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NUMERICAL SOLUTION OF REACTION–DIFFUSION EQUATIONS BY COMPACT OPERATORS AND MODIFIED EQUATION METHODS

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SUMMARY

A system of reaction–diffusion equations which governs the propagation of an ozone decomposition laminar flame in Lagrangian co-ordinates is analysed by means of compact operators and modified equation methods. It is shown that the use of fourth-order accurate compact operators yields very accurate solutions if sufficient numbers of grid points are located at the flame front, where very steep gradients of temperature and species concentrations exist. Modified equation methods are shown to impose a restriction on the time step under certain conditions. The solutions obtained by means of compact operators and modified equation methods are compared with solutions obtained by other methods; good agreement is obtained.

KEY WORDS Compact Differences Modified Equation Methods Reaction–Diffusion Equations

INTRODUCTION

Numerical methods for analysing reaction–diffusion equations have attracted the attention of many researchers because of their importance in heat transfer and combustion.[1–13] Ramos[1–3] has studied the temporal and spatial accuracy of a number of algorithms applicable to the analysis of reaction–diffusion equations. The methods evaluated by Ramos include a finite element scheme and a number of explicit and implicit finite-difference procedures. Techniques based on time linearization and operator-splitting were also evaluated. Ramos[1–13] noted that a fourth-order accurate, in both space and time, method of lines and a fourth-order accurate time linearization scheme which uses compact differences for the spatial derivatives yielded the most accurate temperature profiles and flame speeds for a variety of time steps and grid spacings.

The use of high order methods, such as those reported by Ramos,[2,3] for analysing the reaction–diffusion equations that govern flame propagation problems is a relatively unexplored research area. To our knowledge, Morgolis[4] is the first researcher who used high order methods to analyse flame propagation phenomena; he applied sixth-order accurate B-splines to the analysis of the ozone-decomposition flame. Ramos[5] also studied the ozone-decomposition flame by means of high order methods, including a fourth-order accurate method of lines, a fourth-order accurate operator-splitting scheme and three fourth-order accurate partial time-linearization procedures.

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Other investigators who have studied the ozone-decomposition flame have all employed lower order accurate methods.[6-13]

In this paper, two high order methods are used to study the reaction–diffusion equations that govern one-dimensional flame propagation problems. The methods evaluated here are fourth-order accurate in space. One method achieves fourth-order accuracy by using compact operators. The other methods, referred to as the modified equation methods, achieve fourth-order (or any other order of) accuracy by appending terms to the finite-difference equations in order to reduce truncation errors.

It is noted that the manner in which the compact operators are used in the present study is different from the procedure used by Ramos[5] and Kopal.[14] The procedures employed by Ramos[5] and Kopal[14] can only be used if there is only one type of spatial derivative, e.g. only first-order or second-order derivatives, in each partial differential equation. The procedure employed here for implementing compact operators does not impose restrictions on the number or type of spatial derivatives in the partial differential equations.[15-19]

Modified equation methods have been used by several investigators to develop more stable and/or more accurate numerical methods for analysing shock waves.[20-24] Modified equation methods do not seem to have been used to increase the accuracy of finite-difference methods for flame propagation problems. In this paper, three modified equation methods are developed for analysing the reaction–diffusion equations which arise in one-dimensional flame propagation phenomena.

In this paper, compact operators and modified equation methods are used to calculate the laminar ozone-decomposition flame speed. The ozone-decomposition flame was chosen because it has been studied by means of finite element, partial time-linearization and finite-difference schemes.[5,13] The flame speeds calculated by means of the schemes presented in this paper are compared with those or References 5 and 13 in order to assess the accuracy of compact operator and modified equation methods on the numerical solution of reaction–diffusion equations.

In the next section, the equations governing the propagation of a laminar ozone-decomposition flame in Lagrangian co-ordinates are briefly presented; these equations have been derived in greater detail in References 5 and 13. In the third section, an account is given of compact operators and modified equation methods. The third section is followed by the presentation of results and comparisons with solutions obtained with other methods.

PROBLEM FORMULATION

The equations which govern the propagation of a one-dimensional laminar flame through an oxygen–ozone mixture are presented in References 3–8 and 25. Here, we briefly review the assumptions made in deriving the governing equations in Lagrangian co-ordinates.

The propagation of a one-dimensional laminar flame through a mixture composed of 25 per cent (by volume) of ozone and 75 per cent (by volume) of oxygen at a temperature of 300 K is considered. For such a mixture, the flame speed is much smaller than the speed of sound and the pressure can be assumed to be constant. The mixture is considered to be ideal and the thermal conductivity and specific heat at constant pressure are assumed constant. Body forces, viscous dissipation and Soret and Dufour effects are neglected and the species are assumed to have equal diffusion coefficients, which are inversely proportional to the square of the mixture density. Under these conditions, the continuity, energy and species equations need to be solved together with the equation of state.

The system of one-dimensional mixed hyperbolic–parabolic conservation equations in Eulerian co-ordinates can be transformed into a system of reaction–diffusion equations in Lagrangian co-ordinates. The system of reaction–diffusion equations can be written as[5]

$$\frac{\partial \mathbf{U}}{\partial \tau} = \alpha \frac{\partial^2 \mathbf{U}}{\partial \psi^2} + \mathbf{S}, \tag{1}$$

where

$$\mathbf{U} = (Y_1, Y_2, T)^{\mathrm{T}}, \tag{2}$$

$$\mathbf{S} = \left(\frac{\dot{w}_1}{\rho}, \frac{\dot{w}_2}{\rho}, - \sum_{i=1}^{3} \frac{\dot{w}_i h_i^0}{\rho C_p} \right)^{\mathrm{T}}. \tag{3}$$

Y_1 and Y_2 are the mass fractions of ozone and oxygen, respectively; T is the temperature; τ is the time; $\alpha = \rho^2 D = \text{constant}$; ρ is the density; D is the diffusion coefficient; C_p is the specific heat at constant pressure; h_i^0 is the enthalpy of formation of species i at $T_0 = 298{\cdot}15\,\mathrm{K}$; T_0 is a reference temperature; $\dot{w}_i$ is the reaction rate of species i; the superscript T denotes transpose and ψ is the mass co-ordinate given by

$$\frac{\partial \psi}{\partial x} = \rho, \tag{4}$$

$$\frac{\partial \psi}{\partial t} = -\rho u. \tag{5}$$

In equations (4) and (5), x is the Cartesian co-ordinate, u is the flow velocity and $t = \tau$.

The values of the reaction rates, diffusion coefficients and initial and boundary conditions are given in References 3–5, and are not repeated here.

FINITE-DIFFERENCE METHODS

In order to obtain finite-difference solutions to the governing equations formulated in the previous section, the computational domain was replaced by a system of equally spaced grid points and equally incremented time levels. The time derivative in equation (1) was approximated by the following second-order accurate difference formula:

$$\frac{\mathbf{U}_i^{n+1} - \mathbf{U}_i^n}{\Delta \tau} = \frac{1}{2}\left[\left(\frac{\partial \mathbf{U}}{\partial \tau} \right)_i^{n+1} + \left(\frac{\partial \mathbf{U}}{\partial \tau} \right)_i^{n} \right], \tag{6}$$

where $\mathbf{U}_i^n$ denotes the value of $\mathbf{U}$ at the grid point $\psi = i\Delta\psi$ and time level $\tau = n\Delta\tau$, and $\Delta\psi$ and $\Delta\tau$ are the grid spacing and the time step, respectively. Substitution of equation (6) into equation (1) yields

$$\frac{\mathbf{U}_i^{n+1} - \mathbf{U}_i^n}{\Delta \tau} = \frac{1}{2}\left[\left(\alpha \frac{\partial^2 \mathbf{U}}{\partial \psi^2} + \mathbf{S} \right)_i^{n+1} + \left(\alpha \frac{\partial^2 \mathbf{U}}{\partial \psi^2} + \mathbf{S} \right)_i^{n} \right]. \tag{7}$$

In the above equation, $\mathbf{S}^{n+1}$ is a non-linear function of $\mathbf{U}^{n+1}$. Here $\mathbf{S}^{n+1}$ is linearized with respect to $\mathbf{U}^{n+1}$ as follows:[26,27]

$$\mathbf{S}_i^{n+1} = \mathbf{S}_i^n + \left(\frac{\partial \mathbf{S}}{\partial \mathbf{U}} \right)_i^n (\mathbf{U}_i^{n+1} - \mathbf{U}_i^n). \tag{8}$$

In equation (8) the source term has been linearized with respect to all the dependent variables, whereas in the partial linearization methods developed by Ramos[5] the source term is only linearized with respect to the dependent variable whose equation is being solved, i.e.

$$\mathbf{S}_i^{n+1} = \mathbf{S}_i^n + \left[\operatorname{diag}\left(\frac{\partial \mathbf{S}}{\partial \mathbf{U}} \right)_i^n \right] (\mathbf{U}_i^{n+1} - \mathbf{U}_i^n). \tag{9}$$

Equation (8) represents a second-order accurate approximation which is consistent with the order of accuracy of equation (6).

Substitution of equation (8) into equation (7) yields

$$\frac{\mathbf{U}_i^{n+1}-\mathbf{U}_i^n}{\Delta\tau}=\frac{1}{2}\left[\left(\alpha\frac{\partial^2\mathbf{U}}{\partial\psi^2}\right)_i^{n+1}+\left(\alpha\frac{\partial^2\mathbf{U}}{\partial\psi^2}\right)_i^n+2\mathbf{S}_i^n+\left(\frac{\partial\mathbf{S}}{\partial\mathbf{U}}\right)_i^n(\mathbf{U}_i^{n+1}-\mathbf{U}_i^n)\right]. \tag{10}$$

Before numerical solutions can be obtained, the spatial derivatives appearing in equation (10) must be approximated. Here we evaluate two methods for approximating the spatial derivatives in equation (10): compact operators (or compact differences) and modified equation methods.

Compact operators

When compact operators are used, all spatial derivatives are treated as dependent variables. Accordingly, the following new dependent variable is defined in equation (10):

$$\mathbf{F}=\frac{\partial^2\mathbf{U}}{\partial\psi^2}. \tag{11}$$

A new dependent variable requires a new independent equation. Such an equation can be obtained from the following fourth-order accurate difference formula:[15,18]

$$\mathbf{F}_i=\left(\frac{\partial^2\mathbf{U}}{\partial\psi^2}\right)_i=\frac{1}{\Delta\psi^2}\frac{\delta^2}{1+\delta^2/12}\mathbf{U}_i, \tag{12}$$

where

$$\delta^2\mathbf{U}_i=\mathbf{U}_{i+1}-2\mathbf{U}_i+\mathbf{U}_{i-1}. \tag{13}$$

Multiplying both sides of equation (12) by $1+\delta^2/12$ gives, after some algebraic manipulations, the desired equation relating $\mathbf{F}$ to $\mathbf{U}$:

$$\mathbf{F}_{i+1}+10\mathbf{F}_i+\mathbf{F}_{i-1}=\frac{12}{\Delta\psi^2}[\mathbf{U}_{i+1}-2\mathbf{U}_i+\mathbf{U}_{i-1}]. \tag{14}$$

$$\begin{bmatrix}0 & 0\\ -\dfrac{12}{\Delta\psi^2} & 1\end{bmatrix}\begin{bmatrix}\mathbf{U}_{i+1}^{n+1}\\ \mathbf{F}_{i+1}^{n+1}\end{bmatrix}+\begin{bmatrix}1-\dfrac{\Delta\tau}{2}\left(\dfrac{\partial\mathbf{S}}{\partial\mathbf{U}}\right)_i^n & -\dfrac{\alpha}{2}\Delta\tau\\ \dfrac{24}{\Delta\psi^2} & 10\end{bmatrix}\begin{bmatrix}\mathbf{U}_i^{n+1}\\ \mathbf{F}_i^{n+1}\end{bmatrix}$$

$$+\begin{bmatrix}0 & 0\\ -\dfrac{12}{\Delta\psi^2} & 1\end{bmatrix}\begin{bmatrix}\mathbf{U}_{i-1}^{n+1}\\ \mathbf{F}_{i-1}^{n+1}\end{bmatrix}=\begin{bmatrix}\left[1-\dfrac{\Delta\tau}{2}\left(\dfrac{\partial\mathbf{S}}{\partial\mathbf{U}}\right)_i^n\right]\mathbf{U}_i^n+\dfrac{\alpha\Delta\tau}{2}\mathbf{F}_i^n+\Delta\tau\mathbf{S}_i^n\\ 0\end{bmatrix}, \tag{15}$$

which is a system of linear equations with a 6×6 block tridiagonal coefficient matrix.

The solution of equation (15) yields the values of $\mathbf{U}$ and $\mathbf{F}$ at each grid point, whereas the compactor operator scheme developed by Ramos[5] results in a 3×3 block tridiagonal matrix, the solution of which only yields the value of $\mathbf{U}$ at each grid point. Furthermore, all the dependent variables are linearly coupled in equation (15), whereas in the partial time linearization schemes used by Ramos[5] the dependent variables are uncoupled because of the diagonalization of the source terms, cf. equation (9). Because of the uncoupling of the dependent variables, partial time

linearization methods require smaller time steps than the time linearization methods represented by equation (10).

Equation (15) is the desired finite-difference form of equation (1) when the spatial derivative is approximated by compact operators. Equation (15) is second-order accurate in time and fourth-order accurate in space and involves the dependent variables (**U** and **F**) at only three grid points.

The second-order spatial derivative **F** is zero at the upstream and downstream boundaries and equation (15) is solved by the Thomas algorithm in conjunction with **LU** decomposition for inversion of the 6×6 blocks.

Modified equation methods

Modified equation methods can be used to increase the temporal and/or the spatial accuracy of existing finite-difference equations by appending terms to these equations in order to reduce the truncation errors. Here a modified equation method is used to increase the spatial accuracy of the following second-order accurate, in both space and time, finite-difference representation of equation (1):

$$\frac{\mathbf{U}_i^{n+1}-\mathbf{U}_i^n}{\Delta\tau}=\frac{1}{2}\left[\alpha\frac{\delta^2\mathbf{U}_i^{n+1}}{\Delta\psi^2}+\alpha\frac{\delta^2\mathbf{U}_i^n}{\Delta\psi^2}+2\mathbf{S}_i^n+\left(\frac{\partial\mathbf{S}}{\partial\mathbf{U}}\right)_i^n(\mathbf{U}_i^{n+1}-\mathbf{U}_i^n)\right]. \tag{16}$$

In order to determine the terms that need to be appended to equation (16) to increase its spatial accuracy from second-order to fourth-order, we proceed to derive the modified equation of equation (16), i.e. the partial differential equation truly represented by equation (16). Expanding $\mathbf{U}_{i+1}^{n+1}$, $\mathbf{U}_i^{n+1}$, $\mathbf{U}_{i-1}^{n+1}$, $\mathbf{U}_{i+1}^n$ and $\mathbf{U}_{i-1}^n$ in Taylor series around $[(n+1/2)\Delta\tau, i\Delta\psi]$ and substituting of the resulting expansions into equation (16) yields

$$\begin{aligned}\frac{\partial\mathbf{U}}{\partial\tau}+\frac{\Delta\tau^2}{24}\frac{\partial^3\mathbf{U}}{\partial\psi^3}+O(\Delta\tau^4)=\alpha\frac{\partial^2\mathbf{U}}{\partial\psi^2}+\mathbf{S}+\alpha\frac{\Delta\psi^2}{12}\frac{\partial^4\mathbf{U}}{\partial\psi^4}\\ +\frac{\Delta\tau^2}{8}\frac{\partial^2}{\partial\tau^2}\left[\alpha\frac{\partial^2\mathbf{U}}{\partial\psi^2}+\mathbf{S}+\alpha\frac{\Delta\psi^2}{12}\frac{\partial^4\mathbf{U}}{\partial\psi^4}\right]+O(\Delta\psi^4,\Delta\tau^4,\Delta\tau^4\Delta\psi^2).\end{aligned} \tag{17}$$

The leading spatial truncation error in equation (17) is $O(\Delta\tau^2\Delta\psi^2)$. This error can be eliminated by subtracting $(\Delta\tau^2/8)\{\partial^2[\text{equation (17)}]/\partial\tau^2\}$ from equation (17). This results in the following equation:

$$\frac{\partial\mathbf{U}}{\partial\tau}-\left(\alpha\frac{\partial^2\mathbf{U}}{\partial\psi^2}+\mathbf{S}\right)=\text{TE}, \tag{18}$$

where TE is the truncation error, which can be written as

$$\text{TE}=\frac{\alpha\Delta\psi^2}{12}\frac{\partial^4\mathbf{U}}{\partial\psi^4}+O(\Delta\tau^2,\Delta\psi^4,\Delta\tau^4\Delta\psi^2) \tag{19}$$

Other time derivative terms can be eliminated from equation (17) in a similar manner.[23]

It can readily be seen from equations (18) and (19) that if the term $(\alpha\Delta\psi^2/12)(\partial^4\mathbf{U}/\partial\psi^4)$ is eliminated from the truncation error, the resulting finite-difference equation will be fourth-order accurate in space. In this paper, we eliminate $(\alpha\Delta\psi^2/12)(\partial^4\mathbf{U}/\partial\psi^4)$ from the truncation error by appending it, with opposite sign, to equation (16). This results in the following finite-difference equation:

$$\frac{\mathbf{U}_i^{n+1}-\mathbf{U}_i^n}{\Delta\tau}=\frac{\alpha}{2\Delta\psi^2}[\mathbf{U}_{i+1}^{n+1}-2\mathbf{U}_i^{n+1}+\mathbf{U}_{i-1}^{n+1}+\mathbf{U}_{i+1}^n-2\mathbf{U}_i^n+\mathbf{U}_{i-1}^n]$$
$$+\left[\mathbf{S}_i^n+\frac{1}{2}\left(\frac{\partial\mathbf{S}}{\partial\mathbf{U}}\right)_i^n(\mathbf{U}_i^{n+1}-\mathbf{U}_i^n)\right]-\frac{\alpha\Delta\psi^2}{12}\frac{\partial^4\mathbf{U}}{\partial\psi^4}, \tag{20}$$

where the fourth-order spatial derivative is evaluated as

$$\frac{\alpha\Delta\psi^2}{12}\frac{\partial^4\mathbf{U}}{\partial\psi^4}=\frac{\alpha}{12\Delta\psi^2}(\mathbf{U}_{i+2}-4\mathbf{U}_{i+1}+6\mathbf{U}_i-4\mathbf{U}_{i-1}+\mathbf{U}_{i-2})+O(\Delta\psi^4). \tag{21}$$

Equation (20) yields an $O(\Delta\tau^2,\Delta\psi^4)$ truncation error if the appended term is evaluated at $(n+1/2)\Delta\tau$, i.e. in a Crank–Nicolson manner; however, if the appended term is evaluated explicitly (at $n\Delta\tau$) or implicitly (at $(n+1)\Delta\tau$) the truncation error of equation (20) is $O(\Delta\tau^2,\Delta\tau\Delta\psi^2,\Delta\psi^4)$.

The accuracy of an explicit or implicit treatment of the appended term in equation (20) can be improved if the diffusion number, i.e. $\alpha\Delta\tau/\Delta\psi^2$ is $O(1)$. In this case, the truncation error proportional to $\Delta\tau\Delta\psi^2$ becomes

$$\pm\frac{\Delta\tau}{2}\frac{\alpha\Delta\psi^2}{12}\frac{\partial^4\mathbf{U}}{\partial\psi^4}=O(\Delta\psi^4), \tag{22}$$

where the plus (minus) sign corresponds to an explicit (implicit) treatment of the appended term in equation (20).

Equation (20) can be written in a general form as

$$\frac{\mathbf{U}_i^{n+1}-\mathbf{U}_i^n}{\Delta t}=\frac{\alpha}{2\Delta\psi^2}[\delta^2\mathbf{U}_i^{n+1}+\delta^2\mathbf{U}_i^n]+\mathbf{S}_i^n$$
$$+\frac{1}{2}\left(\frac{\partial\mathbf{S}}{\partial\mathbf{U}}\right)_i^n(\mathbf{U}_i^{n+1}-\mathbf{U}_i^n)-\frac{\alpha\beta}{12\Delta\psi^2}[\theta\delta^4\mathbf{U}_i^{n+1}+(1-\theta)\delta^4\mathbf{U}_i^n], \tag{23}$$

where

$$\delta^4\mathbf{U}_i=\mathbf{U}_{i+2}-4\mathbf{U}_{i+1}+6\mathbf{U}_i-4\mathbf{U}_{i-1}+\mathbf{U}_{i-2}. \tag{24}$$

$\theta(0\leqslant\theta\leqslant 1)$ is a parameter which denotes the explicit ($\theta=0$), implicit ($\theta=1$) and Crank–Nicolson ($\theta=1/2$) treatments of the appended terms and β is a parameter ($\beta=0,1$) which indicates whether the appended term is considered ($\beta=1$) or disregarded ($\beta=0$) in equation (20). For $\beta=0$, the standard second-order, in both space and time, time linearization method is obtained.

Equation (23) with $\beta=1$ and $\theta=0$ corresponds to a modified equation method in which the appended term is evaluated explicitly. This treatment has the advantage of maintaining the 3×3 block tridiagonal structure of the coefficient matrix inherent in equation (16). The disadvantage of an explicit treatment of the appended term is that it may cause numerical instability if the time step is not sufficiently small.[12,28]

Equation (23) with $\beta=1$ and $\theta=1$ corresponds to a modified equation method in which the appended term is evaluated implicitly. This treatment does not cause numerical instability; however, the 3×3 block tridiagonal structure inherent in equation (16) is destroyed. Equation (23) with $\beta=1$ and $\theta=1$ has a coefficient matrix with bandwidth greater than three. Thus, an implicit treatment of the appended term is computationally much more expensive than an explicit treatment.

Equation (23) with $\beta=1$ and $\theta=1/2$ corresponds to a modified equation method in which the

appended term is evaluated in a Crank–Nicolson manner, i.e. at $(n + 1/2)\Delta\tau$. This method is $O(\Delta\tau^2, \Delta\psi^4)$ and yields a coefficient matrix with bandwidth greater than three. Thus, a Crank–Nicolson evaluation of the appended term is computationally more expensive than an explicit evaluation.

Equation (23) is the desired finite-difference form of modified equation methods for one-dimensional reaction–diffusion equations. This equation is solved by the Thomas algorithm in conjunction with **LU** decomposition for the inversion of the 3×3 blocks. Iterations are needed when the appended term is evaluated implicitly or in a Crank–Nicolson manner. No iterations are required if the appended term is evaluated explicitly, although the time step may have to be reduced for stability reasons.

RESULTS

The compact operator and modified equation methods described in the previous section were used to calculate the propagation of a laminar ozone-decomposition flame. Specifically, the temperature and the mass fractions of ozone, molecular oxygen and atomic oxygen were calculated as a function of position and time. For both methods, calculations were terminated once the flame speed reached a steady-state value. The steady-state flame speed, V, was calculated by the following equation:

$$V = \int_0^{\psi_T} \mathbf{S}[\mathbf{U}(\tau, \psi)]\,\mathrm{d}\psi / (\mathbf{U}(\tau, 0) - \mathbf{U}(\tau, \psi_T)) \tag{25}$$

obtained by integrating equation (1) in a co-ordinate system moving with the flame.[29] In equation (25), ψ_T is the length of the computational domain[5] ($\psi_T = 0{\cdot}00025239$ g/cm^2).

Compact operators

Figures 1–4 show some results obtained by using compact operators, 121 grid points and a time step of 1 μs. In these Figures, the temperature and mass fractions are plotted as functions of the non-dimensional Lagrangian coordinate (ψ/ψ_0) and the normalized Eulerian co-ordinate (X) where the Eulerian coordinate X is defined as

$$X = \frac{x\rho_0}{\psi_0} = \frac{\rho_0}{\psi_0} \int_0^{\psi} \frac{\mathrm{d}\psi}{\rho} \tag{26}$$

ρ_0 is the density of the unburned gases and $\psi_0 = \psi_T/50$.

Figures 1–4 illustrate the diffusion of heat and mass and the flame propagation at different times in both Eulerian and Lagrangian co-ordinates.

The results shown in Figures 1–4 are almost identical (differences less than 0·1 per cent) to those reported by Ramos,[5,13] who employed a variety of fourth-order accurate methods. The results computed with the compact operator and modified equation methods presented in this paper are shown in Table I. Table I also shows the flame speeds computed by means of the partial time linearization, majorant operator-splitting and method of lines techniques presented in Reference 5.

Table I indicates that the steady-state flame speeds calculated with compact operators are as accurate as those reported by Margolis[4] who used a sixth-order B-spline finite element method.

Table I also shows that the flame speed computed with the compact operator technique presented in this paper is in good agreement with those calculated by means of adaptive finite-difference[8–10] and finite element methods.[13]

Table I indicates that the compact operator method yields a flame speed of 49·6 cm/s when 121 grid points and a time step of 1 μs are used in the calculations. This speed is in excellent agreement

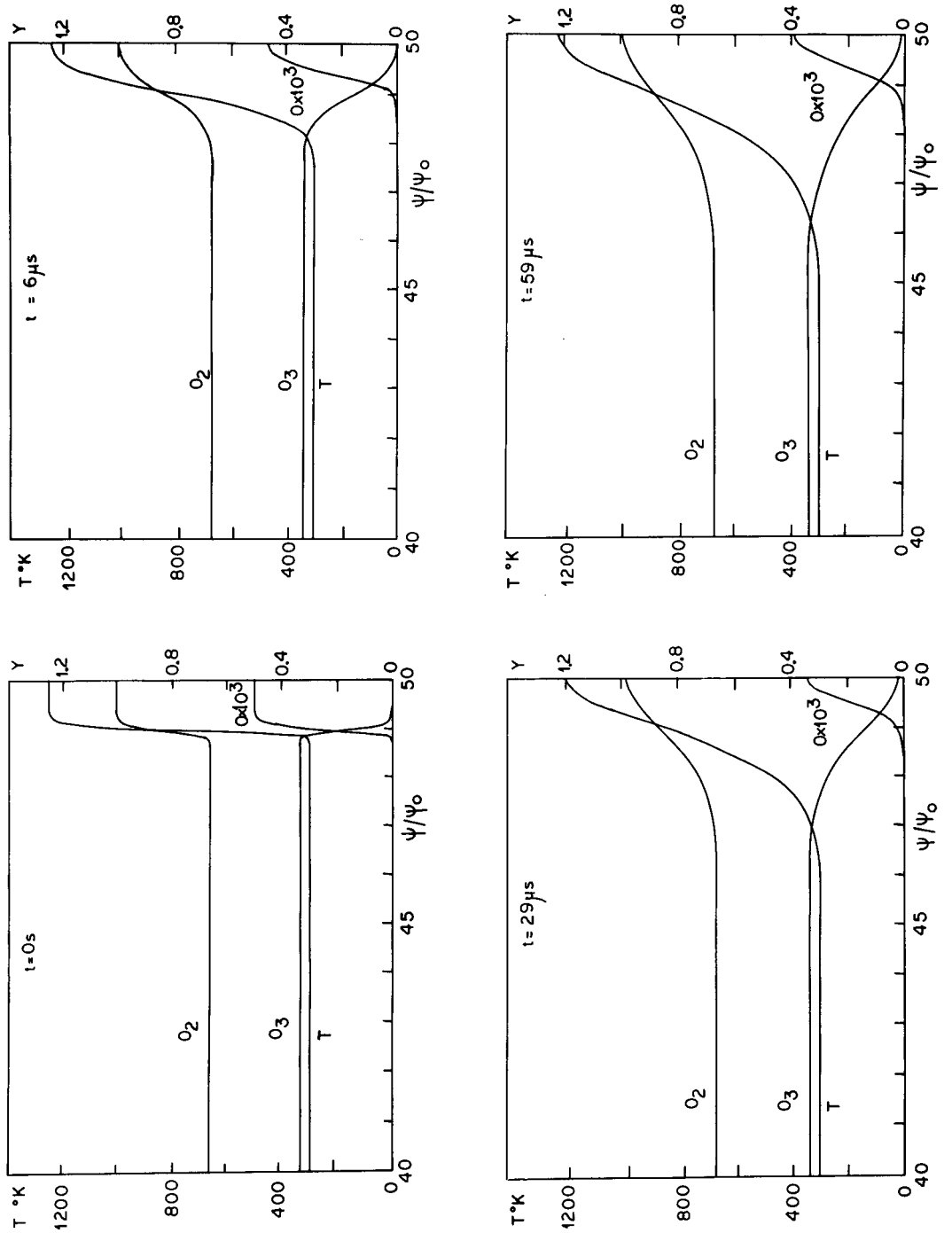

Figure 1. Species mass fractions and temperature profiles as functions of ψ/ψ_o

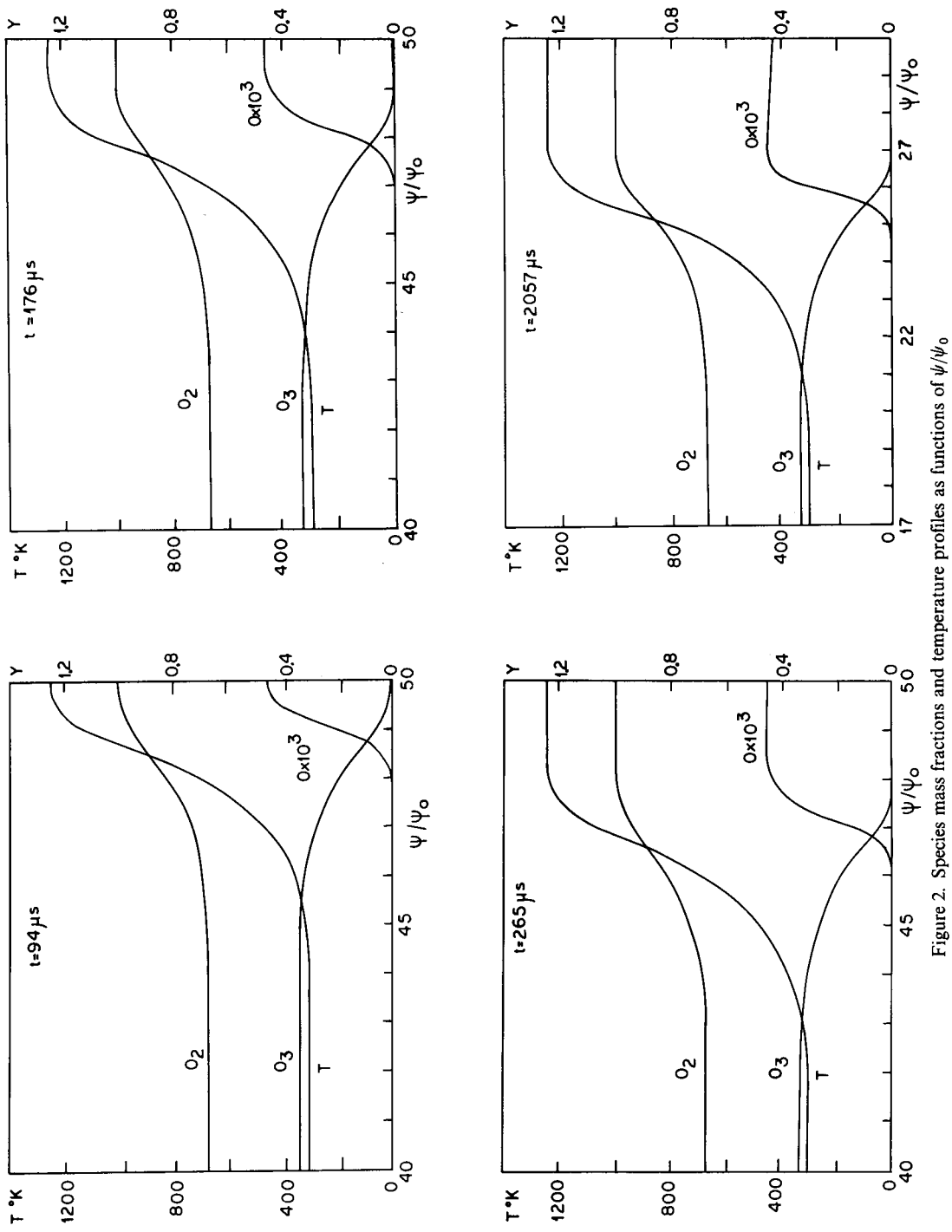

Figure 2. Species mass fractions and temperature profiles as functions of ψ/ψ_0

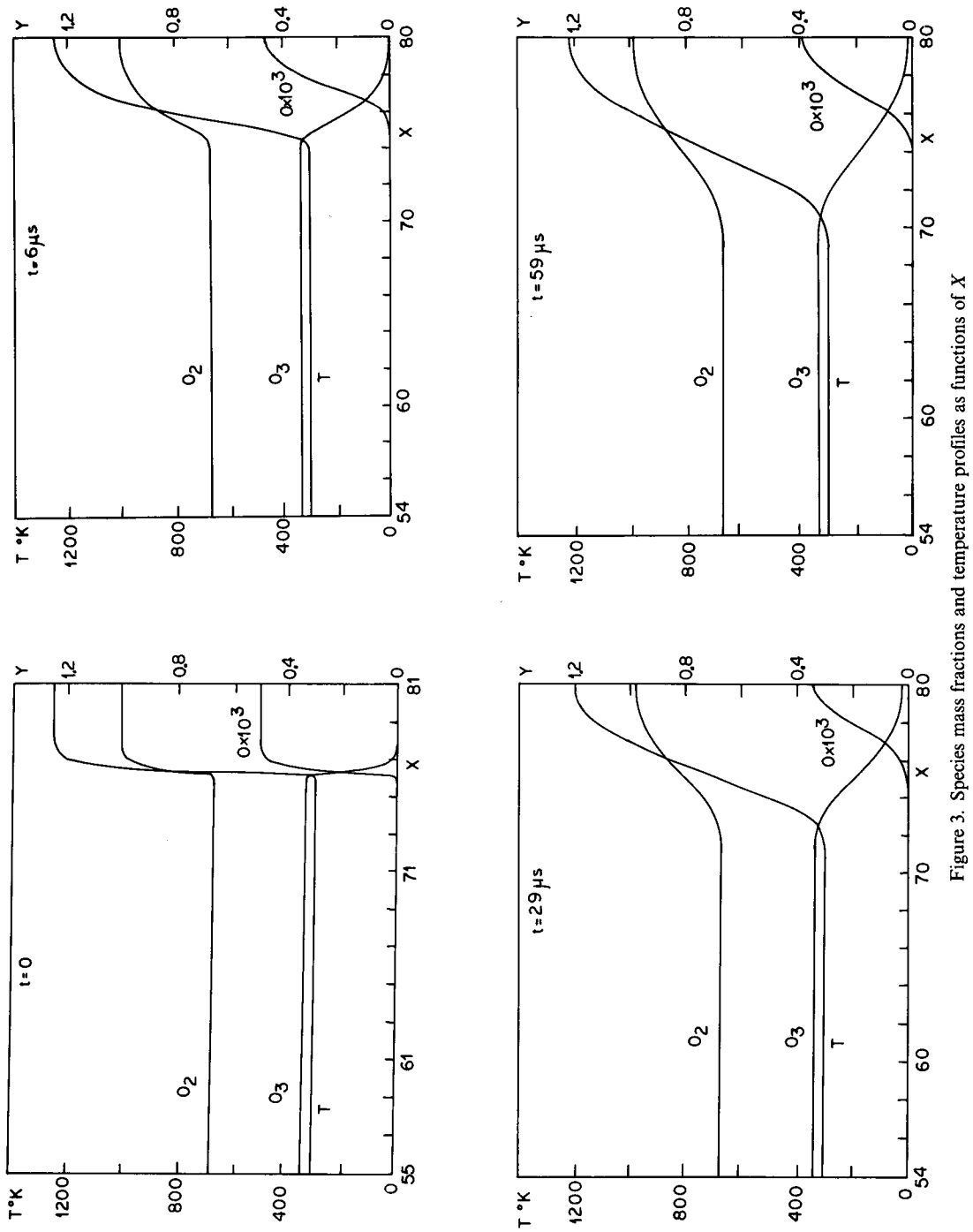

Figure 3. Species mass fractions and temperature profiles as functions of X

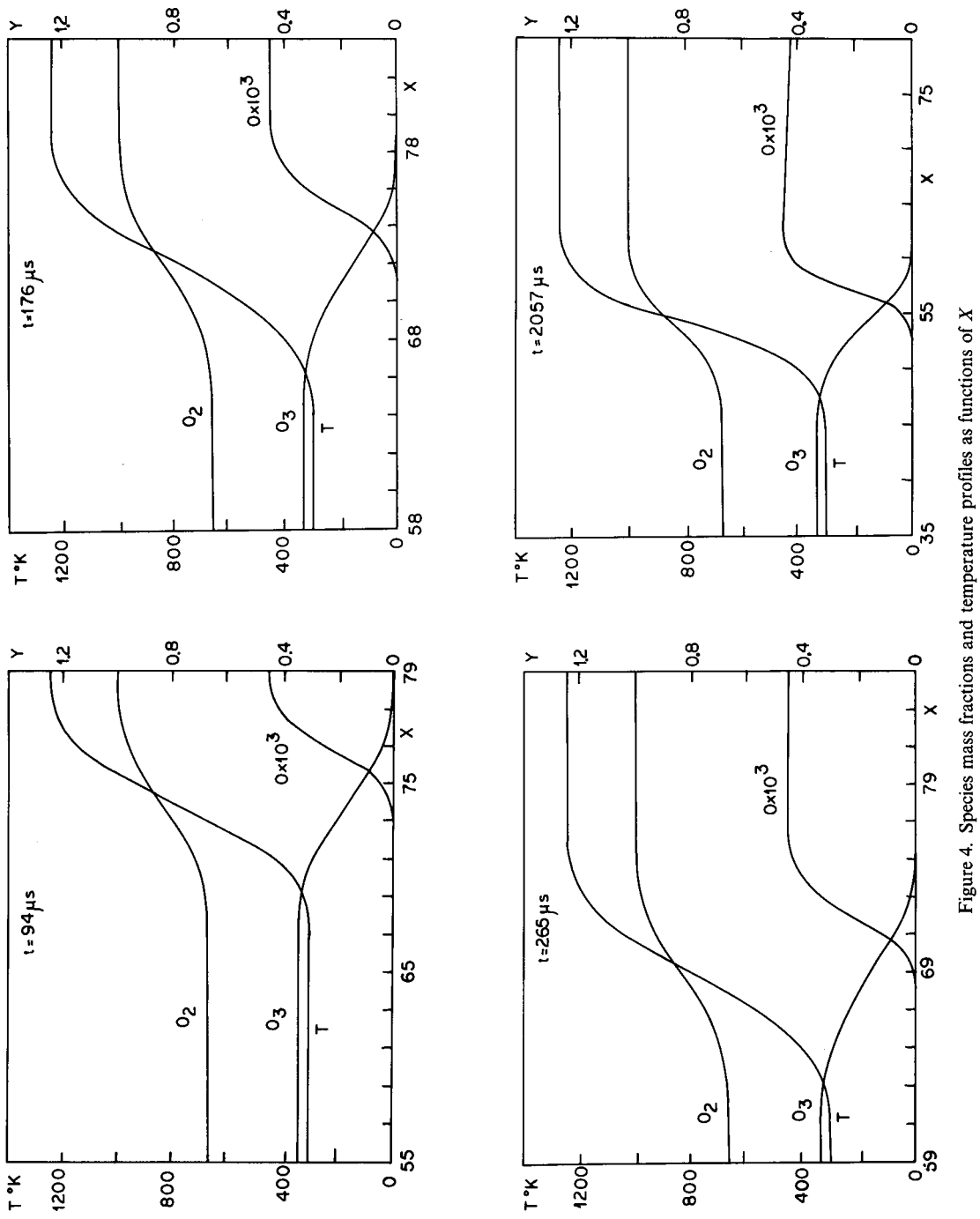

Figure 4. Species mass fractions and temperature profiles as functions of X

Table I. Computed flame speeds

Method	Reference	Wave speed (cm/s)	Number of grid point
Second-order linearization	Equation (10)*	49·20	121
Compact operator	Equation (15)	49·60	121
Modified equation† ($\theta = 0$)	Equation (23)	49·27	121
Modified equation† ($\theta = 1$)	Equation (23)	49·38	121
Modified equation† ($\theta = 1/2$)	Equation (23)	49·53	121
PDECOL	4	49·70	270‡
Partial time linearization	5[Equation (27)]	48·91	121
Partial time linearization	5[Equation (29)]	48·97	121
Partial time linearization	5[Equation (32)]	49·38	121
Fourth-order majorant operator-splitting	5[Equation (22)]	49·51	121
Fourth-order method of lines	5[Equation (19)]	49·57	121

* Also equation (23) with $\beta = 0$
† $\beta = 1$.
‡ Collocation points.

with the value of 49·7 cm/s obtained by Margolis[4] who used a sixth-order B-spline finite element technique and 270 collocation points.

The accuracy of compact operator methods deteriorates as the number of grid points used in the calculations is decreased. Although compact operators have smaller truncation errors than second-order accurate techniques, compact operators must use a sufficient number of grid points to resolve the flame structure. In addition, the accuracy of the compact operator method presented in this paper (cf. equation (15)) deteriorates as large time steps are used in the calculations because of the linearization of the non-linear reaction terms (cf. equation (8)). When the reaction terms or their derivatives with respect to time are large, time linearization methods require small time steps and the delta formulation of Beam and Warming[26] may yield oscillatory temperature and species mass fraction profiles.[30] These oscillations can be eliminated by reducing the time step employed in the calculations.

The results shown in Table I indicate that the second-order time linearization method (cf. equation (10)) presented in this paper is more accurate than the first- (cf. equation (27)) and second-order (cf. equation (29)) partial time linearization schemes presented in Reference 5. Although partial time linearization schemes result in tridiagonal matrices for the dependent variables, their accuracies are lower than those of time linearization methods because of the uncoupling of the dependent variables (cf. equation (9)). Table I also shows that the compact operator method presented in this paper is more accurate than the partial time linearization compact operator scheme presented in Reference 5.

The accuracy of the fourth method of lines and fourth-order majorant operator-splitting technique[5] is slightly lower, but comparable to, that of the compact operator method presented in this paper.

Modified equation methods

The steady-state flame speeds computed with the modified equation methods presented in the previous section are shown in Table I.

The modified equation method described by equation (23) with $\beta = 1$ and $\theta = 0$, i.e. with an explicit evaluation of the appended term, was found to be conditionally stable, as expected.[12,20]

This method yielded a flame speed of 49·27 cm/s with 121 grid points and a time step of 0·1 μs. This time is an order of magnitude smaller than that used in the compact operator algorithm.

The flame speed calculated with the modified equation method and $\theta = 0$ (cf. equation (23)) is slightly more accurate than that computed with the second-order time linearization scheme (cf. equation (10)) and more accurate than those computed with partial time linearization algorithms which do not use compact differences. However, the fourth-order method of lines, the fourth-order majorant operator-splitting method and the compact operator techniques are more accurate than the modified equation method with $\theta = 0$. This comparison indicates that the accuracy of the modified equation method with $\theta = 0$ is somewhere in between second-order and fourth-order.

Modified equation methods with $\theta = 1$ and $\theta = 1/2$ are more stable and accurate than modified equation schemes with $\theta = 0$. The accuracy of modified equation methods which use Crank–Nicolson evaluations for the appended terms is higher than that of those which employ explicit or implicit evaluations for the appended term.

The results shown in Table I indicate that modified equation methods with $\theta = 1/2$ are not as accurate as compact operator techniques. Furthermore, modified equation methods with implicit or Crank–Nicolson evaluations of the appended term require iterations and involve five grid points. Compact operator schemes with time linearization of the reaction terms only involve three grid points and do not require iterations. However, they do require the inversion of 6×6 block matrices, whereas modified equation schemes require the inversion of 3×3 block matrices. Modified equation methods are also difficult to implement in confined flame propagation problems near the boundaries because they involve five grid points.

CONCLUSIONS

A compact operator technique and three modified equation schemes have been developed and applied to study a one-dimensional laminar ozone-decomposition flame.

The compact operator technique was shown to yield as accurate flame speeds as those obtained by using a sixth-order B-spline finite element method. However, it was found that even though compact operators have very small truncation errors, grid spacings cannot be larger than those used by lower order accurate methods when analysing phenomena of very small length scales, such as a flame. This is because in order to resolve the flame structure, grid points must be located inside the very thin flame front.

The aforementioned problem, however, is not insurmountable. It is believed that the number of grid points required can be reduced considerably in problems involving very small length scale phenomena if compact operators are used in conjunction with adaptive grid generation techniques.

Modified equation methods were also found to yield accurate solutions. An explicit treatment of the appended term was found to cause numerical stability problems. Implicit and Crank–Nicolson treatments of the appended term did not cause numerical instability; however, in the present problem, implicit treatments required much more computational effort per time step than that required by the explicit treatment.

Modified equation methods were found to be less accurate than compact operator techniques. However, their accuracy improves with the order of discretization used to evaluate the appended terms.

Modified equation methods yield 3×3 block matrices, involve five grid points and require iterations if the appended terms are evaluated implicitly or in a Crank–Nicolson manner.

Time-linearized compact operator schemes yield 6×6 block matrices, involve only three grid

points and do not require iterations. Compact operator schemes are, therefore, easier to implement in confined flame propagation problems than modified equation techniques. However, the accuracy of time linearization schemes depends on the magnitude of the non-linear reaction terms and on the rate of change of the reaction terms with respect to time.

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