JOURNAL OF THERMOPHYSICS AND HEAT TRANSFER
Vol. 21, No. 1, January–March 2007

Operating Regions for Discrete Models Based on Physical Reality of Diffusion Problems

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DOI: 10.2514/1.24658

The implementation of the discrete numerical schemes for transient heat-conduction problems quite likely yields oscillatory results and also violates the physical reality during the first few steps of the solution process. This unwanted behavior is completely omitted by applying the criteria based on the positive coefficients rule of a physical phenomenon, which displays temperature monotony in the time dimension. The Cholesky factorization at difference recurrence formula is used in deriving the criteria. The critical time-step size limit is directly determined using the stable, nonoscillatory and physical reality requirements. These requirements are summarized to give operating regions for finite element, finite difference, and finite volume formulations. A numerical example is presented to show validity and usefulness of the criteria.

Nomenclature

$[A]$	=	combination of $[K]$ and $[C]$ in the form $[C] + \theta\Delta t[K]$
a_p	=	coefficient of a central grid point
a_{pn}	=	coefficients of neighbor grid points
$[C]$, $[K]$	=	global capacitance and conductance matrices
$[C^{(e)}]$, $[K^{(e)}]$	=	element capacitance and conductance matrices
c	=	specific heat capacity
G	=	amplification factor, η^{n+1}/η^n
k	=	thermal conductivities
L, A	=	length and area of the rod
$[N^{(e)}]$, $[B^{(e)}]$	=	element shape functions and gradient matrices
$[P]$	=	combination of $[K]$ and $[C]$ in the form $[C] - (1-\theta)\Delta t[K]$
q	=	heat flux
r	=	Fourier number, $\alpha\Delta t/\Delta x^2$
T_n	=	temperatures of neighbor grid points
T_j^n	=	temperature at node j and time step n
T_p	=	temperature of a central grid point
$T(x,t)$, T	=	temperature function
$\{T^{(e)}\}$, $\{F^{(e)}\}$	=	element nodal temperatures and force vectors
t	=	time
x	=	space coordinate
α	=	thermal diffusivity
Δt	=	time interval
Δx	=	element length
ε_j^n	=	error grid function at node j and time step n
η^n	=	error amplitude at time step n
θ	=	weighting factor
λ_j	=	eigenvalues of $[C]^{-1}[K]$ matrix
λ_N	=	largest value of λ_j
λ_θ	=	eigenvalues of $[A]^{-1}[P]$ matrix
ρ	=	density

Introduction

USING a finite element formulation in a transient heat-conduction problem converts the partial differential equation to a system of ordinary differential equations. The mathematical discrete model applied to this conversion causes some difficulties in the temperature analysis solution and generally yields oscillatory results. The previous investigations performed on the stability and oscillation characteristics of finite element methods did not succeed in guaranteeing the physical reality of heat diffusion in solids. However, satisfaction of stable, nonoscillatory and physical reality requirements in finite difference and finite volume methods can be readily achieved with time-step size-controlling strategy.

Gresho and Lee [1] observed that the results of using lumped matrix method were no more accurate and, as they showed no leap in the output, their results were, wrongly, accepted as an accurate solution compared with the consistent discretizing methods. Segerlind [2] showed the errors in finite element method for the time-dependent field problems and proposed that lumped discretizing methods be used in finite element formulation in order to eliminate such errors. Rank et al. [3] concluded that small time steps are due to the violation of a discrete maximum principle (DMP) in transient analysis and lead to physically unreasonable results in finite element approximations. Vermeer and Verruijt [4] observed that spatial oscillation of the results was often found to occur and acquired the minimum time-step size for the one-dimensional consolidation problem. Ouyang and Xiao [5] derived the criteria based on physical law of heat-conduction for ensuring temperature monotony, which is equivalent to eliminating oscillation in finite element solutions. Thomas and Zhou [6] presented two requirements that have to be satisfied for the diffusion problem in order to avoid the oscillation phenomenon and derived the minimum time-step size for various kinds of elements.

In this paper, we derived the criteria based on the positive coefficients rule of a physical phenomenon using the Cholesky factorization at difference recurrence formulas and presented the stable, nonoscillatory and physical reality requirements that have to be satisfied for the transient heat-conduction problem. The operating regions for consistent and lumped finite element formulations of linear and quadratic one-dimensional elements will be first obtained by these requirements. The operating regions are then developed for finite difference and finite volume formulations and are compared with the finite element operating regions. We will show that the backward-difference scheme that was introduced to eliminate oscillatory results by a number of researchers on finite element modeling of diffusion problems violates the physical reality and generates unrealistic results at very small time-step sizes when using the consistent formulations and the formulations of high-order elements. Finally, numerical results of a simple one-dimensional transient heat-conduction problem are presented to verify the criteria.

Problem Definition

As an example, the temperature distribution in an insulated rod for which the initial temperature is zero could be discussed as a rod in

Received 17 April 2006; revision received 31 July 2006; accepted for publication 1 September 2006.

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which the heat input at the left end and the right end is insulated (Fig. 1).

The one-dimensional transient Fourier heat-conduction equation for an isotropic material is

$$k\frac{\partial^2 T(x,t)}{\partial x^2} = \rho c\frac{\partial T(x,t)}{\partial t} \tag{1}$$

The period of interest in this study is the transient period, which occurs between the starting of physical process and reaching the steady state conditions for the region presented by Eq. (1). The analytical solution to this problem by separation of variables method with thermal diffusivity, $\alpha = k/\rho c$, will be

$$T(x,t) = \left(\frac{\alpha q}{kL}\right)t + \left(\frac{2q}{kL}\right)\sum_{m=1}^{\infty}\cos\left(\frac{m\pi}{L}x\right)(1 - e^{-\alpha(\frac{m\pi}{L})^2 t})/\left(\frac{m\pi}{L}\right)^2 \tag{2}$$

Consistent and Lumped Finite Element Formulations

The variational statement of the problem is used in finite element technique to obtain the system of differential equations. The functional formulation that is equivalent to Eq. (1) is

$$I = \int_{\Omega}\frac{1}{2}\left[k\left(\frac{\partial T}{\partial x}\right)^2 + 2\rho c\frac{\partial T}{\partial t}T\right]\mathrm{d}v + \int_{\Gamma}\mathrm{q}T\,\mathrm{d}s \tag{3}$$

where Ω is the domain of the body and Γ is the boundary surface. The function for T is continuous, but defined by several equations over the region. The individual equations $T^{(e)}$ are defined over subregions called elements and the preceding equations should be separated into integrals over the individual elements. The temperature in each element is given by

$$T^{(e)} = N_i^{(e)}T_i + N_j^{(e)}T_j + \cdots + N_m^{(e)}T_m = [\boldsymbol{N}^{(e)}]\{T^{(e)}\} \tag{4}$$

A subscript e on the left of the equal sign implies that all the quantities on the right-hand side are to be interpreted on an element basis. The temperature gradient could be written in terms of the interpolation function as

$$\begin{gathered}\{\partial T^{(e)}/\partial t\} = [B^{(e)}]\{T^{(e)}\} \\ [B^{(e)}] = [\,\partial N_i^{(e)}/\partial x \quad \partial N_j^{(e)}/\partial x \quad \cdots \quad \partial N_m^{(e)}/\partial x\,]\end{gathered} \tag{5}$$

Introducing Eq. (5) into the functional and performing the minimization gives the matrix differential equations:

$$[C^{(e)}]\{\partial T^{(e)}/\partial t\} + [K^{(e)}]\{T^{(e)}\} = \{F^{(e)}\} \tag{6}$$

$$[C^{(e)}] = \int_{\Omega}\rho c[N^{(e)}]^T[N^{(e)}]\,\mathrm{d}v \tag{7}$$

$$[K^{(e)}] = \int_{\Omega}k[B^{(e)}]^T[B^{(e)}]\,\mathrm{d}v \tag{8}$$

$$\{F^{(e)}\} = \int_{\Gamma}\mathrm{q}[N^{(e)}]^T\,\mathrm{d}s \tag{9}$$

The preceding three integrals are evaluated over each element and the element contributions are added using the direct stiffness procedure. In consistent formulations, subdividing the region into identical linear elements gives the element matrices, using the shape functions $N_1 = (1 - x/\Delta x)$ and $N_1 = x/\Delta x$:

$$[K^{(e)}] = \frac{kA}{\Delta x}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix} = \begin{bmatrix}2 & -2\\ -2 & 2\end{bmatrix} \tag{10}$$

$$[C^{(e)}] = \frac{\rho cA\Delta x}{6}\begin{bmatrix}2 & 1\\ 1 & 2\end{bmatrix} = \begin{bmatrix}8 & 4\\ 4 & 8\end{bmatrix} \tag{11}$$

In lumped formulations, in order to calculate the capacitance matrix with reduced order of the element shape functions, the element matrix $[C^{(e)}]$ will be

$$[C^{(e)}] = \frac{\rho cA\Delta x}{2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} = \begin{bmatrix}12 & 0\\ 0 & 12\end{bmatrix} \tag{12}$$

The element matrices for quadratic 1-D elements using the shape functions $N_1 = (1 - 2x/\Delta x)(1 - x/\Delta x), N_2 = 4(1 - x/\Delta x)x/\Delta x$, and $N_3 = -(1 - 2x/\Delta x)x/\Delta x$ are given as follows:

$$[k^{(e)}] = \frac{kA}{3\Delta x}\begin{bmatrix}7 & -8 & 1\\ -8 & 16 & -8\\ 1 & -8 & 7\end{bmatrix} = \frac{1}{3}\begin{bmatrix}14 & -16 & 1\\ -16 & 32 & -16\\ 1 & -16 & 14\end{bmatrix} \tag{13}$$

$$[C^{(e)}] = \frac{\rho cA\Delta x}{30}\begin{bmatrix}4 & 2 & -1\\ 2 & 16 & 2\\ -1 & 2 & 4\end{bmatrix} = \frac{1}{15}\begin{bmatrix}48 & 24 & -12\\ 24 & 192 & 24\\ -12 & 24 & 48\end{bmatrix} \tag{14}$$

Hence, within the frame of the consistent and lumped formulations, a time-dependent system of ordinary differential equations of general form is

$$[C]\{T\} + [K]\{\dot{T}\} = \{F\}; \qquad \dot{T} = \partial T/\partial t \tag{15}$$

Difference Recurrence Formula

The system of first-order linear differential equations (15) and the vector of the zero initial values defines the transient heat-conduction problem. Any kind of exact solutions to the differential systems are so complicated for large systems that they are seldom used. The usual solution procedure is to integrate differential equations. Obtaining a numerical solution to the equation given by Eq. (15) is based on the finite difference approximation in the time domain. The procedure moves ahead in time according to the relation

$$\{T\}_n = \{T\}_{n-1} + [\theta\{\dot{T}\}_n + (1-\theta)\{\dot{T}\}_{n-1}]\Delta t \tag{16}$$

where n represents the time-step index. The time difference parameter gives a weighted average time derivative over the time interval, where $\theta = 0, 1/2, 2/3$, and 1 for Euler, central difference, Galerkin, and backward-difference schemes, respectively. In applying Eq. (16) to the finite element problem, premultiplying it by $[C]$ and using Eq. (15) to eliminate the time derivates, regardless of which value is specified for θ, the final system of equations has the general form

$$[A]\{T\}_n = [P]\{T\}_{n-1} + \{F^*\} \tag{17}$$

where $[A]$ and $[P]$ are dependent on the material properties and Δt, and the vector $\{\boldsymbol{F}^*\}$ is a combination of $\{\mathrm{F}\}_{n-1}$ and $\{\mathrm{F}\}_n$.

$$[A] = [C] + \theta\Delta t[K] \tag{18}$$

$$[P] = [C] - (1-\theta)\Delta t[K] \tag{19}$$

$$\{\boldsymbol{F}^*\} = (1-\theta)\Delta t\{F\}_{n-1} + \theta\Delta t\{F\}_n \tag{20}$$

Matrix Stability of the Finite Element Formulations

Equation (17) can be solved for the new temperatures $\{T\}_n$, giving

$$\{T\}_n = [A]^{-1}[P]\{T\}_{n-1} + [A]^{-1}\{\boldsymbol{F}^*\} \tag{21}$$

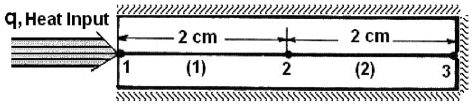

Fig. 1 Insulated rod with heat input; $q = 5$ W, $k = 4$ W/cm · °C, $\rho c = 12$ J/cm^3 · °C, and $A = 1$ cm^2.

$$\{T\}_n = ([A]^{-1}[P])^n\{T\}_0 + \{([A]^{-1}[P])^{n-1} + \cdots + [A]^{-1}[P] + [I]\}[A]^{-1}\{F^*\} \tag{22}$$

In the right-hand side of the preceding equation, the force vector has no role in the stability investigation (see Trujillo [7]) and the term $([A]^{-1}[P])^n$ alone is sufficient for stability investigations. The remaining terms are stable as long as $[A]^{-1}[P]$ is stable. The influence of the forcing term is reflected in the variable coefficients of the solution related to the homogeneous part and the analysis can be done using Eq. (15) with the right-hand side at zero. The initial temperature $\{T\}_0$ is expanded in terms of the eigenvectors $\{x_1\}$, $\{x_2\}$, …, $\{x_n\}$ of a general eigenvalue problem $[A]\{x_j\} = \lambda_\theta[P]\{x_j\}$. Therefore, Eq. (22) can be written as

$$\{T\}_n = ([A^{-1}[P])^n(c_1\{x_1\} + c_2\{x_2\} + \cdots + c_n\{x_n\}) = \sum_{j=1}^{n} c_j\lambda_\theta^n\{x_j\} \tag{23}$$

For this system to be stable the magnitude of each eigenvalue λ_θ must be less than or equal to one. So, the stability condition will be $|\lambda_\theta| \prec 1$. To avoid numerical oscillations, the quantity of λ_θ must be bounded between zero and one, $0 \prec \lambda_\theta \prec 1$. Substituting Eqs. (18) and (19) in the general eigenvalue problem $[P]\{x_j\} = \lambda_\theta[A]\{x_j\}$ yields

$$([C] - (1-\theta)\Delta t[K])\{x_j\} = \lambda_\theta([C + \theta\Delta t[K])\{x_j\} \tag{24}$$

Multiplying through by $[C]^{-1}$ and comparing the result with the general eigenvalue problem $[K]\{x_j\} = \lambda_j[C]\{x_j\}$ gives $\lambda_\theta = [1 - (1-\theta)\Delta t\lambda_j]/(1 + \theta\Delta t\lambda_j)$. All of the eigenvalues of $[C]$ and $[K]$ are positive and real; thus, only the largest value of λ_j, λ_N, needs to be considered when applying the stability criteria. This consideration gives the stability and nonoscillatory stable conditions $0 \prec \Delta t \prec 2/(1-2\theta)\lambda_N$ and $0 \prec \Delta t \prec 1/(1-\theta)\lambda_N$, respectively, which must be applied to provide the optimal time-step control for numerical schemes. The variation of λ_θ with respect to $\phi = \lambda_N\Delta t$, for different values of θ, is shown in Fig. 2. It can be shown that for a small time step, all four schemes are identical and the solution begins to differ as the time step increases.

Derivation of Criteria Based on Concept of Positive Coefficients Rule

The numerical solution of the algebraic equations should be bounded within some limits that usually have a physical origin. Analysis of the stability from physical considerations has been developed by several researchers. Dusinberre [8] states in his stability criteria that negative coefficients in the difference equation should be avoided to enforce stability. Also, the rule of positive neighbor coefficients restriction developed by Patankar [9] guarantees the convergence of numerical solutions to discrete schemes.

It is easy to think of Eq. (17) as having the form $T_p = \sum_{n=1}^{r} a_{pn}T_n + f_p$, where a_{pn} is a coefficient in $[A]^{-1}[P]$, f_p is the coefficient in $[A]^{-1}\{F^*\}$, and T_p is in the region influenced by the values of r nodal points. An increase in the temperature of a node, other than node P, while maintaining the rest of the nodes at their same temperature (excluding node P) means that T_p must increase. The aforementioned discussion leads to the fact that the neighboring coefficients must be positive. A simple rule is "avoid negative coefficients in any row of $[A]^{-1}[P]$." This rule is used when analyzing elements criteria for the necessary requirements. The coefficients a_{pn}, which come from $[A]^{-1}[P]$, have to be nonnegative, as do the elements in $[A]^{-1}$. One way to guarantee that the positive coefficients rule is satisfied is to require negative off-diagonal terms in matrix $[A]$ and positive coefficients in matrix $[P]$. Knowing that every symmetric positive definite matrix has a unique Cholesky decomposition, the matrix $[A]$ can be decomposed into the product of a lower and an upper triangular matrix, $[A] = [L][L]^T$. Using the general formula for Cholesky factorization,

$$l_{ii} = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^2\right)^{1/2}, \qquad l_{ij} = \left(a_{ij} - \sum_{k=1}^{i-1} l_{ik}l_{jk}\right)/l_{jj} \tag{25}$$

it can be shown by induction that every diagonal of $[A]$ is positive and all off-diagonal coefficients are negative. Also, the inverse matrix of $[L]$ is a lower triangular matrix with all positive coefficients. As a result, the matrix $[A]^{-1}$, which is equal to $[L]^{-T}[L]^{-1}$ has positive coefficients.

The evaluation criteria used in this study are the coefficients of $[A]^{-1}[P]$, and $[A]^{-1}$ must be positive; thus, $[A]$ must have positive diagonal and negative off-diagonal coefficients and $[P]$ must have positive coefficients. These criteria are applied as a sufficient condition for the physical reality and it is also expressed that the matrix $[P]$ must be singular or positive definite.

Operating Region for Consistent and Lumped Formulations of Linear 1-D Elements

As mentioned in the preceding section, the largest eigenvalue of the system $[K]\{x_j\} = \lambda_j[C]\{x_j\}$ is needed to determine the stability and nonoscillation criteria. The maximum eigenvalue of consistent formulations is $\lambda_n = 12\alpha/\Delta x^2$. Therefore, the stability and nonoscillation requirements are, respectively, as p_1: $r \prec 1/6(1-2\theta)$ and p_2: $r \prec 1/12(1-\theta)$, where the Fourier number is defined as $r = \alpha\Delta t/\Delta x^2$. The matrices $[A]$ and $[P]$, according to Eqs. (18) and (19), are given by

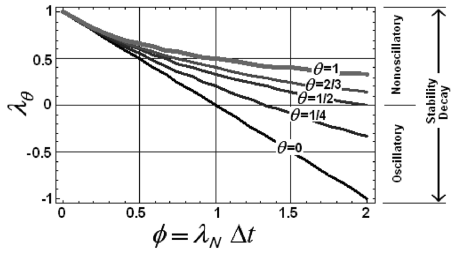

Fig. 2 Variation of λ_θ with respect to ϕ for the various schemes.

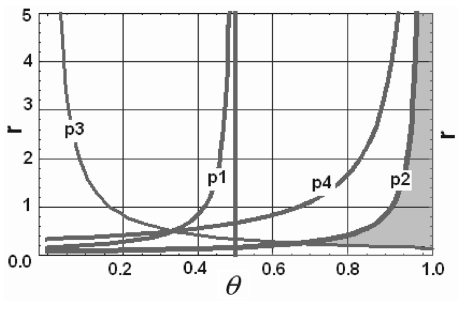

Fig. 3 Operating region for consistent finite element formulations of linear 1-D elements.

$$[A] = \rho cA\Delta x \begin{bmatrix} 1/3 + r\theta & 1/6 - r\theta & 0 \\ 1/6 - r\theta & 2/3 + 2r\theta & 1/6 - r\theta \\ 0 & 1/6 - r\theta & 1/3 + r\theta \end{bmatrix}$$
$$[P] = \rho cA\Delta x \begin{bmatrix} 1/3 + r(-1+\theta) & 1/6 + r(1-\theta) & 0 \\ 1/6 + r(1-\theta) & 2/3 + 2r(-1+\theta) & 1/6 + r(1-\theta) \\ 0 & 1/6 + r(1-\theta) & 1/3 + r(-1+\theta) \end{bmatrix} \tag{26}$$

The criteria based on the positive coefficients rule require the positive diagonal and negative off-diagonal elements in $[A]$ and the positive elements in $[P]$. Thus, Dusinberre's analysis requires p_3: $r \succ 1/6\theta$ and p_4: $r \prec 1/3(1-\theta)$. The requirements p_1, p_2, p_3, and p_4 are plotted in Fig. 3 to obtain the operating region indicated, for stable, nonoscillatory and Dusinberre's criteria.

The requirements yield the following critical time-step size limit for consistent formulations of linear elements:

$$\frac{\Delta x^2}{6\theta\alpha} \le \Delta t \le \frac{\Delta x^2}{12(1-\theta)\alpha} \tag{27}$$

The minimum time-step size given by Eq. (27) is the same as that given by [3–6] and the maximum time-step size is smaller than that given by Ouyang and Xiao [5]; thus, the temperature monotony will remain in a satisfactory safety condition.

In the lumped formulations, the largest eigenvalue of the system $[K]\{x_j\} = \lambda_j[C]\{x_j\}$ is $\lambda_n = 4\alpha/\Delta x^2$ and the stability and nonoscillation requirements are given, respectively, as p_1: $r \prec 1/2(1-2\theta)$ and p_2: $r \prec 1/4(1-\theta)$. Also, the matrices $[A]$ and $[P]$ are given by

$$[A] = \rho cA\Delta x \begin{bmatrix} 1/2 + r\theta & -r\theta & 0 \\ -r\theta & 1 + 2r\theta & -r\theta \\ 0 & -r\theta & 1/2 + r\theta \end{bmatrix}, \qquad [P] = \rho cA\Delta x \begin{bmatrix} 1/2 + r(-1+\theta) & r(1-\theta) & 0 \\ r(1-\theta) & 1 + 2r(-1+\theta) & r(1-\theta) \\ 0 & r(1-\theta) & 1/2 + r(-1+\theta) \end{bmatrix} \tag{28}$$

By applying the positive coefficients rule, Dusinberre's requirement will be p_3: $r \prec 1/2(1-\theta)$. Finally, the operating region for stable, nonoscillatory and Dusinberre's criteria is determined by the requirements p_1, p_2, and p_3. This region is shown in Fig. 4 for the lumped formulations. Hence, it shows that the consistent formulations are more restrictive relative to selecting a time step than the lumped formulations.

From the preceding operating region, the following critical time-step size limit is obtained for lumped formulations of linear elements:

$$0 \le \Delta t \le \frac{\Delta x^2}{12(1-\theta)\alpha} \tag{29}$$

Also from Eq. (29), in lumped formulations, the upper bound of the time-step size limit obtained with the criteria previously described is smaller than that given by Ouyang and Xiao [5] and ensures a sufficient safety condition for oscillatory events.

Operating Region for Consistent and Lumped Formulations of Quadratic 1-D Elements

In the consistent formulations of quadratic elements, the largest eigenvalue of the system $[K]\{x_j\} = \lambda_j[C]\{x_j\}$ is $\lambda_n = 60\alpha/\Delta x^2$ and the stability and nonoscillation requirements are given by, respectively, p_1: $r \prec 1/30(1-2\theta)$ and p_2: $r \prec 1/60(1-\theta)$. Also, the matrices $[A]$ and $[P]$ are given.

$$[A] = \frac{\rho cA\Delta x}{30} \begin{bmatrix} 4 + 70r\theta & 2 - 80r\theta & -1 + 10r\theta \\ 2 - 80r\theta & 16 + 160r\theta & 2 - 80r\theta \\ -1 + 10r\theta & 2 - 80r\theta & 4 + 70r\theta \end{bmatrix}$$
$$[P] = \frac{\rho cA\Delta x}{30} \begin{bmatrix} 4 + 70r(-1+\theta) & 2 - 80r(-1+\theta) & -1 + 10r(-1+\theta) \\ 2 - 80r(-1+\theta) & 16 + 160r(-1+\theta) & 2 - 80r(-1+\theta) \\ -1 + 10r(-1+\theta) & 2 - 80r(-1+\theta) & 4 + 70r(-1+\theta) \end{bmatrix} \tag{30}$$

By the sufficient condition for physical reality, Dusinberre's criterion is not satisfied. According to the necessary condition, the coefficients of $[A]^{-1}[P]$ must be positive.

Therefore, Dusinberre's requirements will be

$$p_3\text{: } r \prec (13 - 36\theta - \sqrt{169 - 336\theta + 576\theta^2})/120\theta(-5 + 6\theta)$$

p_4: $r \prec 7/60\theta$, and p_5: $r \prec 1/20(1-3\theta)$. The operating region for stable, nonoscillatory and Dusinberre's criteria is determined by the requirements p_1, p_2, p_3, p_4, and p_5. This region is shown in Fig. 5 for the consistent formulations of quadratic 1-D elements.

The operating region determined for consistent formulations of quadratic 1-D elements gives the following critical time-step size limit:

$$\frac{7\Delta x^2}{60\theta\alpha} \le \Delta t \le \frac{\Delta x^2}{60(1-\theta)\alpha} \tag{31}$$

In this formulation, the lower bound of the time-step size limit is greater than that given by Thomas and Zhou [6] and shows the necessary safety condition is more certain than in their formulation.

In the lumped formulations of quadratic elements, the largest eigenvalue of the system $[K]\{x_j\} = \lambda_j[C]\{x_j\}$ is $\lambda_N = 24\alpha/\Delta x^2$ and the stability and nonoscillation requirements are given by, respectively, p_1: $r \prec 1/12(1-2\theta)$ and p_2: $r \prec 1/24(1-\theta)$. The matrices $[A]$ and $[P]$ are given as follows:

$$[A] = \frac{\rho cA\Delta x}{3} \begin{bmatrix} 1 + 7r\theta & -8r\theta & r\theta \\ -8r\theta & 1 + 16r\theta & -8r\theta \\ r\theta & -8r\theta & 1 + 7r\theta \end{bmatrix}, \qquad [P] = \frac{\rho cA\Delta x}{3} \begin{bmatrix} 1 + 7r(-1+\theta) & -8r(-1+\theta) & r(-1+\theta) \\ -8r(-1+\theta) & 1 + 16r(-1+\theta) & -8r(-1+\theta) \\ r(-1+\theta) & -8r(-1+\theta) & 1 + 7r(-1+\theta) \end{bmatrix} \tag{32}$$

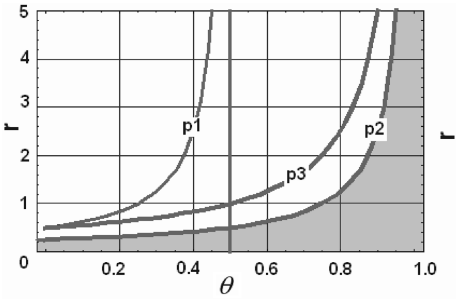

Fig. 4 Operating region for lumped finite element formulations of linear 1-D elements.

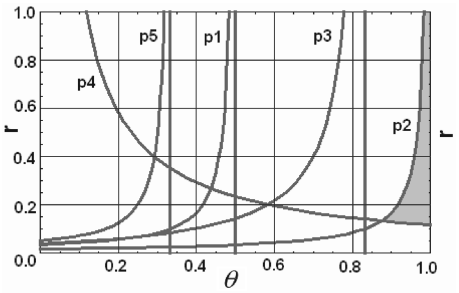

Fig. 5 Operating region for consistent finite element formulations of quadratic 1-D elements.

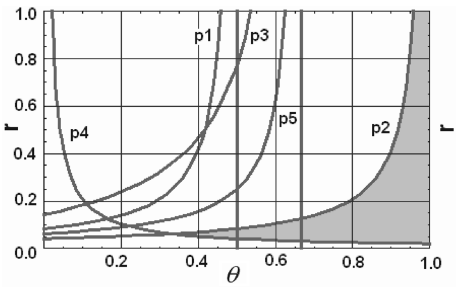

Fig. 6 Operating region for lumped finite element formulations of quadratic 1-D elements.

Dusinberre's requirements, which are given by applying the necessary condition of the physical reality, yield

$$p_3\colon\ r \prec (7 - 30\theta - \sqrt{49 - 36\theta + 324\theta^2})/2\theta(-96 + 144\theta)$$

$p_4\colon\ r \prec 7/48\theta$ and $p_5\colon\ r \prec 1/8(2 - 3\theta)$. The operating region for stable, nonoscillatory and Dusinberre's criteria (which is determined by the requirements p_1, p_2, p_3, p_4, and p_5) is shown in Fig. 6 for the lumped formulations of quadratic 1-D elements.

In lumped formulations of quadratic 1-D elements, the operating region gives the following inequality limit access to critical time-step size:

$$\frac{\Delta x^2}{48\theta\alpha} \le \Delta t \le \frac{\Delta x^2}{24(1-\theta)\alpha} \tag{33}$$

According to Figs. 3–5 and 5, it is concluded that the operating region of the critical time-step size selection in lumped finite element formulations is wider than consistent finite element formulations, and linear elements are wider than quadratic elements.

Finite Difference Formulations and Operating Region

The finite difference method obtains an approximate solution for $T(x, t)$ at a finite set of x and t for the discrete model of the problem, as shown in Fig. 7. Let T_j^n be the numerical approximation to $T(x_j, t_n)$; The discrete x and t are uniformly spaced in the intervals

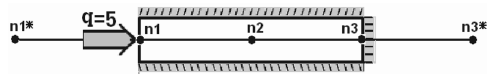

Fig. 7 Discrete finite difference model of the problem.

$0 \le x \le L$ and $0 \le t \le t_{\max}$, respectively, such that $x_j = j\Delta x$; $j = 0, 1, 2, \ldots, M$, and $t_n = n\Delta t$; $n = 0, 1, 2, \ldots, N$, where M and N are the total number of spatial nodes and the number of time steps.

To solve the heat-conduction problem numerically, we consider an application of conventional finite difference schemes. After discretization, the governing equation can be approximated numerically in the following recursive form:

$$\left(T_j^{n+1} - T_j^n\right)/\Delta t = \alpha[\theta\left(T_{j+1}^{n+1} - 2T_j^{n+1} + T_{j-1}^{n+1}\right) + (1-\theta)\left(T_{j+1}^n - 2T_j^n + T_{j-1}^n\right)]/\Delta x^2 \tag{34}$$

According to the boundary condition of the governing equation, the discrete boundary equation on the left side of the model can similarly be derived as follows:

$$\theta\left(T_{j+1}^{n+1} - T_j^{n+1}\right) + (1-\theta)\left(T_{j+1}^n - T_j^n\right) = -q\Delta x/k \tag{35}$$

Assume the error grid function $\varepsilon_j^n = \eta^n e^{i\alpha j\Delta x}$ from the characteristic equation of discrete Eq. (34), where $\eta^n = \eta(n\Delta t)$ is the error amplitude and $i = \sqrt{-1}$. Substituting ε_j^n into the recurrence formula [Eq. (34)] and defining an amplification factor $G = \eta^{n+1}/\eta^n$, we find that

$$G = [1 - 4\sin^2(\alpha\Delta x/2)(1-\theta)r]/[1 + 4\sin^2(\alpha\Delta x/2)\theta r] \tag{36}$$

The criterion $|G| \prec 1$ is the von Neumann necessary condition [10] for linear computational stability. Also, the condition that ensures the nonoscillatory results is $0 \prec G \prec 1$. Thus, these requirements can be shown as $p_1\colon\ r \prec 1/2(1-2\theta)$ and $p_2\colon\ r \prec 1/4(1-\theta)$. A slight improvement in computational efficiency can be obtained with a small rearrangement of Eqs. (34) and (35), given, respectively, as follows:

$$(1/r + 2\theta)T_j^{n+1} = \theta T_{j-1}^{n+1} + \theta T_{j+1}^{n+1} + (1/r + 2\theta - 2)T_j^n + (1-\theta)T_{j-1}^n + (1-\theta)T_{j+1}^n \tag{37}$$

$$\theta T_j^{n+1} = \theta T_{j+1}^{n+1} + (1-\theta)(T_{j+1}^n - T_j^n) + q\Delta x/k \tag{38}$$

where $r = \alpha\Delta t/\Delta x^2$. Note that all the precding expressions can all be generically written as

$$a_p T_p = \sum_{n=1}^{r} a_{pn} T_n + f_p \tag{39}$$

where the summation is to be taken over all neighbors. From the basis rules of Patankar [9], it follows that a_p must equal the sum of the neighbor coefficient a_{pn} and all must be the same sign. According to the positive coefficients rule, let us decide to have a positive sign in all of the coefficients. The criteria enforced on the matrices $[A]$ and $[P]$ conform to the consequence of this physical phenomenon.

If we wish to represent the specified heat flux boundary condition at $x = 0$ and the adiabatic surface boundary condition at $x = L$, it is necessary to introduce the fictitious temperatures T_{1^*} and T_{3^*} at the external nodes $n1^*$ and $n3^*$, as shown in Fig. 7, by imaging the rod to be extended very slightly.

The linear system of equations can be represented in multiplication matrix form as recurrence relation (17). For the specific case under consideration, the nodal temperatures vector is $\{\boldsymbol{T}\}_n^T = \{T_{1^*}^n, T_1^n, T_2^n, T_3^n, T_{3^*}^n\}$ at $t - n$ and the matrices $[A]$ and $[P]$ are derived as follows:

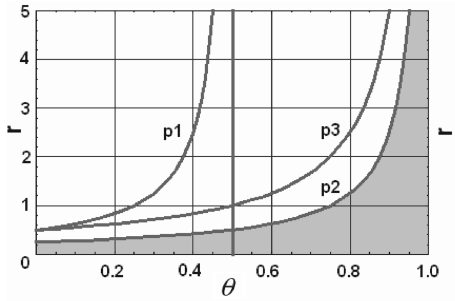

Fig. 8 Operating region for 1-D finite difference models.

$$[A]=\begin{bmatrix} \theta & -\theta & 0 & 0 & 0 \\ -\theta & 1/r+2\theta & -\theta & 0 & 0 \\ 0 & -\theta & 1/r+2\theta & -\theta & 0 \\ 0 & 0 & -\theta & 1/r+2\theta & -\theta \\ 0 & 0 & 0 & -\theta & \theta \end{bmatrix}$$

$$[P] = \begin{bmatrix} \theta-1 & 1-\theta & 0 & 0 & 0 \\ 1-\theta & 1/r+2\theta-2 & 1-\theta & 0 & 0 \\ 0 & 1-\theta & 1/r+2\theta-2 & 1-\theta & 0 \\ 0 & 0 & 1-\theta & 1/r+2\theta-2 & 1-\theta \\ 0 & 0 & 0 & 1-\theta & \theta-1 \end{bmatrix} \tag{40}$$

The criteria that are required to satisfy the positive coefficients rule yield the requirement p_3: $r \prec 1/2(1-\theta)$ for internal nodes $n1$, $n2$, and $n3$. It should be noted that the positive coefficients rule cannot be satisfied at the external nodes $n1^*$ and $n3^*$, according to the first and fifth rows of the matrix $[P]$. On the other hand, the fictitious temperatures T_{1^*} and T_{3^*} violate the physical reality.

In the finite difference formulations, according to the stable, nonoscillatory and physical reality requirements, p_1, p_2, and p_3, the operating region will be obtained as shown in Fig. 8.

Finally, the following critical time-step size limit is obtained for 1-D finite difference formulations and it is concluded that the limit is equal to that for lumped finite element formulations of linear 1-D elements:

$$0 \le \Delta t \le \frac{\Delta x^2}{12(1-\theta)\alpha} \tag{41}$$

Finite Volume Formulations and Operating Region

Finite volume methods are based on the idea of integrating the dependent variables over a finite control volume and applying the conservation principle to the integrated variables. The volume and the points necessary for further development are sketched in Fig. 9.

Part of the integration process of the differential governing equation is shown in the following equations:

$$\int_t^{t+\Delta t}\int_{x_j-\frac{\Delta x}{2}}^{x_j+\frac{\Delta x}{2}} \frac{\partial^2 T_j}{\partial x^2}\,\mathrm{d}x\,\mathrm{d}t = \int_t^{t+\Delta t}\int_{x_j-\frac{\Delta x}{2}}^{x_j+\frac{\Delta x}{2}} \frac{1}{\alpha}\frac{\partial T_j}{\partial t}\,\mathrm{d}x\,\mathrm{d}t \tag{42}$$

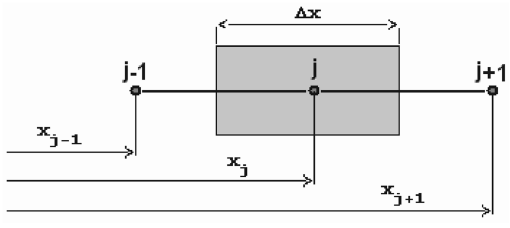

Fig. 9 Discrete finite volume model of the problem.

$$\int_t^{t+\Delta t}\left(\left.\frac{\partial T_j}{\partial x}\right|_{x_j+\Delta x/2} - \left.\frac{\partial T_j}{\partial x}\right|_{x_j-\Delta x/2}\right)\mathrm{d}t = \int_{x_j-\Delta x/2}^{x_j+\Delta x/2}\frac{1}{\alpha}(T_j|_{t+\Delta t} - T_j|_t)\,\mathrm{d}x \tag{43}$$

The derivatives appearing after the application of the finite volume method are given by $\partial T_j/\partial x = (T_{j+1}-T_j)/\Delta x$ at $x_j + \Delta x/2$ and $\partial T_j/\partial x = (T_j - T_{j-1})/\Delta x$ at $x_j - \Delta x/2$. A very general proposition is to assume that the integral is given by time-weighted averages as follows:

$$\int_t^{t+\Delta t} T_j\,\mathrm{d}t = \left(\theta T_j^{n+1} + (1-\theta)T_j^n\right)\Delta t \tag{44}$$

where θ is between 0 and 1. Finally, the following algebraic discretized equation is obtained:

$$(1/r+2\theta)T_j^{n+1} = \theta T_{j-1}^{n+1} + \theta T_{j+1}^{n+1} + (1/r+2\theta-2)T_j^n + (1-\theta)T_{j-1}^n + (1-\theta)T_{j+1}^n \tag{45}$$

According to the von Neumann stability analysis discussed in the previous section, the stability and nonoscillation requirements for finite volume formulations are given by, respectively, p_1: $r \prec 1/2(1-2\theta)$ and p_2: $r \prec 1/4(1-\theta)$. One algebraic boundary equation like the following, relating the values of T at three contiguous nodes, is obtained at the left side of the model:

$$(1/2r+\theta)T_j^{n+1} = \theta T_{j-1}^{n+1} + (1/2r+\theta-1)T_j^n + (1-\theta)T_{j-1}^n + q\Delta x/k \tag{46}$$

The discrete equations (45) and (46) have the general form given in Eq. (39). The positive coefficients rule take into consideration the positive signs in a_p and a_{pn}. This physical law of heat diffusion is satisfied by applying the criteria. In this case, the system of equations can be represented by the recurrence relation (17), in which the nodal temperatures vector is $\{\boldsymbol{T}\}_n^T = \{T_1^n, T_2^n, T_3^n\}$ and the matrices $[A]$ and $[P]$ are as follows:

$$[A]=\begin{bmatrix} 1/2r+\theta & -\theta & 0 \\ -\theta & 1/r+2\theta & -\theta \\ 0 & -\theta & 1/2r+\theta \end{bmatrix}$$
$$[P]=\begin{bmatrix} 1/2r+\theta-1 & 1-\theta & 0 \\ 1-\theta & 1/r+2\theta-2 & 1-\theta \\ 0 & 1-\theta & 1/2r+\theta-1 \end{bmatrix} \tag{47}$$

The criteria that are derived indicate that $[A]$ must have positive diagonal and negative off-diagonal elements and $[P]$ must have positive elements. Thus, Dusinberre's analysis requires p_3: $r \prec 1/2(1-\theta)$. Finally, the operating region for finite volume formulations is obtained (Fig. 10).

The requirements are summarized to give the following critical time-step size limit obtained for 1-D finite volume formulations and they conclude that the limit is equal to that for lumped finite element formulations of linear 1-D elements:

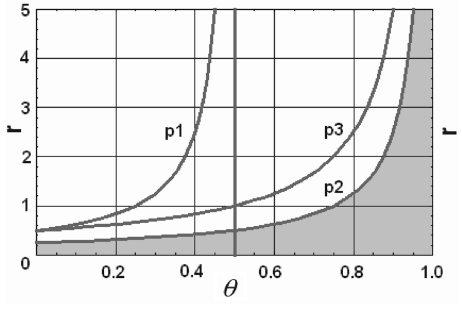

Fig. 10 Operating region for 1-D finite volume models.

$$0 \le \Delta t \le \frac{\Delta x^2}{12(1-\theta)\alpha} \tag{48}$$

Numerical Results for Various Formulations

All of the following figures compare the temperature distribution vs time at adiabatic surface $x = 4$ and backward-difference scheme $\theta = 1$ for various time-step sizes $\Delta t = 4, 3, 2.4, 1, 0.5, 0.2$, and 0.1 related to the Fourier numbers $r = 0.3333, 0.25, 0.2, 0.0833, 0.0416, 0.0166$, and 0.0083, respectively. The analytical solution is also plotted in all figures.

Figure 11a plots the temperature distribution vs time for consistent finite element formulation of linear 1-D elements. According to Eq. (27), the physical reality is violated and temperature monotony is not displayed in Fig. 11a for the time-step size less than two, related to the Fourier number 0.1666. It is concluded that the violation of physical reality and unrealistic results are observed at the time-step sizes 1, 0.5, 0.2, and 0.1 and temperature distribution goes below the zero initial temperature. This is physically unreasonable in an insulated rod with zero initial condition, because a heating boundary cannot cause cooling at adiabatic surface. Results of the lumped finite element formulation of linear 1-D elements and finite difference and finite volume formulations, as shown in Fig. 11b. are physically realistic and never go below the zero initial temperature. Furthermore, the temperature distributions vs time for lumped finite element formulation when using linear elements (and finite difference and finite volume formulations) have the same behavior for a given mesh size.

Figures 11c and 11d are the comparison of the temperature distribution vs time at adiabatic surface $x = 4$ and backward-difference scheme $\theta = 1$ for consistent and lumped formulations of quadratic 1-D elements when different time-step sizes are used. According to Eqs. (31) and (33), the minimum time-step sizes for consistent and lumped formulations of quadratic 1-D elements are 1.4 and 0.25, related to the Fourier numbers 0.1166 and 0.1458, respectively. Thus, the physical reality is violated in Fig. 11c for the time-step sizes 1, 0.5, 0.2, and 0.1 and in Fig. 11d for the time-step sizes 0.2 and 0.1. It could be concluded that violation of the physical reality and unrealistic results are observed in consistent and lumped finite element formulations of quadratic 1-D elements when very small time-step sizes are used. According to our computations and the operating regions that were well presented, this result will simply be able to develop for all the various scheme implementations and high-order elements.

Conclusions

In this study, the operating regions for discrete numerical modeling of one-dimensional transient heat-conduction problems were presented. These regions, which can directly determine the critical time-step size limit, were obtained using the criteria based on the positive coefficients rule of a physical phenomenon.

The positive coefficients criteria require negative off-diagonal and positive diagonal elements in $[A]$ and positive elements in $[P]$, where $[A]$ and $[P]$ are dependent on the material properties and the time interval.

It is observed that the operating region of the critical time-step size selection in consistent finite element formulations is lower than lumped finite element formulations. Also, we concluded that the operating region of quadratic 1-D elements is lower than that given by linear 1-D elements. On the other hand, using the consistent

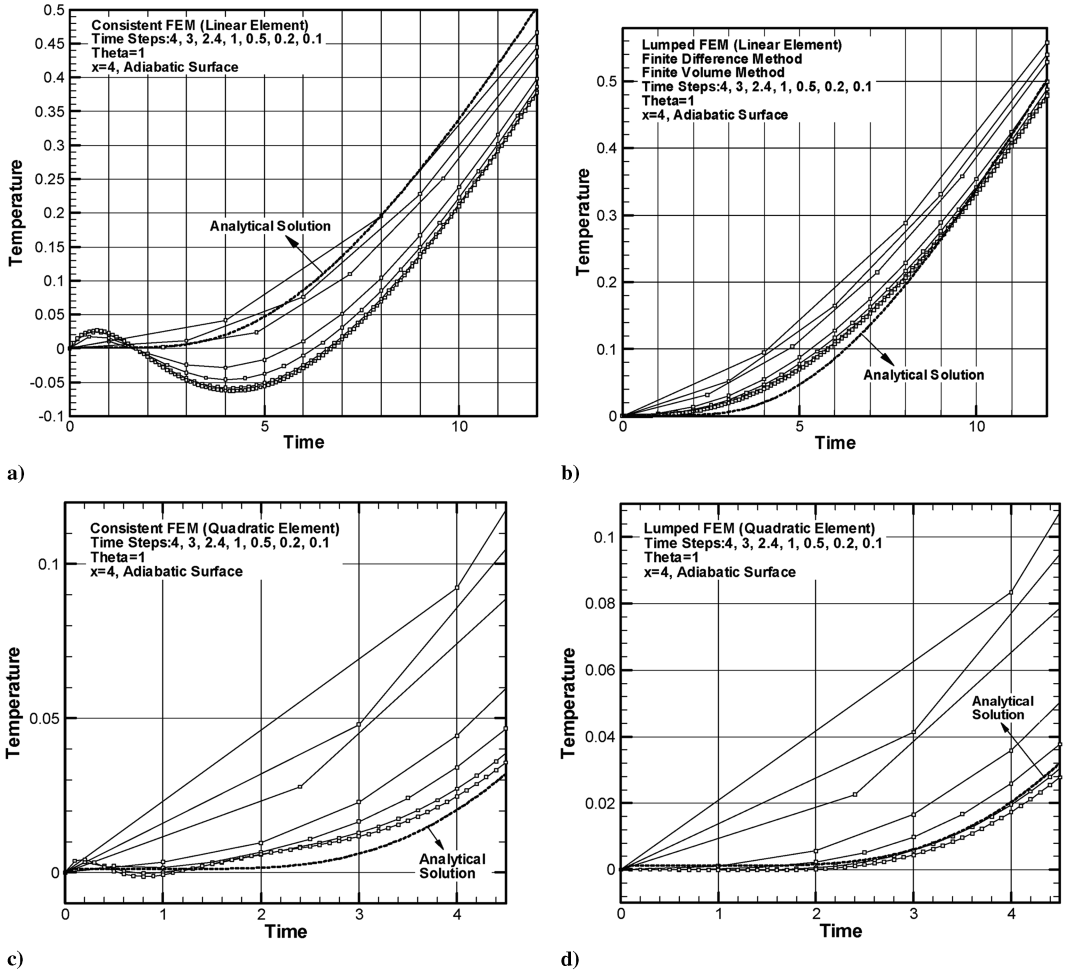

Fig. 11 Temperature distribution vs time at $x = L$ and $\theta = 1$ and various time steps.

formulations and the formulations of high-order elements restricts the critical time-step size limit compared with the lumped formulations and low-order elements.

When backward differences are used, the scheme is stable in all formulations that were discussed, but in consistent finite element formulations and the formulations of high-order elements, the physical reality is violated when very small time-step sizes are used for various scheme implementations.

Lumped finite element formulations of linear elements (and finite difference and finite volume formulations) have the same behavior using the different numerical schemes and their operating regions are equal; hence, the temperature monotony lead to a more satisfactory safety condition than that seen with consistent finite element formulations.

The numerical solution of the temperature distribution in an insulated rod showed that the results of the lumped finite element formulations of linear elements (and finite difference and finite volume formulations) results are physically realistic, whereas the consistent finite element formulations and the formulations of quadratic elements generate unrealistic results for small values of time. Therefore, it is very difficult to meet positive coefficients criteria using consistent formulations and high-order elements during the first few steps of solution process.

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