Numerical Solution for the Problem of Flame Propagation by the Random Element Method

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A numerical, grid-free algorithm is presented for the one-dimensional reaction-diffusion model of laminar flame propagation in premixed gases. It is based on the random element method developed by the authors for the analysis of diffusional processes. The effect of combustion is taken into account by applying the principle of fractional steps to separate the process of diffusion, modeled by the random walk of computational elements, from the exothermic effects of chemical reaction monitoring their strength. The validity of the algorithm is demonstrated by application to flame propagation problems for which exact solutions exist. The flame speed evaluated by its use oscillates around the exact value at a relatively small amplitude, while the temperature and species concentration profiles are self-correcting in their convergence to the exact solution. A satisfactory resolution is obtained by the use of a small number of computational elements which automatically adjust their distribution to fit sharp gradients.

Introduction

FUNDAMENTAL properties of the reaction-diffusion model of a laminar flame have stimulated a good deal of interest among mathematical physicists. The ground work was laid down by Zeldovich and Frank-Kamenetskii,[1] Zeldovich et al.,[2] and Barenblatt et al.,[3] systematized by Spalding,[4] exposed by Williams,[5] and verified in terms of rigorous mathematical analysis by Fife[6] and Lin,[7] and, with particular reference to the use of random walk modeling of diffusion, by McKean.[8]

Recently, this model provided basic incentive for numerous investigations involving numerical computations of the propagation and structure of laminar flames in premixed gases. Included prominently among them are the studies of Dwyer et al.,[9-11] Westbrook,[12] Warnatz,[13] Margolis,[14] Reitz,[15] Ramos,[16] and Lee and Ramos.[17]

Of particular relevance to this study are the papers of Otey and Dwyer[10] and Ramos,[16] which treated the propagation of planar and spherical flames, respectively. The first presents a comprehensive exposition of a wide variety of finite difference methods, including a comparison between their degree of accuracy as well as computational efficiency expressed in terms of the computer time required and the number of grid points used to achieve the same precision in the flame speed. One of the most convenient devices used by the authors is the operator splitting technique, which received an extensive analysis by Yanenko,[18] whereby the diffusion and reaction parts of the governing equations are solved independently, thus permitting the application of the most efficient numerical algorithm to compute each part. The major disadvantage of this procedure, however, is the inherent numerical decoupling between the two processes, during each elementary time step, that would otherwise occur simultaneously, and which imposes a strict limit on the size of the integration step.

Ramos,[16] on the other hand, applied the same principles to the point-symmetrical case of a spherical flame front. In the course of his study as many as nine various finite difference schemes, based on second-order spatial approximation, were employed, thus providing a critical evaluation of their applicability to the analysis of laminar flames, including a direct comparison with the finite element method as well as with exact solutions of simple cases.

Chorin,[19] on the other hand, suggested the use of random walk to solve the reaction-diffusion equation as an extension of the vortex sheet method.[20] Hald[21] provided a convergence proof for this procedure when the random walk is restricted on a grid.

The essential difficulties encountered in the integration of the reaction-diffusion equations modeling laminar flames can be summarized as follows:

1) The need to resort to implicit schemes for discretizing the diffusional part of the equations in order to guarantee numerical stability while using large time steps. It becomes necessary, therefore, to use relatively expensive matrix inversion routines to solve the resulting set of algebraic equations.

2) The boundary-layer-like nature of the flame, whereby the zone of steep gradients is extremely thin in comparison with the overall size of the flowfield under study. The fact that this zone moves at an unknown speed is particularly troublesome, necessitating the use of adaptive gridding techniques[11] to follow the zone of sharpest gradients during the course of the computations.

3) The stiffness of the equations modeling the reaction due to the existence of a wide range of chemical time scales.

4) The application of boundary conditions in terms of a vanishing derivative of temperature and species concentration at infinity, requiring the extension of the computational domain large distances on both sides of the flame.

Presented here is a numerical algorithm to integrate the reaction-diffusion equations for a laminar flame that circumvents most of these difficulties in a straightforward and natural way. Its major advantage lies in avoiding the need to discretize the governing equations on a grid. The method yields an explicit solution for the diffusion part of the model, providing an exact solution in a statistical sense, while its

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stability is independent of the time step. The amount of computational time is, thus, reduced greatly. The efficiency and accuracy of the method is particularly good for the case of Lewis number equal to one, since only one diffusion equation has to be solved for all of the dependent variables.

The principle of operator splitting is used to separate the diffusion part, solved by the random walk of computational elements representing discrete jumps in temperature or species concentration, from the reaction part expressed in terms of ordinary differential equations that modulate the evolution of temperature and species in the moving computational elements.

In its physical sense, this work is a sequel to the authors' previous studies[22] on modeling turbulent flame propagation, in which the flame front was treated as a thin interface separating reactants from products. The exothermic effects of combustion were taken into account by assuming that the interface moves in the direction normal to itself at a prescribed laminar burning speed, which depends on the properties of the mixture, while the effects of expansion were modeled by a line of volumetric sources delineated by the flame front. Meanwhile, Majda[23] provided an interesting analysis of that model and proved that its proper one-dimensional asymptotic limit is a reaction-diffusion system of equations that describes the propagations of a laminar flame. In this paper, a method to evaluate the solution of that limit, namely, the laminar burning speed in a premixed environment given its physical properties in terms of the diffusivities and a chemical kinetic scheme, is furnished.

In what follows, a general formulation of the problem, based on the classical reaction-diffusion model, is presented. Salient features of the random element method recently developed by the authors[24] for the modeling of diffusional processes are then described, and the exposition is culminated by its application to two simple cases of planar laminar flames using temperature-explicit reaction models, a one-reaction model, and a two-reaction model.

Problem

In general, the problem of a plane laminar flame can be expressed in terms of a time-dependent system of reaction-diffusion equations

$$\frac{\partial z}{\partial t} = D\frac{\partial^2 z}{\partial x^2} + F(z) \tag{1}$$

where

$$z = (\theta, c_i)$$

is the vector of dependent variables, whose components are the nondimensional temperature, $\theta \equiv (T-T_u)/(T_b-T_u)$, with subscript u denoting the unburnt and b the burnt medium, and concentrations, c_i, of k chemical species taking part in the combustion reaction. While

$$D = IB$$

is the diffusivity matrix, presented here in its simplest form of a diagonal matrix, $B = (1, Le_i^{-1})$ is the vector of transport coefficients, and Le_i, the Lewis number of the ith species, is defined as the ratio of the thermal diffusivity $\alpha \equiv \lambda/\rho c_p$ and the representative individual diffusivity $\mathfrak{D}_i$; whereas $t \equiv A\tilde{t}$ and

$$x \equiv \tilde{x}\sqrt{A/\alpha}$$

are the nondimensional independent variables, the time and space coordinates, A expressing the frequency factor, a quantity inversely related to the representative chemical time (quantities with a tilde are dimensional). The last term, $F(z)$, represents the sources providing the essential drive for the problem, i.e., the rate of the evolution of exothermic energy for the first component of z, and the rates of generation of the appropriate species for the remaining components of this vector.

Equation (1) is based on the assumption of strictly one-dimensional variation in all the dynamic and thermodynamic variables, while the diffusivities are considered to be constant. The continuity equation as well as the convective terms in the energy and species conservation equations are eliminated by employing a Lagrangian-mass coordinate $(\tilde{x}, \tilde{t})$ defined by the relations

$$\frac{\partial \tilde{x}}{\partial x_p} = \rho/\rho_u$$

and

$$\frac{\partial \tilde{x}}{\partial \tilde{t}} = \rho/\rho_u u$$

where x_p is the physical-Eulerian coordinate, while ρ and u are the density and the flow velocity, respectively. The momentum equation is removed by adapting the widely accepted assumption of negligible pressure variation throughout the flame.

The formulation is completed by specifying initial conditions

$$z(x,0) = z_0(x) \tag{2}$$

and boundary conditions, depending on the geometry of the space where the flame is located. For the planar flame these are

$$\begin{aligned} x &= -\infty \qquad & z &= (1, c_{p_i}) \\ &= +\infty & &= (0, c_{R_i}) \end{aligned} \tag{3}$$

subscript p denoting the products and R the reactants, so that the flame propagates to the right.

For the case of a temperature-explicit reaction, the planar flame problem is reduced to a single scalar equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2} + f(\theta) \tag{4}$$

while the initial and boundary conditions are, respectively,

$$\theta(x,0) = \theta_0(x)$$

$$x = -\infty, \quad \theta = 1; \quad x = +\infty \quad \theta = 0 \tag{5}$$

Here, following Spalding,[4] one may obtain a well-behaved representative solution by assuming that

$$f(\theta) = \theta^n(1-\theta) \tag{6}$$

For the sake of comparison, the same cases as those considered by Lee and Ramos[17] and Ramos[16] are analyzed, namely, $n = 1$ and 2, in which exact solutions exist. In the case of $n = 1$,

$$\theta_0(\xi) = 1/[1+\exp(\xi/\sqrt{6})]^2 \tag{7a}$$

with a wave speed $\omega = 5/\sqrt{6}$, and $\xi = x - \omega t$, while for $n = 2$,

$$\theta_0(\xi) = 1/[1+\exp(\xi/\sqrt{2})] \tag{7b}$$

with a wave speed of $1/\sqrt{2}$.

In a single reaction model of a planar flame one has

$$R \rightarrow P$$

while

$$z = (\theta, c)$$

where c is the concentration of a single representative species, R, and Eq. (1) is reduced for $Le_i = 1$ to

$$\frac{\partial z}{\partial t} = \frac{\partial^2 z}{\partial x^2} + F(z) \tag{8}$$

while the initial and boundary conditions are, respectively,

$$\theta(x,0) = H(x_0); \quad c(x,0) = -H(x_0)$$

that is

$$x = -\infty : \ \theta = \theta_0; \qquad c = 0$$

$$x = +\infty \quad \theta = \theta_0 - 1; \quad c = 1 \tag{9}$$

where H is the Heaviside function.

Again, for the sake of comparison, we are using the same source functions as Otey and Dwyer,[10] namely,

$$F_{\theta,R} = \pm A_1 c \exp(-\theta_1/\theta) \tag{10}$$

where $A_1 = 2.2 \times 10^5$ and $\theta_1 = 4$, the positive sign is for the θ-equation, while the negative sign is for the c-equation. The temperature is nondimensionalized with respect to the activation energy of the reaction.

For more realistic chemical schemes, a two-step reaction is considered. The reaction proceeds from reactants R to products P via an intermediate state I so that

$$R \rightarrow I \rightarrow P \tag{11a}$$

while

$$z = (\theta, c_R, c_I)$$

and the reaction terms are then expressed, as in Otey and Dwyer,[10] by the following relations:

$$F_\theta = \left(\frac{\beta}{1+\beta}\right) A_R c_R e^{-\theta_1/\theta} + \left(\frac{1}{1+\beta}\right) A_I c_I e^{-\theta_2/\theta}$$

$$F_R = -A_R c_R e^{-\theta_1/\theta}$$

$$F_I = A_R c_R e^{-\theta_1/\theta} - A_I c_I e^{-\theta_2/\theta} \tag{11b}$$

where β is the ratio of the heat of combustion of the two reactions.

Method

The authors' technique of solving the diffusion of energy and species has been developed as a generalization of the random vortex method devised by Chorin[19,20,25,26] for numerical solution of the Navier-Stokes equations in turbulent flow. In this method, Chorin exploited the concept of stochastic modeling of diffusion, based on Einstein's studies of Brownian motion,[27] to evaluate the effect of the diffusion of vorticity in a flowfield with a high Reynolds number. The extension of these concepts to the analysis of diffusion of heat and species in one- and two-dimensional fields was accomplished by Ghoniem and Oppenheim.[24] The procedure was developed further by Ghoniem and Sherman[28] to treat the combined diffusion of heat and vorticity in natural convection, where the diffusion of heat stimulates the process of generation of vorticity inside the field by baroclinic effects of gravity.

In the case at hand, the transport of heat and chemical species by diffusion is expressed in terms of a Fourier equation of exactly the same kind as that describing the transport of vorticity in the case of fluid flow. The analogy between these processes is most clearly evident in the case of a one-dimensional problem, as displayed in Table 1.

As one can see in Table 1, the dependent variables of the diffusion equation appear in three differential orders:

1) The primary variable: velocity u, temperature T, or species concentration c, all expressed in the following as a generalized diffusion variable Φ.

2) The secondary variable, defined as the gradient of the primary variable: vorticity ξ, heat flux q, or mass flux G, all denoted by ϕ, the gradient of Φ.

3) The integral variable, determined either as a line integral of the primary variable around the boundary of an area element or as the area integral of the secondary variable over this element (the two being equivalent according to Stokes theorem): circulation γ, internal energy $\dot{e}$, mass of a given species $\dot{m}$.

Here the Fourier equation is expressed as

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2} \tag{12}$$

while the initial conditions specify that

$$\phi(x,0) = \delta(x) \ \text{ or } \ \Phi(x,0) = H(x) \tag{13a}$$

where δ is the Dirac delta function, whereas the boundary conditions imply that

$$\phi(\pm\infty,t) = 0 \ \text{ or } \ \frac{\partial \Phi}{\partial x}(\pm\infty,0) = 0 \tag{13b}$$

The fundamental concept behind the application of the random walk technique to model the solution of Eq. (12),

Table 1 Analogy between diffusional processes

Conserved quantity	Momentum	Energy	Species
Primary variable	u	T	c
Diffusion equation	$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2}$	$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$	$\frac{\partial c}{\partial T} = D \frac{\partial^2 c}{\partial x^2}$
Diffusing element	$f = \int \rho u \mathrm{d}A$	$e = \int \rho c_p T \mathrm{d}A$	$m = \int \rho c \mathrm{d}A$
Conserved quantity	Vorticity	Heat	Mass flux
Secondary variable	$\xi = -\frac{\partial u}{\partial x}$	$q = -k \frac{\partial T}{\partial x}$	$G = -\rho D \frac{\partial c}{\partial x}$
Diffusion equation	$\frac{\partial \xi}{\partial t} = \nu \frac{\partial^2 \xi}{\partial x^2}$	$\frac{\partial q}{\partial T} = \alpha \frac{\partial^2 q}{\partial x^2}$	$\frac{\partial G}{\partial t} = D \frac{\partial^2 G}{\partial x^2}$
Diffusing element[a]	$\gamma = \int \xi \mathrm{d}A$	$\dot{e} = \int q \mathrm{d}A$	$\dot{m} = \int G \mathrm{d}A$

[a] $\mathrm{d}A = \mathrm{d}x$; $\dot{e} = \mathrm{d}e/\mathrm{d}t$.

Table 2 Fundamental idea[a]

Differential equation	$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial y^2}$
Boundary conditions	$\phi(x,0) = \delta(x); \quad \phi(\pm\infty,t) = 0$
Constraint	$\Phi = \int_{-\infty}^{\infty} \phi \mathrm{d}x = 1$
Formal solution	$\phi = \frac{1}{\sqrt{2\pi\sigma}} \exp[-(x/\sigma)^2]; \quad \sigma = \sqrt{2\alpha t}$
Stochastic solution	$\Sigma \delta\Phi_i = 1$
	$x_i(t+\Delta t) = x_i(t) + \eta_i$
	$E(\eta_i) = 0; \quad E(\eta_i^2) = 2\alpha\Delta t$
Local sampling	$\phi = \frac{1}{\delta y} \Sigma \delta\Phi_i \delta(x - x_i)$
Global sampling	$\Phi = \Sigma \delta\Phi_i H(x - x_i)$

[a] H = heaviside step function; δ = Dirac delta function; E = expected value; η = Gaussian random variable; σ = standard deviation.

Table 3 Reaction-diffusion equation

Differential equation	$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + f(T)$
Initial condition	$T(x,0) = T_0(x)$
Boundary conditions	$T(+\infty,0) = 0; \quad T(-\infty,0) = 1$
Solution	
Fractional steps	$T(n\Delta t) = [R(\Delta t) D(\Delta t)]^n T_0$
Reaction	$\frac{\mathrm{d}T}{\mathrm{d}t} = f(T)$
Diffusion	$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$
Deterministic	$\delta T_i(t+\Delta t) = \delta T_i(t) + f(T_i)\Delta t$
Stochastic	$T = \Sigma \delta T_i(t) H(x - x_i)$
	$x_i(t+\Delta t) = x_i(t) + \eta_i$
	$E[n] = 0; \quad E[\eta^2] = 2\Delta t$

subject to the initial and boundary conditions specified in terms of Eqs. (13), is that the formal solution of this problem is identical to the probability density function of a Gaussian random variable with a zero mean and a variance of $(2\alpha t)$. Since the sum of Gaussian variables is itself a Gaussian variable with the same mean and a variance equal to the sum of variances, the solution can be constructed by a sequence of displacements of a set of discrete elements of the diffusing component, $\delta\Phi$, each displacement drawn from a set of Gaussian variables with a variance of $(2\alpha\Delta t)$ and a zero mean.

These elements are generated by partitioning the initial distribution of the primary variable into a number of elements of equal strength $\delta\Phi_i$, while $\Sigma\delta\Phi_i = 1$, representing the total initial distribution. At any instant of time the solution $\phi(x,t)$ is obtained by local sampling over an area element around δx, representing, in effect, the gradient of the diffusing element. The value of the diffusing element itself, $\Phi(x,t)$, can be evaluated by global sampling over the whole field, an integration process whereby a good deal of noise introduced by the intrinsically sporadic displacements of the random walk is smoothed out. Thus,

$$\Phi(x) - \Phi(\infty) = \int_{\infty}^{x} \frac{\partial \Phi}{\partial x} \mathrm{d}x$$

or

$$\Phi(x) = \Phi(\infty) + \sum_i \delta\Phi(x_i) \quad x \leq x_i \leq \infty \tag{14}$$

Salient features of this procedure are presented in Table 2.

In order to implement this procedure in the solution of the reaction-diffusion equation [Eq. (4)] a fractional step scheme is employed. The two processes taking place simultaneously are decoupled each time step into a diffusion fractional step and a reaction fractional step. Equation (4) is thus decomposed in the form

$$\frac{\partial \Phi}{\partial t} = \alpha \frac{\partial^2 \Phi}{\partial x^2} \tag{15a}$$

and

$$\frac{\mathrm{d}\Phi}{\mathrm{d}t} = f(\Phi) \tag{15b}$$

During the diffusion step, existing elements, $\delta\Phi_i$, of temperature, δT_i, or species concentration, δc_i, are given a displacement drawn from a set of independent Gaussian random numbers with zero mean and a variance of $(2\alpha\Delta t)$ where α is one for temperature and Le_i^{-1} for species, thus modeling the solution of Eq. (15a). During the reaction step, Eq. (15b) is integrated for each discrete element $\delta\Phi_i$ to evaluate its new strength in terms of the local value Φ, thus

$$\Phi(x_i, t+\Delta t) = \Phi(x_i, t) + \int_{\Delta t} f(\Phi) \mathrm{d}t \tag{16}$$

$$\delta\Phi_i(t+\Delta t) = \delta\Phi_i(t) + (\Phi(x_i, t+\Delta t) - \Phi(x_i, t))$$

while

$$\delta\Phi_{i+1}(t+\Delta t) = \delta\Phi_{i+1}(t) - (\delta\Phi_i(t+\Delta t) - \delta\Phi_i(t))$$

where $\delta\Phi_{i+1}$ is the element immediately behind the element $\delta\Phi_i$. Table 3 displays the above sequence of steps.

Solution

The method of solution just described was used to evaluate the propagation speed and temperature profiles of a flame modeled by Eq. (4) with initial conditions described by Eqs. (7). In both cases, the initial temperature profile is expressed in terms of a number N of temperature jump elements, δT_i, of equal strength $1/N$, located at $x_i = x_i(\theta_0)$, where $x_i \equiv \theta_0^{-1}$. The position of each of these elements is updated each time step according to

$$x_i(t+\Delta t) = x_i(t) + \eta \tag{17}$$

where $E[\eta] = 0$ and $E[\eta^2] = 2\Delta t$, and E stands for the expected value. In order to accommodate for the energy released by reaction, the total temperature is evaluated at the location of the element x_i using Eq. (14) as

$$T(x_i) = \Sigma \delta T_j(x_j) \qquad x_j \geq x_i \tag{18}$$

and the value of the temperature jump at the element i is then adjusted as

$$\delta T_i(t+\Delta t) = \delta T_i(t) + f(T_i)\Delta t \tag{19}$$

while the strength of the element $i+1$ is reduced by the same amount. For the temperature-explicit reaction, a first-order explicit scheme of integration is utilized to solve Eq. (16). To keep the resolution of the temperature profile within a specified limit, an element with strength $\delta T_i > \delta T_{\max}$ is divided into a number of elements such that δT_i is maintained less than $\delta T_{\max}$. If, on the other hand, $\delta T_i < \delta T_{\min}$, where $\delta T_{\min}$ is a very small number on the order of magnitude of 10^{-4}, the element is removed from the computations, thus keeping the number of elements small and finite at all times.

The method was first tested by solving Eq. (4), using Eq. (6) to express the rate of heat release. The numerical results were compared to the analytical solution provided by Eqs. (7). To separate statistical errors introduced by random walk modeling of diffusion from numerical error caused by operator splitting and numerical integration of the reaction term, analytical integrals of Eq. (16) were used.

Figure 1 shows the solution of Eq. (4) with $f(\theta) = \theta(1-\theta)$, using numerical integration in Fig. 1a and analytical integration in Fig. 1b. In both cases, $\delta T_{\max} = 0.002$ and N was 500, while $\Delta t = 0.01$. The diagrams indicate clearly that the random walk error is essentially statistical in nature; causing the numerical solution to oscillate around the exact solution. The average location of the flame, however, is predicted properly. When a first-order numerical integration scheme was used to evaluate the reaction term the error increased substantially and the predicted wave structure deviated from the exact structure, demonstrating that the error stems primarily from the numerical integration of the reaction term. The average wave speed, evaluated each time step as an integral of the solution

$$S_u = \frac{1}{T_\infty - T_{-\infty}} \frac{\mathrm{d}}{\mathrm{d}t} \int_{T-\infty}^{T+\infty} x \mathrm{d}T$$

$$= \frac{1}{T_b - T_u} \frac{1}{\Delta t} \left\{ \sum_{t+\Delta t} x_i \delta T_i - \sum_{t} x_i \delta T_i \right\} \tag{20}$$

is 2.05 for Fig. 1a and 1.86 for Fig. 1b, while its exact value is 2.04.

A typical variation of the wave speed at steady-state conditions is shown in Fig. 2 for $f(\theta) = \theta^2(1-\theta)$. The analytical solution yields a value of 0.707, while the average numerical value is 0.706.

The extension of the procedure to a two- or three-equation model is achieved by using a set of elements to represent the distribution of the concentration profile for each species. The change in the strength of these elements is monitored by the integration of the reaction part of the corresponding conservation equation. The diffusion is still modeled by displacing these elements at each time step using a set of random numbers of a Gaussian distribution, with zero mean and a variance $(2\alpha\Delta t)$ where α is 1 for temperature elements and $1/Le_k$ for each of the species k.

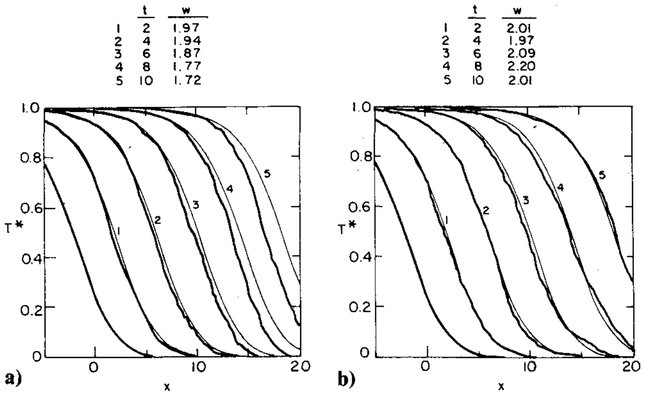

Fig. 1 Temperature profiles as a function of time for the solution of Eqs. (4) and (7b). The reaction term is integrated using a first-order scheme on the left-hand side, while analytical integration is used on the right-hand side.

The case of $Le = 1$ is of special interest here because of the simplifications it introduces and the insight it provides into the meaning of the suggested algorithm. For equal diffusivities of energy and mass, the diffusion equations for temperature and species are identical and the same set of random numbers can, therefore, be used to displace all different elements—a considerable simplification of the calculations, helping also to reduce the statistical error. Since the location of different elements is identical, only one set of elements is used and one diffusion equation is solved to relocate the elements at every time step. The strength of each element is specified by $(\delta T, \delta c_i)$. It is adjusted with time by integrating the equation

$$\frac{\mathrm{d}z}{\mathrm{d}t} = F(z)$$

where $z = (T, c_i)$. Thus, an element represents a finite amount of reactants that enters the flame zone at the temperature of the unburnt mixture. The temperature and concentration of the reactants, as well as of the intermediate and product species, change in this element as it crosses the flame by the action of diffusion, modeled by its displacement from a point with a value $z = z_1$ to another that has $z = z_2$, and by the reaction inside the element itself that changes its strength by $\delta z = F(z)\Delta t$. When all the reactants have been converted into products and the element has exited the reaction zone, it is ignored in the computations from then on, while it is normally replaced by new elements that have entered the flame zone at the same time. Figure 3 illustrates these processes schematically.

Solutions for the one-reaction model are shown in Fig. 4. To compare with the results of Otey and Dwyer,[10] we used $A_R = 2.2 \times 10^5$ and $\theta_I = 4$. In this case, $\Delta t = 10^{-5}$ and the computations started with $\delta T = 0.01$ while at steady state, its value reached the level of 0.002. To overcome the stiffness of the equation that models the reaction part, Gear[29] and Hindmarsh[30] integration package was employed.

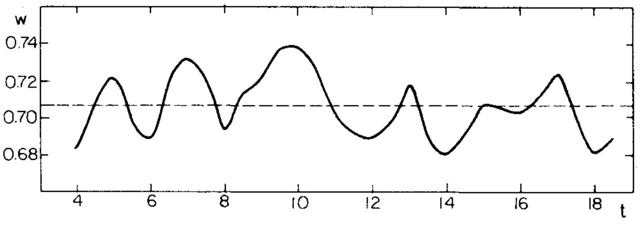

Fig. 2 Variation of the steady-state wave speed with time for the case of Eqs. (4) and (7a). The exact value is indicated by the dotted line.

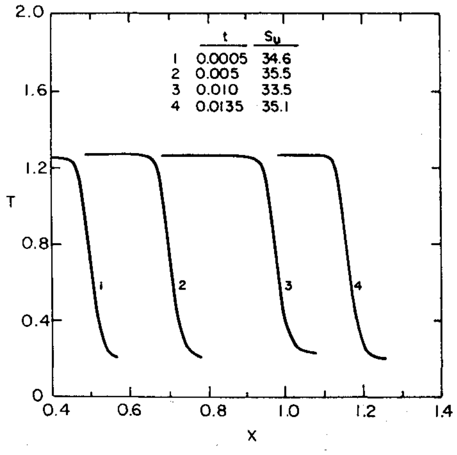

Fig. 3 Temperature profiles for the one-reaction model at steady state.

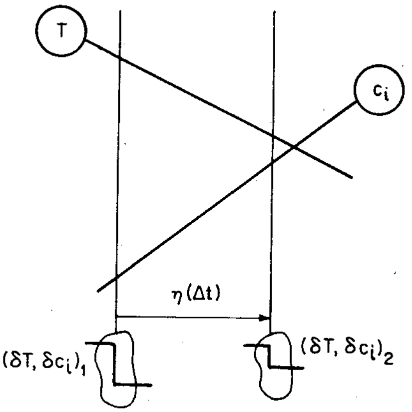

Fig. 4 The displacement of an element by diffusion denoted by $\eta(\Delta t)$ exposes it to a different temperature and species concentration, while its own composition and energy contents, defined in terms of (δT, δc_i), is changing by internal reaction.

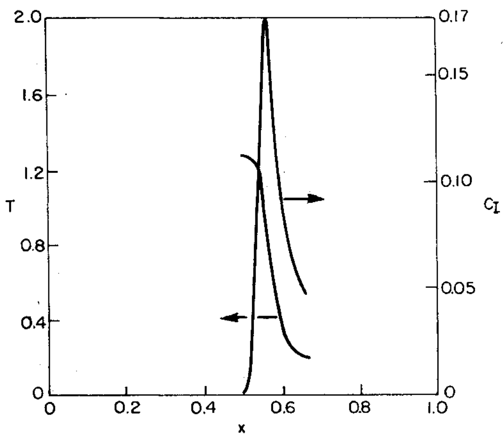

Fig. 5 Temperature and intermediate species concentration for a two-reaction flame model. Results are shown after 1000 time steps of computations.

The steady-state value of the temperature behind the flame reached 1.26 with an error of about 5%, which was most probably an integration error that could be reduced by taking smaller time steps. The average flame speed in the one-reaction model, evaluated using Eq. (19) after steady state is reached, is 34.06, while the value given by Otey and Dwyer[10] is 35.2.

The accuracy of the model in predicting the concentration of intermediate species is tested by solving the two-reaction flame model described by Eqs. (8), (11a), and (11b). This reaction scheme provides an example in which the concentration of the intermediate species c_I depends directly on the relative speed of the two reactions. If Eq. (8) is approximated by neglecting the effect of diffusion, and the reaction scheme, Eq. (11b), is assumed independent of temperature, it can be shown that $c_I/c_R = 0(A_R/A_I)$. While diffusion is expected to decrease the concentration of the species, the relative order of magnitude should be the same for equal diffusivities.

Two sample calculations were performed. Both had $\theta_R = \theta_I = 4$ and $A_R = 2.2\times 10^5$, while $N = 500$ and $\Delta t = 10^{-6}$. In the first example, $A_I = 2.2\times 10^{10}$ and $\beta = 0$, which corresponds to a very fast intermediate reaction while the first reaction is adiabatic. From the above simplified analysis $c_I = 0(10^{-5})$, while Otey and Dwyer[10] report a value of 9×10^{-6} for $c_{I_{\max}}$, our calculations yield 11.8×10^{-6}. The second case was computed for $A_I = 2.2\times 10^5$ and $\beta = 1$, and the distribution of both the temperature and the concentration of I is shown in Fig. 5. The nonmonotonic nature of the concentration profile of I is reproduced by generating elements δc_I of both positive and negative signs according to the sign of the reaction term in the third equation of Eq. (11b). An element can change its sign if it jumps during a diffusion step from the rising side of the profile to the decaying side or vice versa. The average flame speed is calculated using Eq. (19) and found to be 29.07, while Otey and Dwyer[10] had 27.8.

Conclusion

A novel numerical algorithm is presented for the computation of the structure and propagation speed of laminar flames in premixed gases modeled by a set of reaction-diffusion equations representing the conservation of energy and chemical species. The algorithm is based on the use of random walk in modeling the effect of diffusion by moving computational elements that carry discrete quantities of energy and species, while the reactions govern the change of the concentration of these quantities in the existing elements. The two processes, diffusion and reaction, are decoupled by the use of operator splitting in the course of each computational time step. The resulting numerical procedure is time-dependent and spatially adaptive; the computational elements are used only where sharp gradients exist.

The accuracy of the method was checked by applying it to a set of problems for which exact solutions are available. Using relatively large time steps, the computed temperature profiles exhibited a wavy character oscillating around the exact solution—a consequence of the statistical error introduced by the random walk of a finite number of computational elements. However, this error is reduced substantially by the use of smaller time steps—a necessary requirement for integrating complicated chemical kinetic schemes in which chemical time scales are much smaller than those of diffusion.

Using random walk to model diffusion is a simple and explicit procedure, thus allowing the same time step to be employed for the change in the temperature and composition of the reacting medium and the solution of the diffusion equation in a fractional step scheme. Using the time same step reduces the effect of decoupling the two processes, which also facilitates the computational procedure. The efficiency of the method is improved further in the case of a Lewis number of unity, since then only one diffusion equation applies to both temperature and species.

Results for the flame speed using one- and two-reaction models are in good agreement with those of Otey and Dwyer[10] who used, for this purpose, several versions of finite difference methods.

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