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Quasi-Analytical Transient Conduction Solution

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Nomenclature

$[A]$	= matrix coefficient of finite difference or element model
A_{ij}	= elements of $[A]$
$[D]$	= diagonal matrix consisting of eigenvalues of $[A]$
F	= column matrix representing internal heat generation
L_i	= dimensions of laminated slab used in numerical example
M	= half bandwidth of $[A]$
N	= size of $[A]$
R_m	= remainder formula
$[S]$	= matrix composed of eigenvectors of $[A]$
T^*	= amplitude of prescribed surface temperature, Eq. (22)
T	= column matrix representing nodal temperatures
T_i	= temperature of ith node
T_0	= column matrix representing initial nodal temperatures
x_i	= Cartesian coordinates of laminated slab (see Fig. 1.)
ζ	= complex spatial portion of temperature field
θ_{ij}	= fiber orientations
$\kappa_{ij}/(\rho c_p)$	= thermal diffusivity (ft^2/sec)
Ω	= period of prescribed surface temperature, Eq. (22)
$Re\{\ \}$	= real part of $\{\ \}$
$\|\ \|$	= absolute value
$\|\|\ \|\|$	= norm ($\|\|[A]\|\| = \|A_{11}\| + \|A_{12}\| + \ldots + \|A_{NN}\|$)

Introduction

ALTHOUGH a great number of transient conduction problems have been solved, only a limited number of geometrical shapes and only those boundary conditions which can easily be expressed mathematically (Dirichlet) have been handled. Hence, for most transient conduction problems, one must resort to a numerical technique. Generally finite element and difference procedures are most prominently used. For such numerical models, the transient problem has been handled using numerical integration (predictor-corrector), Euler (forward), Crank-Nicolson (mid-difference), Galerkin algorithms, finite element,[1] and least squares stepping schemes[2] etc. As many of these procedures are conditionally or unconditionally stable, the choice of different time steps will lead to a variety of solution degradations. Recently, as an alternative approach, Dodd and Gupta[3] and Bahar[4]have used the state space procedures of atuomatic controls to obtain numerical solutions for several boundary value problems. Such procedures stem from a direct utilization of formal procedures of classical ODE theory. Based on one such formal solution, the present Note will develop a transient numerical procedure which will not be subject to the numerical degradation of the previously noted time stepping schemes. In fact, akin to Monte Carlo techniques,[5] the given procedure has the added capability of handling the temperature at a given node and/or nodes. As will be seen, this is possible without performing simultaneous calculations at all the nodes of the given model as is required of time stepping schemes.

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Equations and Solution

As a starting point, consider the following system of first-order ODE

$$dT/dt = [A]\ T + F(t);\ T(0) = T_0 \tag{1}$$

such that $[A]$ and $F(t)$ stem from either finite element or difference models wherein T represents the nodal temperatures, and T_0 is the initial condition column matrix. Following Ref. 6, assuming that $[A]$ is nonsingular, the formal exact solution of Eq. (1) is given by

$$T(t) = e^{t[A]}T_0 + \int_0^t e^{(t-\mu)\ [A]}F(\mu)\,d\mu \tag{2}$$

For the case in which the eigenvalues of $[A]$ are known, $e^{t[A]}$ can be reduced to the following canonical form,[6] namely

$$e^{t[A]} = [S]e^{t[D]}\ [S]^{-1} \tag{3}$$

As $[A]$ is in general a large matrix, the accurate evaluation of all of its eigenvalues and associated eigenvectors usually represents a formidable numerical problem. Hence, most investigators have resorted to a variety of time stepping schemes as noted earlier. For this Note, the numerical evaluation of Eq. (2) is obtained by formally expanding $e^{t[A]}$ in Maclaurin series, namely

$$e^{t[A]} = \sum_{n=0}^{\infty} (t^n/n!)\ [A]^n \tag{4}$$

Furthermore, to evaluate the convolution integral appearing in Eq. (2), since F is generally in the form of tabulated data, without loss in generality, the following polynomial spline fit is used for $t \epsilon [t_{i-1}, t_i]$, hence

$$F_i(t) \cong \sum_{\ell=0}^{L} F_{i\ell}t^{\ell} \tag{5}$$

such that

$$t_i = \sum_{j=0}^{i} \Delta t_j$$

In terms of Eqs. (4 and 5), Eq. (2) formally reduces to

$$T\cong \sum_{n=0}^{\infty} (t^n/n!)\ [A]^n T_0$$

$$+ \sum_{i=1}^{I} \int_{t_{i-1}}^{t_i} \sum_{n=0}^{\infty} ((t-\mu)^n/n!)\times [A]^n \sum_{\ell=0}^{L} F_{i\ell}\mu^\ell \, d\mu \qquad (6)$$

where as will be shown later, since the series of Eq. (6) is uniformly and absolutely convergent,

$$\int \sum_{n=0}^{\infty} \equiv \sum_{n=0}^{\infty} \int$$

therefore

$$T\cong \sum_{n=0}^{\infty} [A]^n \{ (t^n/n!) T_0 + \sum_{i=1}^{I} \sum_{\ell=0}^{L} \Gamma_{ni\ell}(t) F_{i\ell} \} \qquad (7)$$

such that

$$\Gamma_{ni\ell} = \int_{t_{i-1}}^{t_i} (t-\mu)^n \mu^\ell/n! \, d\mu \qquad (8)$$

To verify the formal convergence of Eq. (7), the properties of its normed version are considered, namely

$$\|T\| \le \sum_{n=0}^{\infty} \|[A]\|^n ((|t|^n/n!)\|T_0\| + \sum_{i=1}^{I} \sum_{\ell=0}^{L} |\Gamma_{ni\ell}(t)|\,\|F_i\| \qquad (9)$$

Since $\|[A]\|$ and $\|F_{i\ell}\|$ are assumed to be bounded and

$$|\Gamma_{ni\ell}(t)| \le \int_{t_{i-1}}^{t_i} (t^n\mu^\ell/n!)\,d\mu \cong 0(t^n/n!) \qquad (10)$$

applying the ratio test to Eq. (9) yields

$$\lim_{n\to\infty} \|[A]\|^{n+1} \Big[|t|^{n+1}/(n+1)!\|T_0\| + \sum_{i=1}^{I} \sum_{\ell=0}^{L} |\Gamma_{n+1i\ell}(t)|\,\|F_{i\ell}\| \Big] /$$

$$\|[A]\|^n \Big[|t|^n/n!\|T_0\| + \sum_{i=1}^{I} \sum_{\ell=0}^{L} |\Gamma_{ni\ell}(t)|\,\|F_{i\ell}\| \Big]$$

$$\le \lim_{n\to\infty} \|[A]\| 0[t/(n+1)] \to 0 \qquad (11)$$

Hence, the series in Eq. (7) is seen to be absolutely and uniformly convergent for all $t\epsilon(0,\infty)$.

For $t \gg 0$, since Eq. (7) will require a large number of terms for adequate convergence, to reduce the computational effort, expansion in Taylor series about τ yields the following more convenient version, namely

$$T(t) \cong \sum_{n=0}^{\infty} \Big\{ ((t-\tau_I)^n/n!) e^{\tau_I[A]} [A]^n T_0 + \sum_{i=1}^{I} \sum_{\ell=0}^{L} \Gamma_{ni\ell}(t-\tau_i) e^{\tau_i[A]} [A]^n F_{i\ell} \Big\} \qquad (12)$$

wherein

$$\tau_i = \Delta t_i/2 + \sum_{j=0}^{i-1} \Delta t_j \qquad (13)$$

Equations (7) and (12) both have the interesting feature that because of their basic form, the transient solution for a given node can be obtained without involving calculations at other nodes. Hence, in terms of Eq. (7), the temperature at a given node takes the form

$$T\cong \sum_{n=0}^{\infty} \sum_{i_1=1}^{N} \sum_{i_{n-1}=1}^{N} \sum_{j=1}^{N} A_{ii_I} \times (\prod_{\ell=1}^{n-2} A_{i_\ell i_{\ell+1}}) A_{i_{n-1}j} ((t^n/n!) T_{j0} + \sum_{k=1}^{I} \sum_{\ell=0}^{L} \Gamma_{nkl}(t) F_{jkl}) \qquad (14)$$

Compared to Eqs. (7) or (12), Eq. (14) requires only $1/N$ the number of total calculations.

Although Eqs. (7, 12 and 14) are absolutely convergent, it is certainly of importance to establish a convergence check. For the present series, this will be possible through the development of a remainder formula for the global set, Eq. (7) or (12). To start, Eq. (9) is recast as

$$\|T\| \le \sum_{n=0}^{\infty} \|[A]\|^n (t^n/n!)\ (\|T_0\| + \|F^*\|) \qquad (15)$$

where

$$\|F^*\| = \sum_{i=1}^{I} \sum_{\ell=0}^{L} \int_{t_{i-1}}^{t_i} \mu^\ell d\mu \|F_{i\ell}\| \qquad (16)$$

Since Eq. (15) represents a Taylor expansion of the function

$$\|T\| \le (\|T_0\| + \|F^*\|) e^{\|[A]\|t} \qquad (17)$$

it follows that an upper bound for the remainder formula of Eq. (7) is given by

$$R_m \le (t^n/n!) \|[A]\|^n (\|T_0\| + \|F^*\|) e^{\|[A]\|\mu} \qquad (18)$$

where $\mu\epsilon[0,t]$. To establish the nature of $\|[A]\|^n$, its finite element form will be considered. Assuming that $b = \max(A_{ij})$, then

$$\|[A]\| \le bN^2 \qquad (19)$$

where N *denotes the size of* $[A]$. In terms of Eq. (19), Eq. (18) reduces to the more useful form

$$R_m \le ((tbN^2)^n/n!)\ (\|T_0\| + \|F^*\|) e^{bN^2\mu} \qquad (20)$$

For the case with banding, Eq. (20) can be recast as

$$R_m \le ((tb(2MN-N-M(M-1)))^n/n!)\,(\|T_0\| + \|F^*\|) \times \exp(b(MN-N-M(M-1))\mu) \qquad (21)$$

such that M denotes the half bandwidth. Considering typical engineering materials, since the thermal diffusivity $(\kappa_{ij}/\rho c_p)$ $\epsilon[.1139\times10^{-5},\ .183\times10^{-2}]$ (ft^2/sec),† $|A_{ij}| \ll 1$. Therefore, depending on M and N, fairly good global convergence can be expected for moderate times. This is particularly true for the local case for which a less restrictive R_m can be established.

In terms of Eqs. (7, 12, and 14), the following important advantages are noted for the given procedure: 1) since the series are absolutely convergent, in the context of the numerical model used, the transient temperature field can be

†This follows for metals and most typical inorganic and organic construction materials.

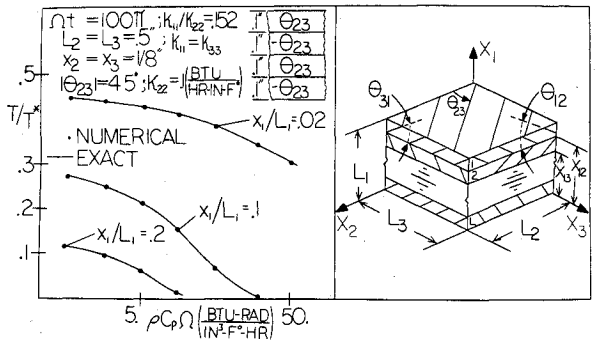

Fig. 1 Effects of $\rho c\Omega$ variations on the temperature field of an x_1 monoclinic alternately laminated slab.

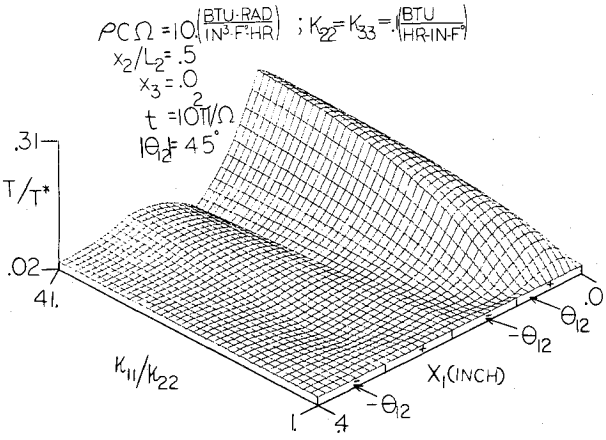

Fig. 2 Effects of conductivity variations (κ_{11}/κ_{22}) on the temperature field of an x_3 monoclinic alternately laminated slab.

obtained to any degree of accuracy required; 2) the series can be used to obtain either an "entire" history or more conveniently, the temperature at several specific time values; 3) in the context of 2), the temperature can be evaluated at a node and/or nodes without requiring calculations to be performed at all nodes; 4) the procedure can be used as a starter for numerical integration techniques for $t>0$; (this of course, would reduce the numerical degradation of time stepping schemes); and 5) upper bounds are available on possible series truncation errors.

Example

To reveal the capabilities of the present procedure, the time dependent temperature distribution of a laminated slab composed of inherently anisotropic laminae is considered, Fig. 1. The boundary-value problem treated is defined by

$$\text{at } x_1=x_{11};T=T^*\cos\left(\frac{m\pi}{L_2}x_2\right)\cos\left(\frac{n\pi}{L_3}x_3\right)\cos\Omega t$$

$$\text{at } x_1=x_{15}\ ;\quad T=0 \tag{22}$$

In terms of the developments of Ref. 7, an eight node 3-D brick element was used to obtain the spacial distribution for the slated problem. For $t\gg 0$, the exact solution to the stated problem was derived by assuming that $T=Re\{\zeta(x_1,x_2,x_3)\,e^{j\Omega t}\}$ where $\zeta(x_1,x_2,x_3)$ was obtained in the manner of Ref. 8. The material properties used for the following numerical experiments were obtained by considering that each lamina of the slab, Fig. 1, consisted of fiber reinforced materials (boron-epoxy).[8] Figure 1 illustrates the main effect of Ω variations on the time dependent temperature field of an x_1 monoclinic alternatively laminated slab $(\theta_{23},-\theta_{23},\theta_{23},-\theta_{23})$. This figure also juxtraposes the "exact" and element generated results. As can be seen, good agreement was possible over a large range of Ω and for all the positions depicted. To reveal the significant effects of x_3 monoclinic material anisotropy, Fig. 2 illustrates the time dependent temperature field of an alternately laminated slab $(\theta_{12},-\theta_{12},\theta_{12},-\theta_{12})$. Here again, excellent accuracy was possible over the entire range of material anisotropy considered.

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Condensed Phase Reactions in Solid Propellants

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Introduction

MOST of the combustion theories, based on analytical models for describing the steady-state combustion process of solid propellants, consider that oxidizer and binder sublime independently and interact in the gas phase while no significant physical or chemical interactions take place in the condensed phase. However, the importance of the condensed phase reactions has been realized in solid propellant combustion.[1-5] It is very likely that combustion may be controlled to a varying extent by reactions taking

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