Delta)(\partial\theta/\partial\eta)]R\Delta\, d\eta. \quad (22)$$

Aside from a multiplicative minus sign, the integral over $S4$ consists of the same terms as those of equation (22).

Attention may now be turned to the volume integral that appears on the left-hand side of equation (5). The volume element dV can be written as

$$dV = 2\pi r\, dr\, dz = 2\pi r_w^3 R\Delta\, d\eta\, d\xi \quad (23)$$

and the total derivative d/dt can be transformed to $d/d\tau$ in accordance with equation (6).

With the aid of the expressions derived in the preceding paragraphs, the general integral energy balance (5) can be specialized to the moving curvilinear control volume defined by the lines ξ = constant, η = constant. For compactness, it is convenient to introduce the abbreviations

$$\Omega = R[-(\chi/\Delta)(\partial\theta/\partial\eta) - \eta\theta Ste(\partial\Delta/\partial\tau)] \quad (24)$$

$$\Lambda = \beta R(\partial\theta/\partial\xi), \quad \Gamma = -R\Delta(\partial\theta/\partial\xi), \quad \psi = \beta R(\partial\theta/\partial\eta). \quad (25)$$

Then, the form of the integral energy balance appropriate to the moving control volume is

$$\frac{d}{d\tau}\left[\int_{\xi_1}^{\xi_2}\int_{\eta_1}^{\eta_2} R\Delta\theta\, d\xi\, d\eta\right]Ste = \int_{\xi_1}^{\xi_2}(\Omega+\Lambda)_{S3}\, d\xi - \int_{\xi_1}^{\xi_2}(\Omega+\Lambda)_{S1}\, d\xi + \int_{\eta_1}^{\eta_2}(\Gamma+\psi)_{S4}\, d\eta - \int_{\eta_1}^{\eta_2}(\Gamma+\psi)_{S2}\, d\eta. \quad (26)$$

As written, equation (26) has the appearance of an energy balance for a fixed control volume across whose faces energy is transferred by both conduction and convection. The terms $-(R\chi/\Delta)(\partial\theta/\partial\eta)$ and $-R\Delta(\partial\theta/\partial\xi)$ are respectively proportional to diffusive heat flows (i.e. conduction) in the positive η- and positive ξ-directions, while the term $-\eta R\theta Ste(\partial\Delta/\partial\tau)$ is proportional to a pseudo-convective energy transfer in the positive η-direction. The Λ and ψ terms can also be thought of as representing heat conduction. Thus, Λ denotes conduction driven across an η face by a temperature gradient in the ξ-direction, while Γ represents conduction across a ξ face driven by an η temperature gradient. Such cross terms are encountered in anisotropic materials [1, p. 38].

The origins of the pseudo-convection and the pseudo-anisotropic diffusion can be readily identified. The former is a consequence of the movement of the control volume, while the latter is due to the non-orthogonal nature of the control volume boundaries.

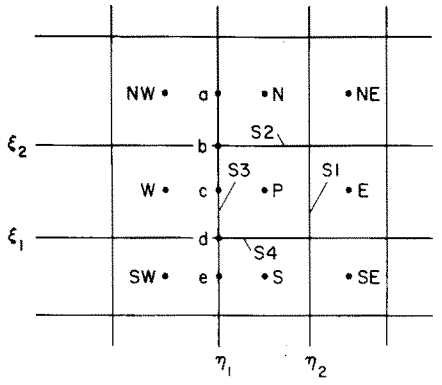

FIG. 2. An array of control volumes in the ξ, η plane.

Finite-difference formulation

A fully implicit finite-difference form of the energy equation (26) will now be deduced. To facilitate the derivation, an array of control volumes in the ξ, η plane is pictured in Fig. 2. The control volume of specific interest is that which surrounds the grid point P. Note that the grid points are centered in the respective control volumes. The superscript τ will denote quantities to be evaluated at time τ, while quantities without the superscript are to be evaluated at time $(\tau + \delta\tau)$. With this notation, a fully implicit form of equation (26) is

$$[R\Delta\theta - (R\Delta\theta)^\tau]_P(\delta\xi\delta\eta Ste/\delta\tau) + (\Omega_{S1} - \Omega_{S3})\delta\xi + (\Gamma_{S2} - \Gamma_{S4})\delta\eta = (\Lambda_{S3} - \Lambda_{S1})\delta\xi + (\psi_{S4} - \psi_{S2})\delta\eta \qquad (27)$$

in which the subscript P denotes quantities evaluated at the grid point P that is centered in the control volume of interest (see Fig. 2).

Whereas equation (27) displays the discretization of the time derivative, the spatial derivatives, which are contained within Ω, Γ, Λ and ψ, remain to be discretized. The choice of a scheme to be employed for the spatial discretization depends on the relative importance of convection relative to diffusion. When convection is small, central differencing (or its counterpart for nonuniform grids) can be used to yield results of high accuracy for a suitably small mesh size. On the other hand, when convection is large, the differencing scheme should account for the special influence of upstream points.

In the physical situations to be considered here, the convective transport is actually a pseudo-convection—due entirely to the movement of the control volumes. The experience of the authors suggests that the convection will generally be small compared with the diffusion, so that the nonuniform-grid-counterpart of central differencing should serve effectively for the spatial derivatives. Therefore, this differencing approach will be the primary one to be discussed here. Later, at the end of the paper, a more encompassing scheme which can handle strong convective influences will be described.

The derivatives $\partial\theta/\partial\eta$ on $S1$ and $S3$ and the derivatives $\partial\theta/\partial\xi$ on $S2$ and $S4$, which appear in the quantities Ω and Γ, respectively, are discretized by employing straight-line temperature distributions between point P and the relevant neighboring grid point. Thus, to find $\partial\theta/\partial\eta$ on $S1$, a straight line is passed between θ_E and θ_P, the slope of which yields $\partial\theta/\partial\eta = (\theta_E - \theta_P)/\overline{PE}$. Corresponding expressions are applicable for $\partial\theta/\partial\eta$ on $S3$ and for $\partial\theta/\partial\xi$ on $S2$ and $S4$. In addition, the θ values needed for the evaluation of Ω on $S1$ and $S3$ are found from these straight-line representations.

The derivatives $\partial\theta/\partial\eta$ and $\partial\theta/\partial\xi$ which appear in the pseudo-diffusion terms Λ and ψ are discretized by an extension of the aforementioned approach. Consider, for example, the discretization of $\beta R(\partial\theta/\partial\xi)$ on $S3$, which comprises the Λ_{S3} term in equation (27). First, the temperature θ_a at point a (Fig. 2) is expressed in terms of θ_N and θ_{NW} by means of a straight-line representation. Similarly, temperatures at c and e are represented in terms of θ_P and θ_W and of θ_S and θ_{SW}, respectively. Then, derivatives $\partial\theta/\partial\xi$ along ca and ec are expressed as

$$(\theta_a - \theta_c)/\overline{ca}, \quad (\theta_c - \theta_e)/\overline{ec}. \qquad (28)$$

The first of these is then multiplied by the value of βR at point b, while the second is multiplied by the βR value at point d. These two quantities are then averaged to yield $\beta R(\partial\theta/\partial\xi)$ on $S3$. All of the terms which appear on the right-hand side of equation (27) are discretized in this manner.

There are two other derivatives in equation (27) whose representations remain to be discussed. One of these is $\partial\Delta/\partial\tau$ which appears in Ω_{S1} and Ω_{S3}. This derivative is discretized as

$$(\Delta - \Delta^\tau)/\delta\tau \qquad (29)$$

where both Δ and Δ^τ correspond to $\xi = \xi_p$. The quantity Δ^τ is a known quantity (from the prior time step), while Δ is unknown. Its value is determined from the thermal boundary condition at the moving boundary of the solution domain, as will be discussed shortly.

The remaining derivative $\partial\Delta/\partial\xi$ appears in both β and χ. The values of this derivative were obtained by differentiation of a second-order spline which was fit to the calculated values of Δ vs ξ. The spline fit also yielded the Δ values needed on the left-hand side of equation (27) and for the evaluation of Ω, Γ and $R = 1 + \eta\Delta$.

The description of the discretization of equation (27) is now complete. The discretized equation, when applied at all grid points where θ is unknown, provides a means for determining θ at time $(\tau + \delta\tau)$. In addition to the geometrical position variables, the inputs required for the solution are the temperature distribution θ^τ and the layer thickness distribution Δ^τ, both from the prior time step, and the layer thickness distribution Δ at the current time step. Whereas θ^τ and

Δ^τ will be available as the solution marches forward in time, the current distribution of Δ is unknown. Therefore, the determination of the current distribution of Δ has to be coupled with the determination of the current distribution of θ. The procedure by which this is accomplished will be described shortly.

Before leaving this section, note may be taken of possible interactions between the discretized form of equation (27) and the thermal boundary conditions at the fixed boundaries. It is not expected that these will require numerical treatment that is out of the ordinary.

THERMAL CONDITIONS AT MOVING BOUNDARY

The thermal boundary condition at the moving boundary of the solution domain reflects the physical processes which are responsible for the motion. Various specific forms for the boundary condition are possible depending on the problem under consideration. Here, a representative physical situation will be considered in order to illustrate how the boundary condition participates in the solution for the temperature distribution in the layer.

Suppose that the physical problem is that of the freezing of a liquid on a cooled vertical tube. At any time t, the solidified material occupies the region $r_w \leq r \leq r_\delta(z, t)$, while the region $r > r_\delta(z, t)$ is occupied by liquid. The solid–liquid interface is at the fusion temperature T^*, while the liquid temperature T_∞ exceeds T^*. When $T_\infty > T^*$, it is highly likely that natural convection will occur in the liquid, with h_{NC} denoting the natural convection heat transfer coefficient at the interface (h_{NC} is assumed to be known).

The thermal condition at such a freezing interface is

$$k\nabla T \cdot \mathbf{n} = \rho\lambda \mathbf{u}_\delta \cdot \mathbf{n} + h_{NC}(T_\infty - T^*). \quad (30)$$

The left-hand side of this equation represents the heat that is conducted into the solid from the interface. On the right-hand side, the first term expresses the energy liberated by the conversion of liquid into solid (λ is the latent heat of fusion, and $\mathbf{u}_\delta$ is the velocity of the moving boundary). The second term on the right is the heat delivered to the interface from the liquid by natural convection.

To rephrase equation (30) into a more convenient form, it may first be noted that the temperature gradient ∇T is normal to the interface, since $T = T^*$ = constant along the interface. This characteristic facilitates the rephrasing of the left-hand side. The first term on the right may be evaluated by following the steps previously used to evaluate $\mathbf{u}_b \cdot \mathbf{n}$ in equation (5). The end result of these operations is

$$k(\partial T/\partial r)[1 + (\partial r_\delta/\partial z)^2]^{1/2} = \rho\lambda(\partial r_\delta/\partial t) \times [1 + (\partial r_\delta/\partial z)^2]^{-1/2} + h_{NC}(T_\infty - T^*). \quad (31)$$

If ΔT_{ref} denotes the temperature difference used to nondimensionalize T and $-\Delta T_{\text{ref}}$ is the temperature difference which appears in the Stefan number Ste, then further transformation of equation (31) yields

$$\partial\Delta^2/\partial\tau = -2(\partial\theta/\partial\eta)[1 + (\partial\Delta/\partial\xi)^2] - (2h_{NC}r_w/k)[(T_\infty - T^*)/\Delta T_{\text{ref}}] \times \Delta[1 + (\partial\Delta/\partial\xi)^2]^{1/2}. \quad (32)$$

The fully implicit finite-difference form of equation (32) is

$$\Delta = [(\text{RHS } 32)\delta\tau + (\Delta^\tau)^2]^{1/2} \quad (33)$$

where RHS 32 denotes the right-hand side of equation (32). Aside from Δ^τ, all of the variables appearing in equation (33) pertain to time $(\tau + \delta\tau)$ and are, therefore, unknown. The role played by equation (33) in the solutions for the temperature field in the layer and the layer thickness Δ will be described in the next section of the paper.

SOLUTION PROCEDURE

A computational procedure will now be described for solving the difference equations that have been derived in the preceding sections of the paper. Suppose that the computations at time τ have been completed, so that the numerical values of $\theta^\tau(\xi, \eta)$ and $\Delta^\tau(\xi)$ are available. Also available at time τ are values of $R = 1 + \eta\Delta$, $\partial\theta/\partial\eta$, and of $\partial\Delta/\partial\xi$, with the latter being obtained from a second-order spline fit of $\Delta^\tau(\xi)$. With these input values, calculations are to be carried out to determine $\theta(\xi, \eta)$ and $\Delta(\xi)$ at time $(\tau + \delta\tau)$.

The computations begin with the interface energy equation (33), which is solved iteratively for Δ by the following procedure. First, the right-hand side of equation (32) is evaluated at each grid point ξ ($\eta = 1$) on the interface by employing known values of $\partial\theta/\partial\eta$, $\partial\Delta/\partial\xi$, and Δ from the solution at time τ. With these, a distribution $\Delta(\xi)$ is computed from equation (33), and $\partial\Delta/\partial\xi$ follows from a spline fit. The just-determined Δ and $\partial\Delta/\partial\xi$ are then employed as input to equations (32) and (33), with $\partial\theta/\partial\eta$ held fixed, and new distributions $\Delta(\xi)$ and $\partial\Delta/\partial\xi$ are obtained. These new distributions are inputed to (32) and (33), yielding still other distributions of $\Delta(\xi)$ and $\partial\Delta/\partial\xi$. In practice, this procedure was found to converge in two or three rounds of iteration.

With tentative values of Δ, $\partial\Delta/\partial\xi$, $R = 1 + \eta\Delta$, $\beta = \eta(\partial\Delta/\partial\xi)$, and $\chi = 1 + \beta^2$ now available at time $(\tau + \delta\tau)$, attention is turned to the solution of the discretized form of equation (27). As already noted, the required inputs to equation (27) from time τ are also available. Thus, only the θ values at the respective grid points appear as unknowns, and these appear linearly. Any number of available methods, either iterative or direct, may be used to solve for the θ distribution. If an iterative method were to be used, it may be convenient to treat the right-hand side of equation (27) as a source term, the value of which is obtained from the θ values of the preceding iteration.

The solution of the discretized form of equation (27) yields the θ distribution throughout the layer, from which $\partial\theta/\partial\eta$ can be determined as a function of ξ at the interface $\eta = 1$. With this information, equations (32) and (33) are revisited to obtain, via iteration, a refined

result for the distributions of $\Delta(\xi)$ and $\partial\Delta/\partial\xi$. When these distributions have been obtained, attention is once again focused on the discretized form of equation (27), from which an updated solution for $\theta(\xi,\eta)$ and for $\partial\theta/\partial\eta$ at $\eta = 1$ can be determined.

This procedure of successive visitations with equations (32), (33) and (27) is continued until convergence to a preselected tolerance is obtained. The resulting distributions $\theta(\xi, \eta)$ and $\Delta(\xi)$, which correspond to time $(\tau+\delta\tau)$, are then used as input to the computations for the next time level.

The starting of the solution at $\tau = 0$ offers no special difficulties provided that the initial transient is not too fast. However, if the transient is initiated by a step change in a boundary condition, it is very difficult to obtain an accurate numerical solution at small values of time (indeed, errors at small times may propagate to larger times). In that event, it is advantageous to seek a small-time solution from a simplified model of the physical situation. Such a small-time solution, evaluated at a suitable $\tau>0$, can serve as a point of departure for the full-blown numerical solution set forth in this paper. An illustration of the use of a small-time solution will be presented in the applications paper which follows on pp. 1345–1357.

ALTERNATE DISCRETIZATION

In the spatial discretization of the control volume energy equation (27), as described earlier in the paper, it was assumed that the pseudo-convective transport was small compared with the diffusive transport. Now, consideration will be given to situations where convection may not be small, so that a central-difference-like discretization of the derivatives is not suitable. The alternate discretization leans heavily on the material set forth in Chapter 5 of [6], and, specifically, makes use of the power-law scheme described on pp. 90–92 of that chapter.

To rephrase equation (27) in a form which enables it to be discretized by comparison with a standard equation presented in [6], the left-hand side of (27) has to be transformed. To this end, $f = 1$ is introduced into equation (2), and $\mathbf{u}_b \cdot \mathbf{n}$ is evaluated as before from equations (17) and (18). The resulting equation is rewritten in implicit finite-difference form, yielding

$$[R\Delta - (R\Delta)^{\tau}]_P(\delta\xi\delta\eta/\delta\tau) = \delta\xi[\eta R(\partial\Delta/\partial\tau)]_{S1} - \delta\xi[\eta R(\partial\Delta/\partial\tau)]_{S3}. \quad (34)$$

Equation (34) can be solved for $R\Delta$, which is then introduced into equation (27). After this substitution, the resulting equation is completely analogous to equation (5.53) of [6], and, in accordance with [6], it can be written as

$$[(R\Delta)^{\tau}(\theta - \theta^{\tau})]_P(\delta\xi\delta\eta Ste/\delta\tau) + a_N(\theta_P - \theta_N) + a_S(\theta_P-\theta_S) + a_E(\theta_P-\theta_E) + a_W(\theta_P-\theta_W) = b \quad (35)$$

where

$$a_N = (R\Delta)_{S2}\delta\eta/(\xi_N - \xi_P),$$
$$a_S = (R\Delta)_{S4}\delta\eta/(\xi_P - \xi_S) \quad (36)$$
$$a_E = D_1A(|P_1|) + \{\{-F_1, 0\}\},$$
$$a_W = D_3A(|P_3|) + \{\{F_3, 0\}\} \quad (37)$$

and

$$D_1 = (\chi R/\Delta)_{S1}\delta\xi/(\eta_E - \eta_P),$$
$$D_3 = (\chi R/\Delta)_{S3}\delta\xi/(\eta_P - \eta_W) \quad (38)$$
$$F_1 = -\delta\xi Ste[\eta R(\partial\Delta/\partial\tau)]_{S1},$$
$$F_3 = -\delta\xi Ste[\eta R(\partial\Lambda/\partial\tau)]_{S3} \quad (39)$$
$$P_1 = F_1/D_1, \quad P_3 = F_3/D_3. \quad (40)$$

Also,

$$A(x) = \{\{0, (1 - 0.1x)^5\}\} \quad (41)$$

in which the notation $\{\{x_1, x_2\}\}$ means that the larger of x_1 and x_2 is to be used.

The quantity b which appears on the right-hand side of equation (35) is equal to the right-hand side of equation (27), the discretization of which has already been discussed. Furthermore, the derivatives $\partial\Delta/\partial\tau$ and $\partial\Delta/\partial\xi$ are also treated in the same way as in the discretization scheme that was described earlier.

Equations (35)–(41), supplemented by the text which follows them, convey a complete statement of the alternate discretization scheme. The computational procedure for solving the resulting algebraic equations is as before.

CONCLUDING REMARKS

In this paper, a methodology has been set forth for the numerical solution of transient two-dimensional diffusion-type problems in which one of the boundaries of the diffusion region moves as time passes. The solution method accommodates moving boundaries that do not lie along coordinate lines (e.g. curved boundaries).

The moving boundary is immobilized by a coordinate transformation, but the transformed coordinates are, in general, not orthogonal. Furthermore, as time passes, the coordinate lines of the new coordinate system sweep across the diffusion region. Therefore, with respect to a given control volume in the new coordinate system, mass appears to pass through the control surface which bounds the volume. This movement of mass brings about a convection-like transport of energy with respect to the given control volume.

The special feature of the present formulation is the use of a control-volume-based energy equation as the starting point for the derivation of the finite-difference equations. The control volume approach facilitates physical interpretation of the novel terms which result from the coordinate transformation, including both pseudo-convection terms and additional diffusion-type terms. Among these, the latter resemble the cross

diffusion terms for an anisotropic medium, whereby, for example, the heat flow in a given direction is driven by a temperature gradient in a different direction. The pseudo-convection is due to the aforementioned movement of the coordinate lines, while the pseudo-anisotropic-diffusion is due to the nonorthogonal nature of the transformed coordinates. The capability of identifying the pseudo-convection terms has relevance in the selection of a differencing scheme, since the suitability of central differencing (or its counterpart for nonuniform grids) depends on whether or not convection is small compared with diffusion.

The energy equation for a moving, nonorthogonal control volume is first derived in general and is then specialized to the transformed coordinate system which immobilizes the moving boundary of the diffusion region. Both the general energy equation and its specialized version are in integral form. A fully implicit scheme is used to discretize the energy equation. With respect to the spatial derivatives, two discretizations are described. The primary discretization is for the case in which the convective transport is small compared with the diffusion transport, so that central differencing (or its nonuniform-grid counterpart) can be used. Experience suggests that for moving boundary problems, the pseudo-convection is small compared with the diffusion. An alternate discretization is also presented which accommodates convection and diffusion transports of comparable magnitude.

Consideration is also given to the energy equation at the moving boundary of the solution domain. This equation reflects the physical processes which are responsible for the movement of the boundary. The boundary energy equation is transformed into the new coordinates and then discretized.

With the discretized equations thus derived, attention is turned to the scheme for their numerical solution. At any time level, the scheme involves a succession of visitations with the energy equations within the solution domain and with the energy equation at the boundary. The specific steps of the solution methodology are described in sufficient detail to facilitate their application.

The use of the control volume formulation and the solution methodology will be illustrated for a specific problem in a companion paper that follows this paper in the journal.

Acknowledgement—This research was performed under the auspices of the U.S. Department of Energy (DOE/DE-AC02-79ER10343), Office of Basic Energy Sciences.

REFERENCES

1. H. S. Carslaw and J. C. Jaeger, *Conduction of Heat in Solids*. Oxford University Press, London (1959).
2. M. N. Ozisik, *Heat Conduction*. John Wiley, New York (1980).
3. T. Saitoh, Numerical method for multi-dimensional freezing in arbitrary domains, *J. Heat Transfer* **100**, 294–299 (1978).
4. J. L. Duda, M. F. Malone, R. H. Notter and J. S. Vrentas, Analysis of two-dimensional diffusion-controlled moving boundary problems, *Int. J. Heat Mass Transfer* **18**, 901–910 (1975).
5. L. M. Hossfeld, A coordinate transformation method for solving a convection phase change problem, Ph.D. Thesis, Department of Mechanical Engineering, University of Minnesota, Minneapolis, Minnesota (1979).
6. S. V. Patankar, *Numerical Heat Transfer and Fluid Flow*. Hemisphere Publishing, Washington, D.C. (1980).

RESOLUTION NUMERIQUE DES PROBLEMES A FRONTIERES MOBILES PAR IMMOBILISATION DE LA FRONTIERE ET UN SCHEMA DE DIFFERENCES FINIES AVEC VOLUME DE CONTRÔLE

Résumé—On établit une méthode de résolution des problèmes de diffusion variable bidimensionnelle (conduction thermique) dans lesquels une des frontières du domaine se déplace en fonction du temps. La frontière mobile est rendue fixe par un changement de coordonnées, mais celles-ci ne sont pas orthogonales en général. Par rapport à un volume de contrôle dans le nouveau système de coordonnées, la masse semble passer à travers la surface de contrôle qui limite le volume et à ce mouvement de masse est lié un transport d'énergie. L'équation d'énergie pour un volume de contrôle mobile et non orthogonal est obtenue et adaptée au système de coordonnées transformées associé à l'immobilisation de la frontière. Un schéma entièrement explicite est utilisé pour discrétiser l'équation d'énergie. Les dérivées spatiales sont discrétisées par l'un des deux schémas suivant la taille de la pseudo-convection relative à la diffusion. Le bilan d'énergie à la frontière mobile est aussi transformé et discrétisé. Une procédure numérique est ensuite développée pour résoudre les équations d'énergie discrétisées. L'utilisation de cette méthode est illustrée dans un article qui suit ce texte dans le même journal.

NUMERISCHE LÖSUNG VON PROBLEMEN MIT WANDERNDER GRENZE DURCH FESTLEGUNG DER GRENZE MIT HILFE EINES FÜR EIN KONTROLLVOLUMEN FORMULIERTEN FINITEN DIFFERENZENVERF AHRENS

Zusammenfassung—Eine Methode zur numerischen Lösung von instationären zweidimensionalen Diffusionsproblemen (z. B. Wärmeleitung) wird entwickelt, bei denen eine der Grenzen des Lösungsgebiets mit der Zeit fortschreitet. Die wandernde Grenze wird durch eine Koordinatentransformation festgehalten, wobei aber die transformierten Koordinaten im allgemeinen nicht rechtwinklig sind. Ferner strömt in bezug auf ein gegebenes Kontrollvolumen in dem neuen Koordinatensystem Masse durch die das Volumen begrenzende Kontrollfläche, und dieser Massenstrom hat einen konvektionsartigen Energiestrom zur Folge. Die Energiegleichung für ein bewegtes nichtorthogonales Kontrollvolumen wird allgemein hergeleitet und dann für das transformierte System in Verbindung mit dem Festhalten der wandernden Grenze speziell entwickelt. Mit einem vollständig impliziten Verfahren wird die Energiegleichung für das Kontrollvolumen diskretisiert. Die räumlichen Ableitungen werden mit einem von zwei Verfahren, die von der Größe des Verhältnisses der Pseudo-Konvektion zur Diffusion abhängen, diskretisiert. Die Energiebilanz an der wandernden Grenze des Lösungsgebiets wird ebenfalls transformiert und diskretisiert. Ein numerisches Verfahren wurde dann zur Lösung dieser diskretisierten Energiegleichungen entwickelt. Die Anwendung des Kontrollvolumenansatzes und der Lösungsmethode wird für einen bestimmten physikalischen Fall in einem Begleitartikel dargestellt werden, der dem vorliegenden Ausfatz in dieser Zeitschrift folgen wird.

ЧИСЛЕННОЕ РЕШЕНИЕ ЗАДАЧ С ДВИЖУЩЕЙСЯ ГРАНИЦЕЙ С ПОМОЩЬЮ КОНЕЧНО-РАЗНОСТНОЙ СХЕМЫ КОНТРОЛЬНОГО ОБЪЕМА ДЛЯ ФИКСИРОВАННОЙ ГРАНИЦЫ

Аннотация — Предложена методика численного решения задач диффузионного типа (например, теплопроводности), в которых положение одной из границ расчетной области изменяется во времени. Движение границы фиксируется преобразованием координат, причем новые координаты, как правило, не ортогональны. При получении контрольного объема в новой системе координат возникает массообмен через контрольную поверхность, ограничивающую рассматриваемый объем, который приводит к конвективному переносу энергии. Уравнение энергии для движущегося неортогонального контрольного объема выводится обычным образом, а затем записывается в системе координат, связанной с фиксацией движущейся границы. При аппроксимации уравнения энергии для контрольного объема используется полностью неявная схема. Пространственные производные аппроксимируются одной из двух схем в зависимости от соотношения между диффузионной и конвективной составляющими. Таким же образом преобразуется и аппроксимируется уравнение баланса для движущейся границы. Приводится численный алгоритм решения разностных уравнений энергии. Методика использования контрольного объема и численного алгоритма иллюстрируется на примере решения частной физической задачи, опубликованной в этом же номере журнала.