ON THE USE OF GREEN'S FUNCTIONS FOR SOLVING MELTING OR SOLIDIFICATION PROBLEMS

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Abstract – An analytical cum computational technique is proposed using Green's functions for solving melting or solidification problems. It is suggested that from a computational viewpoint, this procedure may be very attractive for tackling problems involving non-linear boundary conditions, or multi-component systems.

The application of the technique is illustrated on two examples, the melting ablation of a slab due to convective heat transfer and the dissolution-melting of a slab into a binary liquid mixture.

	NOMENCLATURE
a^{2} ,	thermal diffusivity $[L^2t^{-1}];$
C ₀ , C _B ,	carbon concentration at the sur-
	face and in the bulk respectively,
	in weight fraction;
<i>G</i> ,	Green's function, defined in equa-
	tion (8); $G(x, t \xi, \tau)$;
h,	heat transfer coefficient
	$[QL^{-2}T^{-1}t^{-1}];$
h _D ,	mass transfer coefficient $[Lt^{-1}];$
<i>k</i> ,	integers, appearing as indices;
Ĩ,	thermal conductivity
	$[QL^{-1}T^{-1}t^{-1}];$
<i>l</i> ,	half width of the slab [L];
n, N,	integers;
$S_1, S_2 \ldots S_k$	slopes of the chord connecting
	discrete values of $X[Lt^{-1}]$;
х,	spatial coordinate [L];
X(t),	position of the melt line (solidifi-
	cation front) [L];
Τ,	temperature [T];
$T_{B}, T_{i}(x),$	bulk temperature and initial
	temperature distribution respec-
	tively;
$T_m, T_m(t),$	melting temperature;
α, β,	constants;
ΔH ,	latent heat of melting $(QM^{-1}]$;
ρ.	density $[ML^{-3}];$

ξ,	position of instantaneous source;
τ,	time of occurrence of in-
	stantaneous source;
t _k ,	corresponding time steps with
	$t_1 = 0$, etc.;
X_{k} ,	melting front at t_k ;
P_{k} ,	partition point of the original
	slab thickness [L].

INTRODUCTION

PROBLEMS involving melting or solidification occur frequently both in nature and in systems of technological importance. Ice formation or thawing represent important environmental applications, whereas ingot solidification and scrap melting are significant problems in the metals processing industry.

The mathematical statement of these moving boundary problems is readily given in most instances, but the range of analytical solutions that may be generated is extremely restricted [1]. In general, one is therefore led to consider numerical or semi-analytical techniques. While the finite difference approach to moving boundary problems may be very straight forward in concept, difficulties are frequently encountered in actual computation due to numerical instabilities. These difficulties may be overcome by the choice of fine grids and small "time steps"—this, however, may require excessive computer time.

This state of affairs stimulated alternative approaches, through the use of semi-analytical techniques. Thus Citron [2] suggested the use of successive approximations for the melting of slabs for arbitrary initial temperature distribution and for an arbitrary heat input.

Boley used an "embedding technique" and the concept of the fictitious heat flux to obtain short time and long time solutions for slabs [3] and cylinders [4].

The use of the integral profile technique for moving boundary problems was pioneered by Goodman [5] and has found widespread application to a variety of melting and solidification processes [6, 7].

The techniques described above are attractive because of their simplicity, but their application becomes somewhat cumbersome for multicomponent systems or in situations where transient diffusion of heat flow equations have to be solved for two adjoining phases. meet this criterion. The description and illustration of this technique forms the subject matter of this paper.

While Green's functions have been used extensively for tackling a wide range of diffusion and heat conduction problems [8], their application to moving boundaries appears to be a relatively novel undertaking.

FORMULATION

Let us consider a solid slab, extending from x = -l to x = l of a given initial temperature distribution; at time = 0, the slab is immersed in its own melt and we are interested in the resultant melting or solidification process.

The physical system is sketched in Fig. 1; for constant physical properties, the conservation of heat within the solid phase may be readily expressed by the linear transient heat conduction equation*

$$a^{2} \frac{\partial^{2} T}{\partial x^{2}} - \frac{\partial T}{\partial t} = 0, -X(t) \le x \le X(t)$$
 (1)



FIG. 1. Schematic representation of the system.

The work to be reported in this paper forms part of a project aimed at the study of melting and solidification in multicomponent systems. A rational approach to this class of problems requires a relatively economical computational technique.

In the following we shall describe an analytical cum computational procedure, involving the use of Green's functions, which is thought to where X(t) represents the instantaneous position of the solidification boundary.

The boundary conditions are written as

$$T = T_i(x); t = 0 \tag{2}$$

$$T = T_m(t); x = \pm X(t)$$
 (3), (4)

^{*} The problem considered here assumed symmetry about x = 0; the treatment to be presented may be readily generalized to cover asymetric systems.

and

$$\alpha \frac{\partial T}{\partial x} + \beta T = f(t), x = \pm X(t) \quad (5), (6)$$

with

$$X(t) = l \text{ at } t = 0.$$
 (7)

Here equation (2) expresses the previously stated initial condition, equations (3) and (4) state that the solid is at the melting temperature at the phase boundary. For one component systems, to be considered in the first instance, T_m is a constant; however, in multicomponent systems the melt temperature is composition dependent, and hence will, in general, be a function of time. Equations (5) and (6) constitute a general expression for the conservation of heat at the moving boundary. Here α and β are constants, and the function f(t) is related to the movement of the phase boundary. equation (1) for homogeneous boundary conditions in an infinite medium. After some quite straight forward manipulation, using the properties of Green's functions, the general solution of equations (1)-(7) may be written as [9, 10]

$$T(x,t) = \int_{-1}^{-1} T_i G \Big|_{\tau=0} d\xi + \int_{-X(t)}^{-1} TG \Big|_{-X(t)} d\xi$$

$$+ \int_{t}^{X(t)} TG |_{X(t)} d\xi + a^{2} \int_{t}^{0} \left[G \frac{f(\tau) - \beta T_{m}}{\alpha} - T_{m} \frac{\partial G}{\partial \xi} \right]_{-X(\tau)} d\tau + a^{2} \int_{0}^{t} \left[G \frac{f(\tau) - \beta T_{m}}{\alpha} - T_{m} \frac{\partial G}{\partial \xi} \right]_{X(\tau)} d\tau.$$
(9)



FIG. 2. Technique for advancing the interface.

In order to obtain a formal solution to this problem, let us consider $G \equiv G(x, t | \xi, \tau)$ the Green's function, due to a plane source at $x = \xi$ and at $t = \tau$. G takes the following form

$$G \equiv \frac{1}{2a\sqrt{\pi(t-\tau)}} \exp \left[- [(x-\xi)^2/4a^2(t-\tau)] \right]$$
(8)

and constitutes the fundamental solution of

At this stage equation (9) contains the as yet unknown X(t) i.e. the instantaneous position of the solidification front.

While equation (9) could be integrated directly, such procedure would require inordinately large amounts of computer time and a further difficulty would be posed by the singular point at $t = \tau$ and $x = \xi$. In order to circumvent these difficulties, the following general technique has been developed, which is illustrated in Fig. 2. The actual advancement of the moving phase boundary between positions is approximated by a chord on the plot of X vs. t: let us further designate the slopes of the straight lines connecting X_1 and X_2 , by S_1 ; the slope of the chord connecting X_2 and X_3 by S_2 , etc.

Thus starting from $X_1 = l$, we can find the position $x = X_2(t_2)$, by a few iterations on S_1 ,

$$\frac{\exp^{-[(x-\xi)^{2}/4a^{2}t]} d\xi}{\sqrt{t}} d\xi \simeq \frac{1}{2a\sqrt{\pi}} \sum_{k=1}^{k=N} T_{i}(P_{k}) \int_{P_{k}} \frac{\exp^{-[(x-\xi)^{2}/4a^{2}t]}}{\sqrt{t}} d\xi = \frac{1}{2} \sum_{k=1}^{k=N} T_{i}(P_{k}) \left[\operatorname{erf} \frac{(x-P_{k})}{2a\sqrt{t}} - \operatorname{erf} \frac{(x-P_{k+1})}{2a\sqrt{t}} \right].$$
(11)

The other terms appearing in equation (9) are also readily integrated, and after some algebra we obtain the following expression for the temperature profile

$$T(x,t) = \frac{1}{2} \sum_{k=1}^{k=N} T_i(P_k) \left[E\left(\frac{x-P_k}{2a\sqrt{t}}\right) - E\left(\frac{x-P_{k+1}}{2a\sqrt{t}}\right) \right] + \frac{1}{2} \sum_{k=1}^{k=n} T_m(t_k) \left\{ E\left(\frac{D-A}{\sqrt{QD}}\right) - E\left(\frac{G-A}{\sqrt{QG}}\right) + \left[E\left(\frac{D+A}{\sqrt{QG}}\right) - E\left(\frac{G-A}{\sqrt{QG}}\right) - E\left(\frac{G-A}{\sqrt{QG}}\right) - E\left(\frac{G-A}{\sqrt{QG}}\right) - E\left(\frac{B+D}{\sqrt{QG}}\right) - E\left(\frac{B+D}{\sqrt{QG}}\right) + \left[E\left(\frac{B+D}{\sqrt{QG}}\right) - E\left(\frac{B+D}{\sqrt{QG}}\right) - E\left(\frac{G-A}{\sqrt{QF}}\right) + \left[E\left(\frac{G+A}{\sqrt{QF}}\right) - E\left(\frac{G+A}{\sqrt{QF}}\right) - E\left(\frac{G+A}{\sqrt{QF}}\right) + \left[E\left(\frac{G-A}{\sqrt{QF}}\right) - E\left(\frac{G+A}{\sqrt{QF}}\right) - E\left(\frac{B+F}{\sqrt{QF}}\right) \right] \right] \right\} + \frac{1}{2} \sum_{k=1}^{k=n} T_m(t_k) \left\{ \left[E\left(\frac{G+B}{\sqrt{QG}}\right) - E\left(\frac{F+B}{\sqrt{QG}}\right) \right] e^{4(B/Q)} - E\left(\frac{F+A}{\sqrt{QF}}\right) - E\left(\frac{G+A}{\sqrt{QG}}\right) \right] e^{4(A/Q)} \right\}$$
(12)

by requiring, that equation (9) be satisfied at a position infinitesimally close to the point $x = X_2(t_2)$. Once the position of $X_2(t_2)$ is found, we may proceed to subsequent points in a similar manner.

For each step we may write

$$\tau = t_k + \frac{x_k - \xi}{S_k}, k = 1, 2 \dots n.$$
 (10)

The actual integration indicated in equation (9) is performed by using the technique of "reduction to quadrature." Thus the first term on the right hand side of equation (9) is integrated as follows:

$$\int_{-l}^{l} T_{i}(\xi) G \Big|_{\tau=0} d\xi = \frac{1}{2a\sqrt{\pi}} \int_{-l}^{l} T_{i}(\xi) \frac{1}{\sqrt{t}}$$

where

$$A = (t - t_k)S_k + (x - x_k)$$

$$B = (t - t_k)S_k - (x + x_k)$$

$$D = (t - t_k)S_k^- + (x_{k+1} - x_k)$$

$$F = (t - t_{k+1})S_k$$

$$G = (t - t_k)S_k^-$$

$$Q = 4a^2/S_k \text{ and } S_k = \frac{x_k - x_{k+1}}{t_{k+1} - t_k}$$

$$E(x) \text{ represents erf } (x).$$

It is thus seen, that through the use of equation (12) the advancement of the phase boundary, and the temperature profiles within the solid phase are readily obtained by iterations involving only an algebraic procedure. The actual calculations were performed on the C.D.C. 6400 digital computer of the State University of

New York at Buffalo, the essential components of the flow chart for the program are shown in Fig. 3. The application of the technique for the



Computer flow chart

FIG. 3. Block diagram of the computer program.

solution of actual problems, and typical computed results are shown in the subsequent section.

COMPUTED RESULTS

In order to apply the technique to actual problems, we shall have to specify the constants α and β and the functions, $T_m(t)$ and f(t).

For single component systems $T_m(t) = T_m$, i.e. a constant throughout the melting or solidification period.

For systems where the molten phase is immobile or undergoes regular laminar motion, the quantity f(t) is not given explicitly, but rather, it appears as a coupling between the heat flow equations in the molten and solid phases. Even under these conditions, the technique described above should afford considerable simplification of the overall computing procedure.

However, in the examples to be presented in

the following, we shall confine our attention to systems, where the molten phase is agitated, and where the convective heat transfer coefficient is known between the solid surface and the liquid.

Under these conditions f(t) is explicitly defined in terms of quantities that have appeared in the preceeding formulation.

Example 1

The melting of a steel slab in contact with agitated molten steel. Let us consider a steel slab, initially at a uniform temperature, which at time = 0 is immersed into well agitated, pure molten iron, at some temperature above its melting point.

Under these conditions, $T_m(t) = T_m$, furthermore, symmetry will dictate that the domain $0 \le x \le l$ will behave identically with the region $-l \le x \le 0$, thus only one of these regions will have to be considered.

For such a system equation (5), expressing the conservation of heat at the moving boundary will take the following simple form

$$\tilde{k}\frac{\partial T}{\partial x} - h(T_B - T) = \rho \Delta H \frac{\mathrm{d}X(t)}{\mathrm{d}t} \qquad (13)$$

i.e.

$$\alpha = \tilde{k}, \beta = h, \text{and } f(t) = hT_B + \rho\Delta H \frac{\mathrm{d}X(t)}{\mathrm{d}t}.$$
 (14)

Here \tilde{k} is the thermal conductivity of the solid, h, is the convective heat transfer coefficient between the melt and the solid, ρ is the density, ΔH is the latent heat of melting and T_B is the bulk temperature of the melt.

The following property values were assumed for the purpose of computation

$$l = 1 \text{ in.} T_i = 70^{\circ}\text{F} T_m = 2800^{\circ}\text{F} T_B = 3000^{\circ}\text{F} h = 1,000 \text{ Btu/h ft}^{2\circ}\text{F and} \Delta H = 110 \text{ Btu/lb}, a^2 = 0.018 (in.^2/s) \rho = 445 \text{ lb/ft}^3 \tilde{k} = 20 \text{ Btu/h ft}^{\circ}\text{F}.$$

Some computed curves, giving the transient temperature profiles and the position of the melt line as a function time are given in Figs. 4 and 5 respectively.



FIG. 4. Transient temperature profiles in the solid slab, prior to melting, in Example 1.

It may be shown, that during the premelting stage, the temperature profiles given in Fig. 4 are very close to the asymptotic behaviour for a step change in surface temperature to T_B ; this is to be expected for a relatively large value of the ratio: hl/\tilde{k} .

The position of the melt line, plotted in Fig. 5 appears to be a linear function of time after an initial time period; this again is consistent with the fact, that by that time, all of the slab has been brought to the melting point so that melting would proceed at a uniform rate. This may be readily verified by comparing the numerical value of the melting rate that may be obtained from equation (13) upon setting $(\partial T/\partial x) = 0$, with that given in Fig. 5 for the final stages of the melting process. These numerical values of



FIG. 5. Plot of the position of the melt line against time in Example 1.

of |(dX/dt)| are 1.36×10^{-2} in./s and 1.34×10^{-2} in./s respectively, which are indeed in very good agreement.

Example 2

Melting of a steel slab, immersed in an ironcarbon melt. Let us consider the melting of a pure iron slab, immersed in a melt, consisting of iron and carbon. Let the initial thickness of the slab be one foot, its carbon content zero, and its initial temperature 70°F. Finally, let both the temperature and carbon content of the melt be time dependent, as sketched in Fig. 6. The problem is to find the rate of melting of the slab, as a function of time. Problems of this type arise in the melting of scrap in basic oxygen steelmaking processes.

This problem is rather more complex than that discussed in the previous example, because the melting temperature of the steel slab is no longer constant, but will depend on the carbon composition at the surface. Thus in general, the melting rate will depend on both carbon diffusion (mass transfer) and on heat transfer.



FIG. 6. The time dependence of temperature and of the carbon concentration in the bulk of the melt—Example 2.

By reference to the iron carbon phase diagram [11], let us approximate the effect of carbon content (at the surface) on the melting temperature by the following linear relationship

$$T_{mp} = 2800^{\circ} \mathrm{F} - 1.5 \times 10^{4} \mathrm{C}_{0} \qquad (15)$$

where C_0 is the carbon content at the melt-solid interface in weight fraction. Equation (15) is valid approximately, within the range $0 \le C_0 \le 0.04$.

The surface concentration, C_0 in turn will depend on mass transfer between the melt and the solid surface.

By establishing a carbon balance at the interface, on making the quasi-steady state approximation, we have the following expression for C_0

$$C_0 = \frac{h_D(C_B - C_0)}{\left| (dX/dt) \right| + h_D(C_B - C_0)}$$
(16)

where h_D is the liquid phase mass transfer coefficient, and C_B is the weight fraction of carbon in the bulk. In general,

 $|(dX/dt)| \ge h_D [C_B - C_0]$, therefore equation (16) may be written as:

$$C_0 = \frac{h_D C_B}{h_D + |(dX/dt)|} = \frac{h_D C_B}{h_D + |S_k|}.$$
 (17)

On combining equations (15) and (17) we have

$$T_{mp} = 2800^{\circ} \mathrm{F} - 1.5 \times 10^4 \frac{h_D C_B}{h_D + |S_k|}.$$
 (18)

For a fixed value, or known values of h_D , equation (18) represents and explicit relationship between T_{mp} , C_B and the melting rate, which may be readily incorporated into equation (12) and then computation proceeds in the usual manner.

Some computed results are shown in Figs. 7 and 8. In addition to the previously given $T_B(t)$ and $C_B(t)$ functions, the property values chosen for



FIG. 7. Temperature distribution in the solid, after 0.86 s. Example 2.

the computation were h = 10000 Btu/h ft² °F and $h_D = 0.038$ in./s. Clearly, h and h_D are related through the analogy between turbulent heat and mass transfer. The particular, numerical values chosen are thought to represent typical conditions in the Basic Oxygen Furnace.

Figure 7 shows a plot of the temperature distribution within the slab, very shortly after the commencement of the process. It is seen the surface temperature is very rapidly raised to the melting point. Had carbon diffusion been absent, no melting would have occurred at all, until T_B reached 2800°F, thus in the present case, the lowering of the melting temperature played a very important role in determining the overall rate of the process.

The non-analytical nature of $T_B(t)$, and $C_B(t)$ made a numerical approach mandatory in this case, and the use of the technique outlined in this paper allowed the computation to proceed with considerable economy.



FIG. 8. Position of the melt line as a function of time for Example 2. Also shown is the time dependent melting temperature of the solid.

Figure 8 shows the position of the melt line as a function of time, and the values of the surface temperature (time dependent melting point, due to carbon diffusion) are also shown at certain descrete points. It is seen that the melting rate is almost uniform due to the compensating effects of the gradually increasing T_B and the progressively decreasing C_B ; this latter. of course, leads to a progressively increasing melting temperature for the slab.

DISCUSSION

In the paper a new technique is proposed for the solution of moving boundary problems involving unsteady state heat conduction (or diffusion). The solution is sought in the form of Green's function and the technique involves quite straight forward manipulation of Green's function, but for the fact that the time dependent moving boundary appears in the integrals. The formal integral solution of the problem is then further manipulated to obtain an algebraic expression, in the form of a series summation for the temperature distribution, in terms of the as yet unknown position of the moving boundary. The position of the moving boundary is then determined by an iterative stepwise process, in course of which the moving boundary is advanced to new positions, such that the integral equation is satisfied to within the desired degree of accuracy.

At this stage it may be worthwhile to compare this technique with the alternatives that are available at the present.

The technique described in the paper is helpful as it can readily accommodate non-analytical functions, and quite complex boundary conditions—a feature not possessed by many of the other semi-analytical procedures reported in the literature.

"Straight" finite difference techniques constitute the other alternative. While finite difference techniques may be quite flexible and could certainly accommodate non-linear boundary conditions, they would require considerably more computer time, as constraints posed by stability would mandate fine grids and consequently very small time steps.

During the pre-melt period (fixed boundary) the solution described in the paper involves no iteration, thus the economy achieved over the finite differencing is quite evident.

Furthermore, the advantages of this technique are even more pronounced under conditions of melting, i.e. when the boundary is no longer fixed. Here the Green's function solution requires only the knowledge of the surface temperature, whereas in the finite difference technique the temperature has to be evaluated at all the internal grid points.

ACCURACY OF THE COMPUTED RESULTS

The computational error was estimated by two techniques.

(a) Equation (12) in itself represents an overall heat balance, so that the error is readily estimated by comparing the two sides of equation (12).

In the computation the time step was so chosen that the error, with regard to this overall heat balance, was less than 1.5 per cent. This error could, of course, be readily reduced further, but at the expense of additional computer time.

(b) An error estimate was also available through the comparison of the computed temperature profiles and melting rates with analytical solutions, in the asymptotic regimes.

In the one component system, (Example 1) runs performed with high values of the "outside" heat transfer coefficient agreed very well with analytical solutions calculated for a step change in the surface temperature. Here the percentage error was estimated to be of the order of 20 per cent, however, some of the difference may have been caused by the fact that the analytical asymptote was not exactly valid.*

It was noted, while discussing Example 1, that for this particular case and for long times, the melting rate was almost constant, and corresponded to the rate at which latent heat was supplied by convection, i.e.

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \frac{h(T_B - T_{mp})}{\rho\Delta H} \tag{19}$$

within this region the computed results agreed with equation (19) within an accuracy of 1.0 per cent.

CONCLUDING REMARKS

A new technique, involving Green's functions, is proposed for moving boundary problems, involving the unsteady state transfer of heat or mass. The technique offer considerable computational economy over convectional finite difference procedures and appears to be more flexible for accommodating complex boundary conditions than the semi-analytical methods available at present.

The use of this procedure has been illustrated

^{*} The region of high heat transfer coefficients, approaching the step change asymptote would have caused some computational difficulties, if approached via the conventional finite difference techniques; the use of Green's functions, as done in the paper, avoided this problem.

on two particular examples involving the melting of slabs in one and two component systems; it is thought however, that the principle usefulness of the technique will lie in its application to rather more complex situations.

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SUR L'UTILISATION DES FONCTIONS DE GREEN POUR RÉSOUDRE DES PROBLÈMES DE FUSION ET DE SOLIDIFICATION

Résumé—Une technique analytique et numérique est proposée qui utilise les fonctions de Green pour résoudre des problèmes de fusion ou de solidification. Il est montré que d'un point de vue numérique cette procédure peut être très attrayante pour aborder des problèmes avec des conditions aux limites non linéaires ou des systèmes à plusieurs composants.

L'application de la technique est illustrée par deux exemples, l'ablation par fusion d'une plaque due à un transfert thermique par convection et la dissolution-fusion d'une plaque en un mélange liquide binaire.

DIE ANWENDUNG DER GREENSCHEN FUNKTION AUF SCHMELZ- UND VERFESTIGUNGSPROBLEME

Zusammenfassung – Eine analytische Berechnungsmethode, die sich auf die Greensche Funktion stützt, wird zur Lösung von Schmelz- und Verfestigungsproblemen vorgeschlagen. Von der Berechnung her scheint diese Methode sehr geeignet bei nichtlinearen Randbedingungen oder Vielkomponenten-Systemen. Die Anwendung der Methode wird an zwei Beispielen gezeigt das Abschmelzen eines Stabes bei konvektivem Wärmeübergang und die Auflösung eines Stabes in einer binären Flüssigkeitsmischung.

ОБ ИСПОЛЬЗОВАНИИ ФУНКЦИЙ ГРИНА ДЛЯ РЕШЕНИЯ ЗАДАЧ ПЛАВЛЕНИЯ И ОТВЕРДЕВАНИЯ

Аннотация—Для решения задач плавления и отвердевания предложена методика аналитического расчета с использованием функций Грина, удобная для решения задач с нелинейными граничными условиями или многокомпонентными системами. Возможности методики иллюстрированы двумя примерами. (а) абляция стержня за счет конвективного теплообмена и (б) плавление стержня, сопровождающееся растворением в бинарной жидкой смеси.