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AN INTEGRAL EQUATION APPROACH TO DIFFUSION*

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Abstract—A method of solution of transient diffusion, e.g. heat conduction, problems in homogeneous and isotropic media with internal sources and arbitrary (including nonlinear) boundary conditions and initial conditions is proposed. The method is based on the reduction of the problem to one only involving surface values of temperature and/or heat flux in the form of an integral equation through the introduction of fundamental solutions and the use of Green's theorem. The integral equation is solved numerically for a specific example.

THIS paper is concerned with the analysis of physical problems governed by the linear three-dimensional diffusion equation, e.g. transient heat conduction, for a homogeneous and isotropic material of arbitrary geometry with general initial and boundary conditions including nonlinear boundary relationships such as those corresponding to radiative heat transfer.

The formulation is based on the integral equation form equivalent to the diffusion equation (e.g. see [1]) which allows the reduction of the problem from a form which involved the entire body (i.e. the partial differential equation) to one which only involves surface values (i.e. the integral equation) plus an auxiliary equation which expresses the solution at interior points as a direct quadrature of the surface values. Thus a reduction of one dimension is affected at the price of solving an integral rather than a differential equation. Under the reasonable assumption that such a general problem will undoubtedly require a numerical or approximate mode of solution, such a reduction in dimensionality can offer a substantial economy in solution, especially, as is frequently the case, if only the surface values are sought. Such an approach is particularly attractive for those problems involving bodies whose boundaries do not fall along usable coordinate lines, i.e. are not separable, such that an eigenfunction expansion is not feasible. Since boundary conditions are applied directly at the surfaces involved, the difficulty found so often in finite difference approximations to the differential equation of matching mesh points to boundary points is avoided.

While there are a number of "integral methods" available for the discussion of transient nonlinear heat transfer problems (e.g. Goodman [2] gives a summary of such methods), these are fundamentally different than the one proposed here in that the integrals referred to there represent balances of heat using boundary-layer concepts analogous to those used in fluid mechanics. A transient nonlinear heat-transfer problem in one dimension has been solved by Chambre [3] for a semi-infinite domain by means of a Laplace transform; the boundary condition is a nonlinear relationship between temperature and heat flux; but the similarity to the present approach is again only superficial. A method more closely related to that to be discussed is given by Tolubinskiy [4]. Here the appropriate Green's function for a given region with a thermally insulated boundary is constructed from the fundamental solution by means of "reflections" at the boundary. While an integral equation is obtained for the Green's function, the approach is still significantly different from that to be discussed here in that the present approach will use any convenient Green's function, e.g. the fundamental solution for a point source in an infinite domain, G_∞, regardless of whether or not it satisfies all of the appropriate boundary conditions on the given boundaries. This approach leads to an integral equation which can be expressed completely in terms of surface values of temperature and/or heat flux. Reitzel [5] uses boundary sources in one-dimensional problems reducing these to convolution integrals by introducing a Laplace transform in time but emphasizes the reduction to convolution integrals rather than integral equations involving spatial coordinates as well. Finally, Rizzo and Shippy [6] use a similar approach to the one given here but use an integral equation formulation in a Laplace transform space which is less direct than the present approach. Further details of the present method may be found in [7] along with other examples to illustrate the approach.

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Consider a heat-conduction problem involving a region D with boundary S. The density ρ, the specific heat per unit volume c_v, and the conductivity k are assumed to be constant throughout D. A distributed heat source of strength Q is located within D, while on S there is a specified relationship between the temperature θ and its normal derivative (which is proportional to the surface heat flux). Finally there is an initial temperature distribution at a given time, $t = 0$, specified throughout D. These conditions are described by the following equations [1]:

$$k\nabla^2\theta(\bar{r}, t) + Q = \rho c_v \frac{\partial\theta}{\partial t}\,;\ \bar{r}\in D, t \geqslant 0 \tag{1}$$

$$\mathscr{F}\left(\theta, \frac{\partial\theta}{\partial m}\right) = 0\,;\ \bar{r}\in S, t > 0 \tag{2}$$

$$\theta(\bar{r}, 0) = \theta_0(\bar{r})\,;\ \bar{r}\in D, t = 0. \tag{3}$$

The solution for G for an unbounded three-dimensional space is given in [1] as

$$G_\infty(R, \tau) = \frac{\kappa\,.\,\pi}{2(\kappa\pi\tau)^{3/2}}\exp\left[-\frac{R^2}{4\kappa\tau}\right]H(\tau) \tag{4}$$

where $R = |\bar{r}-\bar{r}_0|^2$, $\tau = t - t_0$, $\kappa = k/(\rho c_v)$ and H is the unit step operator. While this may be the most useful form for G in this discussion, the following derivation is clearly not limited to this particular case. The governing integral equation valid for any G which has an appropriate singularity at $r = r_0$, $t = t_0$ is

$$\begin{aligned}\lambda\kappa\theta(\bar{r}, t) = &\int_{D_0}\theta_0(\bar{r}_0)G(\bar{r}, \bar{r}_0; t, 0)\,\mathrm{d}V_0\\ &+\frac{1}{\rho c_v}\int_0^{t^+}\mathrm{d}t_0\int_{D_0} G\,.\,Q(\bar{r}_0, t_0)\,\mathrm{d}V_0\\ &+\kappa\int_0^{t^+}\mathrm{d}t_0\oint_{S_0}\left\{G\frac{\partial\theta(\bar{r}_0, t_0)}{\partial m_0} - \theta\frac{\partial G}{\partial m_0}\right\}\mathrm{d}S_0\end{aligned} \tag{5}$$

where $\lambda = 4\pi$, 2π, or 0 depending on where $\bar{r}\in D$, $\bar{r}\in S$, or $\bar{r}\notin D$ and S respectively and where m_0 is the outward normal to D_0. As $t\to\infty$, these results should approach the steady state solution. The initial temperature distribution effect vanishes as $t\to\infty$ while the integrations over t_0 for the remaining terms can be carried through assuming that θ and Q no longer depend on t_0 (or equivalently that the contribution to the integral over t_0 from 0 to ∞ from those values of t_0 where θ and Q were still dependent on t_0 is negligible compared to the total integral). Upon carrying out the integration for G as the fundamental solution, G_∞.

$$\int_0^\infty G_\infty\,\mathrm{d}t_0 = 1/R$$

as expected. Then an equation equivalent to equation (5) but for steady state problems is

$$\begin{aligned}\lambda\kappa\theta(\bar{r}) = &\frac{1}{\rho c_v}\int_{D_0}\tilde{G}Q(\bar{r}_0)\,\mathrm{d}V_0\\ &+\kappa\oint_{S_0}\left\{\tilde{G}(\bar{r}, \bar{r}_0)\frac{\partial\theta(\bar{r}_0)}{\partial m_0} - \theta(\bar{r}_0)\frac{\partial\tilde{G}}{\partial m_0}\right\}\mathrm{d}S_0\end{aligned} \tag{6}$$

where the fundamental solution for an unbounded three-dimensional space is now

$$\tilde{G} = 1/R. \tag{7}$$

Consider the geometry shown in Fig. 1(a). An infinitely long cylinder of arbitrary cross-section is cut by a plane x equal to a constant parallel to the cylinder axis, z. On the surface of the cylinder a heat flux, i.e. a normal derivative of the temperature, is specified as a function of time and position; while on the plane surface the temperature is given. If these values are independent of the coordinate z, the problem reduces to a two-dimensional case. By taking the representative Green's function to be the superposition of equal and opposite

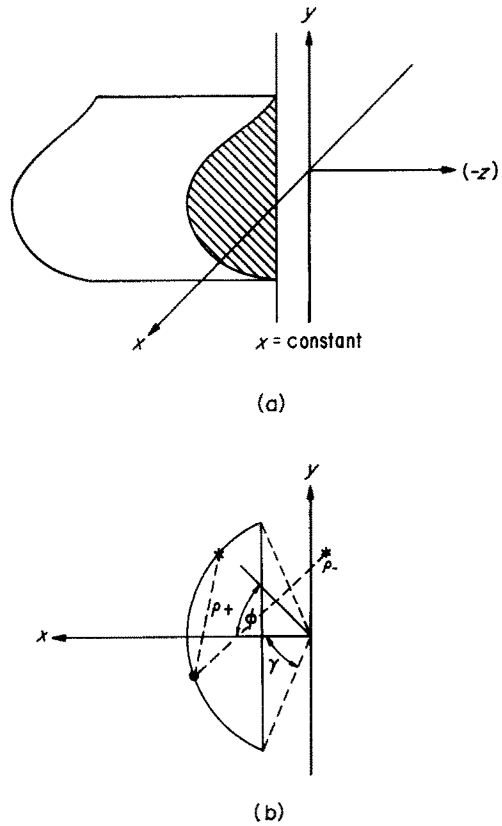

FIG. 1. Geometry for two-dimensional problems: cylinder cut by a plane parallel to the cylinder axis, subjected to heat flux $f(\phi)$ on curved face with constant temperature maintained on plane face.

fundamental solutions placed symmetrically with respect to the plane surface, the integrals over this plane surface will be known leaving the unknown variables appearing only in integrals over the remaining cylinder surface.

As a specific example, consider the cylinder to be circular of radius a in a cross-section with the plane surface cutting off a section of angle 2γ as shown in Fig. 1(b). Take the initial temperature field, the prescribed temperature on the plane surface, and the interior heat source all to be zero. These terms would only contribute known quantities to the calculations if this were not the case. Finally, take the field point to lie on the cylinder surface, $r = a$. Then equation (5) requires

$$2\pi\theta(a, \phi, t) = \int_0^{t^+} \mathrm{d}t_0 \oint_\Gamma \mathrm{d}s_0 \int_{-\infty}^{\infty} \left\{ G\frac{\partial\theta}{\partial m_0} - \theta\frac{\partial G}{\partial m_0} \right\} \mathrm{d}z_0 \quad (8)$$

where Γ is the boundary of that portion of the cylinder cross-section, not including the plane $x = a\cos\gamma$, and lying in the plane $z = 0$ but excluding the field point $\bar{r}$. Since θ is independent of z, the z_0 integration may be carried out leaving an integral equation involving only one spatial coordinate, ϕ. Alternatively, the two-dimensional fundamental solution could have been used. By taking the specific case of the incident heat flux as a step function in time with arbitrary dependence in the remaining spatial coordinate,

$$\frac{\partial\theta}{\partial m}(a, \phi, t) = B.f(\phi).H(t) \quad (9)$$

where the maximum value of $f(\phi)$ is one and $H(t)$ is a unit step. This becomes an integral equation of the Fredholm type in space but of the Volterra type in time.

It is appropriate at this point to non-dimensionalize these equations to facilitate numerical solutions. The length variables shall be scaled to the radius a, time to unit $4\kappa/a^2$, and temperature to a/B, i.e.

$$t' = t.(4\kappa/a^2)$$
$$r' = r/a$$
$$\theta' = \theta/aB.$$

The primes will be dropped in the following equations, and the variable α will be used for $\theta(a, \phi, t)$. Then equation (8) becomes

$$2\pi\alpha(\phi, t) = \int_0^{t^+} \mathrm{d}t_0 \int_{-\gamma}^{\gamma} \left\{ -\alpha(\phi_0, t_0) \frac{\partial G^*}{\partial m_0} + G^*.f(\phi_0) \right\} \mathrm{d}\phi_0 \quad (10)$$

where

$$G^*(r, r_0; \phi, \phi_0; t, t_0) = \frac{1}{\tau}\{\exp[-\rho_+^2/\tau] - \exp[-\rho_-^2/\tau]\} \quad (11)$$

with ρ_+ and ρ_- as shown in Fig. 1(b) representing the distance from the field point to the positive source and negative source points (r_+, ϕ_+) and (r_-, ϕ_-), respectively. These are given in the x_0, y_0 coordinate system. The x_0 coordinates of these points are symmetric about $x = \cos\gamma$ and the y_0 coordinate are equal. Therefore $r_+ \sin\phi_+ = r_- \sin\phi_-$ and $r_+\cos\phi_+ + r_-\cos\phi_- = 2\cos\gamma$ leading to

$$\rho_+^2 = 1 + r_+^2 - 2r_+\cos(\phi_+ - \phi) \quad (12)$$

and

$$\rho_-^2 = 1 + r_+^2 + 2r_+\cos(\phi_+ + \phi) - 4\cos\gamma(\cos\gamma - r_+\cos\phi_+ - \cos\phi). \quad (13)$$

The normal derivative of G^* can be calculated at $r_+ = 1$

$$\frac{\partial G^*}{\partial m_0} = \frac{\partial G^*}{\partial r_+} = \frac{2}{\tau^2}\{-[1-\cos(\phi_+ - \phi)] .\exp[-2[1-\cos(\phi_+ - \phi)]/\tau] + [1+\cos(\phi_+ + \phi) - 2\cos\gamma\cos\phi_+]\exp[-2[1+2\cos(\phi_+ + \phi) + 2\cos\gamma(\cos\gamma - \cos\phi_+ - \cos\phi)]/\tau]\} \quad (14)$$

where ϕ_+ is identical with the ϕ_0 used above. Then equation (9) can be solved numerically for α using G^* from equation (10) and $\partial G^*/\partial m_0$ from equation (14). The integral involving G^* can be reduced somewhat

$$\int_0^{t^+} \mathrm{d}t_0 \int_{-\gamma}^{\gamma} f(\phi_+)G^*\,\mathrm{d}\phi_+ = \int_{-\gamma}^{\gamma} f(\phi_+)\left\{ E_1\left[\frac{2(1-\cos(\phi_+ - \phi))}{\tau}\right] - E_1\left[\frac{2(1+\cos(\phi_+ + \phi) + 2\cos\gamma(\cos\gamma - \cos\phi_+ - \cos\phi))}{\tau}\right]\right\} \mathrm{d}\phi_+ = D(\phi, t) \quad (15)$$

where $E_1(x)$ is the exponential integral function

$$E_1(x) = \int_x^\infty [\exp(-q)/q]\,\mathrm{d}q \tag{15a}$$

but this expression will undoubtedly require numerical evaluation even for simple $f(\phi)$. Clearly the form of the surface flux specified only affects the value of $D(\phi, t)$ leaving the remainder of the solution procedure unchanged. Thus once the computational scheme is established, changes in the form of the incident flux can be included with relatively little effort, i.e. changing one statement card.

While there are many numerical and approximate techniques available for the solution of integral equations (e.g. see [8]), the most direct assumes the dependent variable α to be constant over specified intervals in space (ϕ) and time (t). The integral equation is then replaced by a set of linear (in this case of a linear boundary condition) algebraic equations which are simultaneous in space and successive in time. Since the only values of the dependent variable required are those on a portion of the boundary, the number of space steps used may be relatively small, thereby requiring the solution of a relatively small set of coupled algebraic equations at each successive time step.

The numerical procedure uses IMAX increments in ϕ_+ from $-\gamma$ to $+\gamma$. Each step in ϕ_+ is further divided into N equal increments to carry out the numerical integrations required to determine the coefficient matrix for the set of algebraic equations and the forcing function, $D(\phi, t)$.

Define $\alpha(L, M)$ to be the value of α for $t_{M-1} = \Delta t\,.(M-1) < t < t_M = M\Delta t$ and $\phi_{L-1} = (L-1)\Delta\phi < \phi < \phi_L = L\Delta\phi$. Then equation (9) can be approximated by

$$2\pi\alpha(L, M) = -\sum_{I=1}^{I\mathrm{MAX}} \sum_{J=1}^{M} \alpha(I, J)\,.\,C(L, I; M, J) + D(L, M) \tag{16}$$

where IMAX is the total number of space steps on the boundary, L refers to the location ϕ, I to the location ϕ_+, M to the present time step t, J to the previous time steps, and

$$C(L, I; M, J) = \int_{\phi_{I-1}}^{\phi_I} \mathrm{d}\phi_+ \int_{t_{J-1}}^{t_J} \mathrm{d}t_0 \times \left\{\frac{\partial G^*(\phi_L, \phi_{0I}; t_M, t_{0J})}{\partial m_0}\right\}. \tag{17}$$

Fortunately G^* will always depend on $(t-t_0)$ and C will only involve three indices, 1, I, and $MJ = M-J$ for a uniform time step.

Although α has been assumed to be constant over specified intervals in space and time, there must be some particular choice of ϕ and t to use as representative of the region. The value of ϕ is taken at the midpoint of the interval, $(L-1/2)\Delta\phi$, and the value of t is taken at the end of the time step, $M\Delta t$. Other choices should not change the results appreciably. The expression for C can be simplified somewhat. Define

$$C(L, I, MJ) = F(L, I, MJ) - F(L, I, MJ+1) \tag{18}$$

where F is given by

$$F(L, I, MJ) = \int_{(I-1)\Delta\phi}^{I\Delta\phi} \mathrm{d}\phi_+ \left\{\exp[-\rho_+^2/MJ\Delta t] + \frac{-(2[1+\cos(\phi_+ + \phi) - 2\cos\gamma\cos\phi])}{\rho_-^2} * \exp[-\rho_-^2/MJ\Delta t]\right\} \tag{19}$$

F and D will be evaluated numerically using N increments in each $\Delta\phi$ interval.

Then α may be determined by solving the set of IMAX simultaneous linear algebraic equations at each time step, $t = M\Delta t$

$$\sum_{I=1}^{I\mathrm{MAX}} [2\pi\delta(L, I) + C(L, I, 0)(1-\delta(L, I))]\alpha(I, M) = D(L, M) - \sum_{I=1}^{I\mathrm{MAX}} \sum_{J=1}^{M-1} \alpha(I, J)\,.\,C(L, I, MJ) = \mathrm{RHS}(L, M) \tag{20}$$

where $\delta(L, I)$ is one if $L = I$ and zero otherwise. The total contribution of the field point at the current time to the summation is contained in the $2\pi\alpha(L, M)$ term, and any other contribution of this point at this time must be surpressed. Clearly the coefficients of the current values of α are independent of M, and an inverse coefficient matrix can be defined as

$$\mathrm{CINV}(L, I) = [2\pi\delta(L, I) + C(L, I, 0)(1-\delta(L, I))]^{-1}.$$

Then the temperature on the circular portion of the boundary, Γ, is given by

$$\alpha(L, M) = \sum_{I=1}^{I\mathrm{MAX}} \mathrm{CINV}(L, I)\,.\,\mathrm{RHS}(L, M). \tag{21}$$

The index L in $F(L, J, MJ)$ and $C(L, I, MJ)$ may be surpressed during these calculations thereby reducing the storage requirements. All numerical calculations were done with $N = 9$, $I\mathrm{MAX} = 10$.

Two values of γ were used in the numerical calculations, 90° and 30°, for two forms of incident flux, $f(\phi) = 1{\cdot}0$ and $f(\phi) = (1{\cdot}0 - \sin(\phi))/2$ representing a uniform flux and an asymmetric flux respectively. Results for the 90° case (a semi-cylinder) and a uniform flux are shown in Fig. 2 for time long enough for essentially steady solutions to be obtained. In addition to these numerical solutions for the semi-cylinder, results are given for comparison purposes for a semi-infinite solid and an infinite slab of the same width

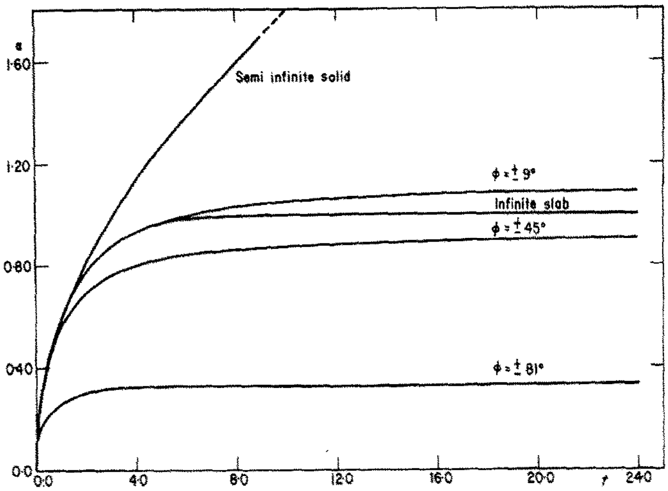

FIG. 2. Surface temperature for $\gamma = \pi/2$ and $f(\phi) = 1{\cdot}0$; $\Delta T = 0{\cdot}05$ compared with analytical solutions for infinite slab and semi-infinite solid.

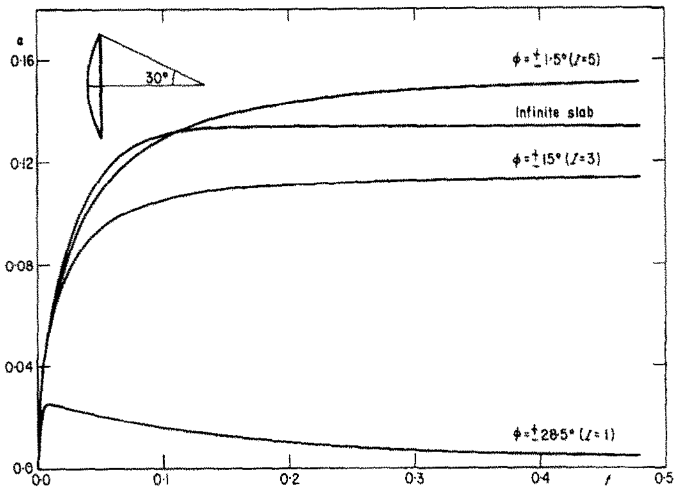

FIG. 3. Surface temperature for $\gamma = \pi/6$ and $f(\phi) = 1{\cdot}0$; $\Delta T = 0{\cdot}002$ compared with analytical solutions for infinite slab.

of the semi-cylinder under the same initial and boundary conditions (e.g. see [9]). The temperature near the center of the perimeter is close to and slightly above the corresponding infinite slab solution as would be expected from the curvature. That near the end, i.e. near the surface of zero temperature, was much lower than the infinite slab surface solution as would be expected.

As γ decreases from 90°, the actual cylinder width decreases as $(1-\cos\gamma)$, and the shape of the cross-section becomes elongated. Results for $\gamma = 30°$ and a uniform incident flux are shown in Fig. 3. Solutions for the corresponding infinite slab are also given, and the results are similar to those found for the $\gamma = 90°$ case described above.

Finally, results for the asymmetric flux $(1{\cdot}0 - \sin\phi)/2$ are given in Figs. 4 for $\gamma = 90°$ and 5 for $\gamma = 30°$.

Since the emphasis in this paper is on method rather than the solution of particular problems, it would seem appropriate in conclusion to compare the approach described to alternative methods of solution. While there are several numerical and/or approximate techniques available, e.g. orthonormal expansions [10] as well as the integral methods and transform methods discussed in the introduction to this paper, the most likely competitor for general geometries would be that based on a finite difference approximation to the original equations (e.g. see [11]).

The number of mesh points in a finite difference

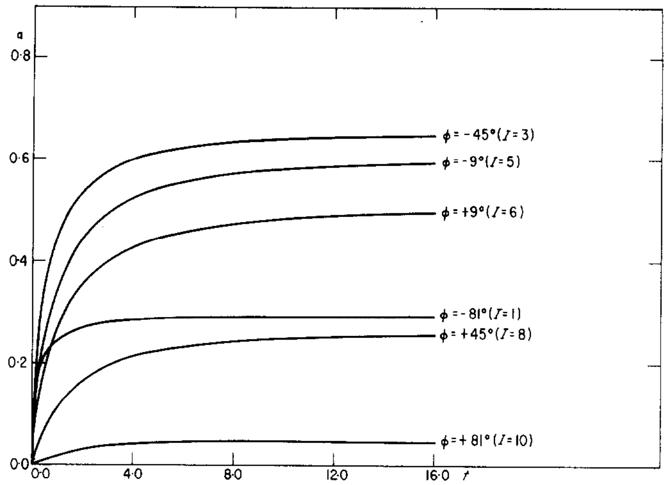

FIG. 4. Surface temperature for $\gamma = \pi/2$ and $f(\phi) = 1/2(1-\sin\phi)$; $\Delta T = 0{\cdot}05$.

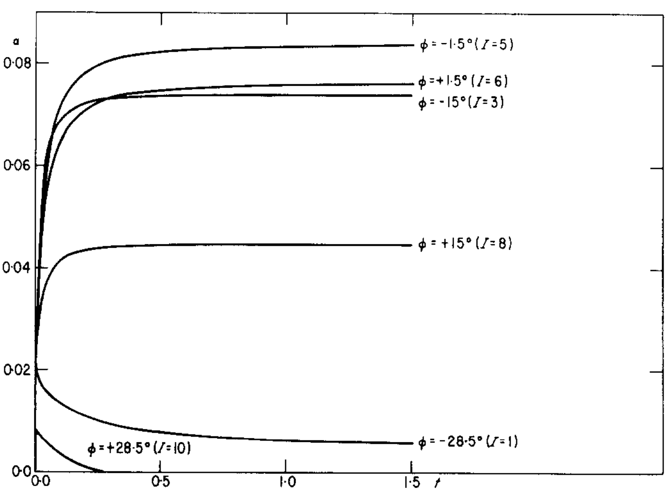

FIG. 5. Surface temperature for $\gamma = \pi/6$ and $f(\phi) = 1/2(1-\sin\phi)$; $\Delta T = 0{\cdot}005$.

method must be greater than the corresponding number in the integral equation approach since the former involves one more dimension. However, the calculations to obtain the coefficients in the integral equation approach are much more complicated. Furthermore the integral equation approach will not immediately give the solution everywhere as would the finite difference scheme. On the other hand, boundary conditions are applied directly on the boundaries rather than being interpolated as in a finite difference method.

If the solution is only sought on the boundary surface (which is frequently the surface of interest), it appears that the integral equation approach has some advantage over the finite difference scheme—particularly if many points (i.e. a fine mesh) are to be used.

Another class of problems in which the integral equation approach is probably superior to finite differences is that involving unbounded media with some internal surface on which boundary conditions are specified. Here the Green's function can be chosen to reduce the problem to involve values only on the interior surface.

On the other hand, the extensions of the integral equation approach to inhomogeneous media seems at this point limited to specific one-dimensional problems using, for example, the fundamental solution of Cholewinski and Haimo [12]. The corresponding extension for finite difference methods does not suffer from this limitation in theory but essentially only involves "more arithmetic," at least in principle.

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UN APPROCHE DE LA DIFFUSION PAR UNE EQUATION INTEGRALE

Résumé—On propose une méthode de résolution des problèmes de diffusion transitoire (conduction thermique en particulier) dans des milieux homogènes et isotropes, avec des sources internes, des conditions aux limites arbitraires (incluant la nonlinéarité) et des conditions initiales. La méthode est basée sur la réduction à un problème de distribution surfacique de température ou de flux thermique sous la forme d'une équation intégrale par l'introduction de solutions fondamentales et par l'utilisation du théorème de Green. L'équation intégrale est résolue numériquement pour un exemple particulier.

EINE INTEGRALGLEICHUNGSNÄHERUNG FÜR DIFFUSION

Zusammenfassung—Eine Lösungsmethode für instationäre Diffusionsprobleme und der Wärmeleitung in homogenen und isotropen Medien mit örtlichen Quellen und beliebigen (auch nichtlinearen) Rand- und Anfangsbedingungen wird vorgeschlagen. Die Methode basiert auf der Reduktion auf ein Problem, das nur noch die Temperaturen und/oder den Wärmestrom in Form einer Integralgleichung enthält, die man durch Einführung von Fundamentallösungen und die Verwendung des Green'schen Theorems erhält. Die Integralgleichung wird numerisch für ein spezifisches Beispiel gelöst.

ИНТЕГРАЛЬНАЯ ФОРМУЛИРОВКА ЗАДАЧИ ДИФФУЗИИ

Аннотация — Предложен метод решения задач нестационарной диффузии, например, теплопроводности в однородных и изотропных средах с внутренними источниками и произвольными (включая нелинейные) граничными и начальными условиями. Метод основан на сведении проблемы к задаче со значениями только температуры и/или теплового потока на поверхности в форме интегрального уравнения путём введения фундаментальных решений и использования теоремы Грина. Интегральное уравнение решено численно для конкретного случая.